

THE BASIC CLOSURES OF FLUID MECHANICS IN FORM CHARACTERISTIC FOR THE FINITE VOLUME METHOD

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Abstract

This short article presents all basic “closures” that are needed to supplement the general set of balance equations in form characteristic for the Finite Volume Method. In subsequent chapters the equation of state, viscous molecular stress tensor, turbulent stress tensor, molecular heat flux, turbulent heat flux and momentum and energy sources were described. This article is a second part of a cycle dedicated for the mathematical basis of Finite Volume Method. The motivation for writing the article follows from the observation that the Finite Volume Method is usually described in greater detail in monographic books, or very briefly in the basic books dedicated to fluid mechanics. This article is an attempt to center justifications of these approaches, so that in the simplest way show the readers the basic knowledge of the so-called Computational Fluid Mechanics. For this reason this article can be treated as a literature review.

Introduction

The basic set of balance equations in Finite Volume Method, described in article (SOBIESKI 2011), has a form:

$$\left\{ \begin{array}{l} \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{v}) = 0 \\ \frac{\partial(\rho \vec{v})}{\partial t} + \operatorname{div}(\rho \vec{v} \vec{v} + p \vec{I}) = \operatorname{div}(\vec{\tau}^m + \vec{\tau}^R) + \rho s_b \\ \frac{\partial(\rho e)}{\partial t} + \operatorname{div}(\rho e \vec{v} + p \vec{I} \vec{v}) = \operatorname{div}[(\vec{\tau}^m + \vec{\tau}^R) \vec{v} + \vec{q}^m + \vec{q}^R] + \rho s_e \end{array} \right. \quad (1)$$

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where:

- ρ – density [kg/m³],
- \vec{v} – velocity [m/s],
- p – static pressure [Pa],
- \vec{I} – unit tensor [-],
- $\vec{\tau}^m$ – viscous molecular stress tensor [Pa],
- $\vec{\tau}^R$ – turbulent Reynolds stress tensor [Pa],
- s_b – source of forces [N/m³],
- e – the sum of kinetic and internal energy [J/kg],
- \vec{q}^m – molecular heat flux [J/(m² · s)],
- \vec{q}^R – turbulent heat flux [J/(m² · s)],
- s_e – sources of heat [J/(m³ · s)].

The set of balance (or transport) equations (1) is not complied and need to be supplemented by many “closures”, this means a specific models describing the individual issues. In current article, the basic “closures” for the equation of state, stress tensors, heat transfer and sources are described. It is a direct continuation of the article (SOBIESKI 2011) and for this reason, the introduction is limited to the minimum. The motivation of this work was a desire to prepare a short and clear introduction to the mathematical model characteristic for the Finite Volume Method (FVM). This follows from the observation that the mathematical model characteristic for the FVM is usually described in greater detail in monographic books, or very briefly in the basic books dedicated to fluid mechanics. This article stems from a desire of averaging these approaches.

Equation of state

The equation of state is a constitutive equation which provides a mathematical relationship between basic quantities in a system such as temperature, pressure and volume. Equations of state are useful in describing the properties of fluids (gases and liquids), mixtures of fluids and even solids. The formula depends on the adopted model of the matter, but must be added to the set (1) in any case as a separate equation. In the literature, one can find many different equations of state; the most common one known is the Clapeyron’s equation (BADUR 2005).

$$pV_m = RT \tag{2}$$

where:

- p – the static pressure [Pa],
- V_m – the volume of 1 mole of gas or liquid [m³],
- R – ideal gas constant equal to 8.314472 [J/(mol · K)],
- T – the temperature [K].

The formula (2) is dedicated for ideal gases; for real gases more appropriate is the Van der Waals equation (WAALS 1910)

$$\left(p + \frac{a}{V_m^2}\right) (V_m - b) = RT \quad (3)$$

where:

a and b are substance-specific constants, taking into account the pressures arising from gas particle vibration and its volume, respectively. In the literature, one can find other formulas for the equation of state, too.

In the case of the liquid flows, it is often assumed that

$$\begin{cases} \rho = \text{const.} \\ u = \text{const.} \end{cases} \quad (4)$$

where:

ρ – is the liquid density [kg/m^3],

u – is the internal energy [J].

Viscous molecular stress tensor

The viscous molecular stress tensor $\hat{\tau}^m$ is one of the important closures in set of equations (1). The form of this tensor depends on the adopted model of fluid. In the numerical analysis is usually adopted the Pascal's model, Newton's model or a non-Newtonian fluid model. The Pascal's model assumes existence of a stress only in perpendicular direction, without taking into account the viscosity and compressibility. In this case $\hat{\tau}^m = 0$. The Pascal's model can be used for ideal gases.

The most popular in the practice is the Newton's model, which may be used in modeling flows of air, water, oil and a lot of other fluids with a simple molecular structure (PUZYREWSKI, SAWICKI 2000). In this model the stress (τ^m) versus strain rate ($\dot{\gamma}$) curve is linear and passes through the origin (Fig. 1a). For one direction flow and Cartesian coordinates (Fig. 1b), it can be written as (PUZYREWSKI, SAWICKI 2000, GRYBOŚ 1998)

$$\tau_{xy}^m = \mu_l \frac{\partial v_x}{\partial y} \quad (5)$$

where:

μ_l – is the constant of proportionality called dynamic viscosity [$\text{Pa} \cdot \text{s}$].

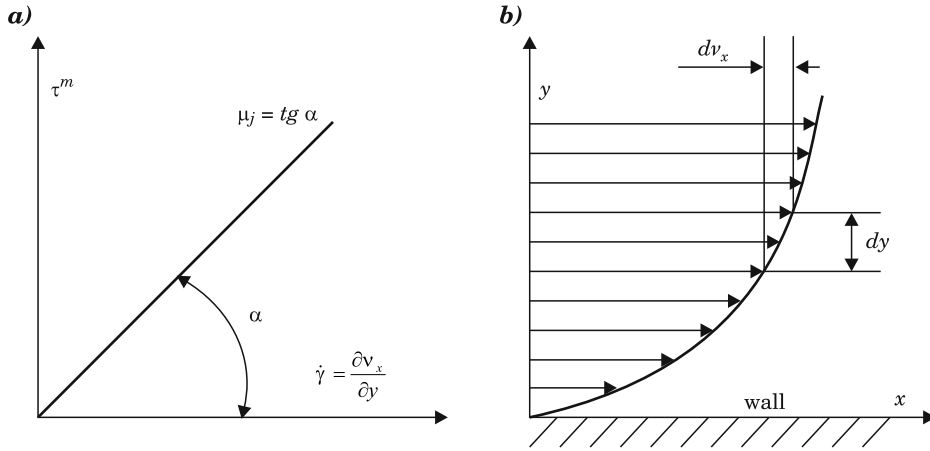


Fig 1. Relationship between stress and strain rate for Newtonian fluid

In general cases, the total stress tensor $\overset{\leftrightarrow}{T}$ for Newtonian fluid may be written in form

$$\overset{\leftrightarrow}{T} = a\overset{\leftrightarrow}{I} + b\overset{\leftrightarrow}{D} \tag{6}$$

where:

a and b are the model constants,

$\overset{\leftrightarrow}{I}$ - is the unit tensor,

$\overset{\leftrightarrow}{D}$ - is the deformation rate tensor.

The first part describes the stress in perpendicular direction, and the second part takes into account the friction caused by viscosity; tensor $\overset{\leftrightarrow}{D}$ is here a three dimensional counterpart of the quotient appearing in the equation (5). In Cartesian coordinates this tensor has a form as follow (PUZYREWSKI, SAWICKI 2000)

$$\overset{\leftrightarrow}{D} = \begin{bmatrix} \frac{\partial v_x}{\partial x} & \frac{1}{2} \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right) \\ \frac{1}{2} \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) & \frac{\partial v_y}{\partial y} & \frac{1}{2} \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) \\ \frac{1}{2} \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right) & \frac{1}{2} \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) & \frac{\partial v_z}{\partial z} \end{bmatrix} \tag{7}$$

Therefore, the formula (6) can be written in form

$$\vec{T} = \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix} + \begin{bmatrix} b \frac{\partial v_x}{\partial x} & b \frac{1}{2} \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) & b \frac{1}{2} \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right) \\ b \frac{1}{2} \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) & b \frac{\partial v_y}{\partial y} & b \frac{1}{2} \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) \\ b \frac{1}{2} \left(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right) & b \frac{1}{2} \left(\frac{\partial v_y}{\partial z} + \frac{\partial v_z}{\partial y} \right) & b \frac{\partial v_z}{\partial z} \end{bmatrix} \quad (8)$$

On the other hand

$$\vec{T} = \begin{bmatrix} T_{xx} & T_{xy} & T_{xz} \\ T_{yx} & T_{yy} & T_{yz} \\ T_{zx} & T_{zy} & T_{zz} \end{bmatrix} \quad (9)$$

Two tensors are the same, if their invariants are equal, then

$$T_{xx} + T_{yy} + T_{zz} = 3a + b \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \right) \quad (10)$$

The expression in brackets describes divergence of the velocity, then

$$T_{xx} + T_{yy} + T_{zz} = 3a + b \operatorname{div}(\vec{v}) \quad (11)$$

After dividing both sides by 3, we obtain

$$\frac{T_{xx} + T_{yy} + T_{zz}}{3} = a + \frac{1}{3} b \operatorname{div}(\vec{v}) \quad (12)$$

The equation describes the average stress perpendicular to the surface – it is the static pressure p (SONIN 2001) (the minus sign results from the orientation of the surface versor), then

$$-p = a + \frac{1}{3} b \operatorname{div}(\vec{v}) \quad (13)$$

From the above equation, one can designate the constant a :

$$a = -p - \frac{1}{3} b \operatorname{div}(\vec{v}) \quad (14)$$

The constant b can be derived by comparison of the T_{xy} component from tangential part of stress tensor formula (8) with the classical form (5), for one direction flow (when $v_y = v_z = 0$)

$$\mu_l \frac{\partial v_x}{\partial y} = b \frac{1}{2} \frac{\partial v_x}{\partial y} \quad (15)$$

and

$$b = 2\mu_l \quad (16)$$

The constants a and b can be included to the formula (6):

$$\overleftrightarrow{T} = -p\overleftrightarrow{I} + 2\mu_l \overleftrightarrow{D} - \frac{2}{3} \mu_l \operatorname{div}(\vec{v}) \overleftrightarrow{I} \quad (17)$$

or in another form

$$\overleftrightarrow{T} = -p\overleftrightarrow{I} + \overleftrightarrow{\tau}^m \quad (18)$$

where

$$\overleftrightarrow{\tau}^m = 2\mu_l \overleftrightarrow{D} - \frac{2}{3} \mu_l \operatorname{div}(\vec{v}) \overleftrightarrow{I} \quad (19)$$

In set of equations (1), the pressure part is transferred to the right side, so as to obtain the separation of convection and diffusion (it was discussed in the previous article (SOBIESKI 2011)).

In flows of very rapid change in velocity (e.g. flows with shock waves) the tensor $\overleftrightarrow{\tau}^m$ needs a correction. The part $-\frac{2}{3} \mu_l$ is replaced by $-\frac{2}{3} \mu_l + \mu_l'$, where μ_l' is the second viscosity or volumetric viscosity (SONIN 2001, Fluent 6.3. User's Guide 2006).

$$\overleftrightarrow{\tau}^m = 2\mu_l \overleftrightarrow{D} - \frac{2}{3} \mu_l \operatorname{div}(\vec{v}) \overleftrightarrow{I} + \mu_l' \operatorname{div}(\vec{v}) \overleftrightarrow{I} \quad (20)$$

Formula (20) is the general formula of viscous molecular stress tensor for Newtonian fluid used to supplement the basic set of equations (1). For non-Newtonian fluid, a different stress tensor must be defined, appropriate to the property of the fluid. In the literature, one can find tens of different models. General non-Newtonian fluids are divided into a few groups due to the relationship between stress and strain rate tensor (Fig. 2a) and on two groups due to the change of the properties at the time (Fig 2b). A more extensive discussion of this issue does not fall within the scope of this article.

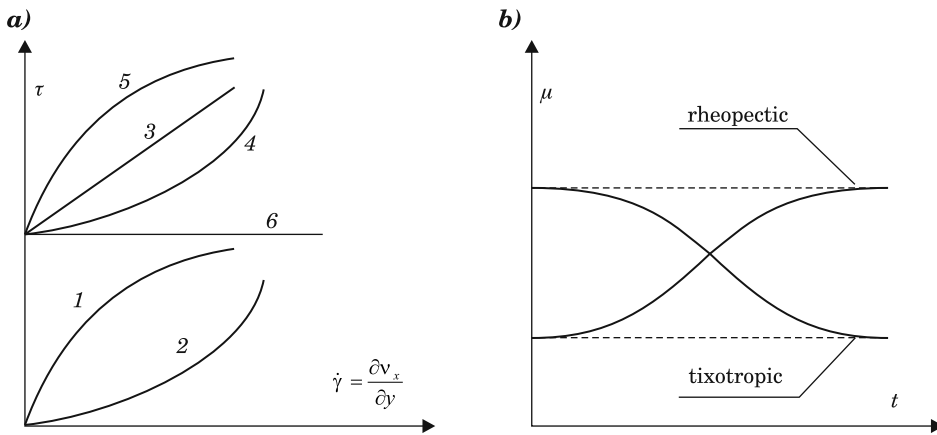


Fig 2. Types of non-Newtonian fluid: 1 – pseudoplastic fluid, 2 – dilatant fluid, 3 – Bingham fluid, 4 – dilatant fluid with yield, 5 – pseudoplastic fluid with yield, 6 – ideal pseudoplastic fluid

Turbulent stress tensor

Turbulence modeling is one of the biggest problems of modern fluid mechanics. In the CFD area, it can be at present to distinguish a few basic approaches to the turbulence modeling (Fig. 3).

Direct Numerical Simulation (DNS) (MOIN 1998, JOSEPH 2005, BOGUSŁAWSKI 2008). It is the most accurate numerical method to solve turbulent flows. In this method all spatial and temporal scales (Fig. 4) are resolved. Hence, computed results are equivalent to those that are obtained experimentally. The disadvantage of the method is enormous computing power requirements – the cost of a simulation goes up to in term of CPU time. Currently, the method can be used only for flows with relatively low Reynolds number.

Large Eddy Simulation (LES) (PIOMELLI et al. 2000, UYGUN et al. 2004). The essence of this method is the division of eddies on the large scale and the subgrid scale, according to the Kolmogorov's theorem (PUZYREWSKI,

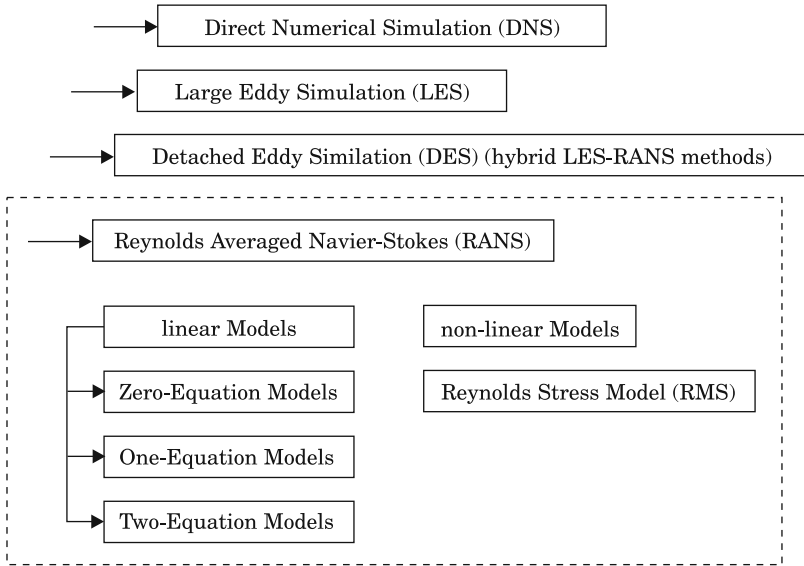


Fig 3. The main group of turbulence models

Source: KACZYŃSKI (1997), UYGUN et al. (2004), SAAD (2011).

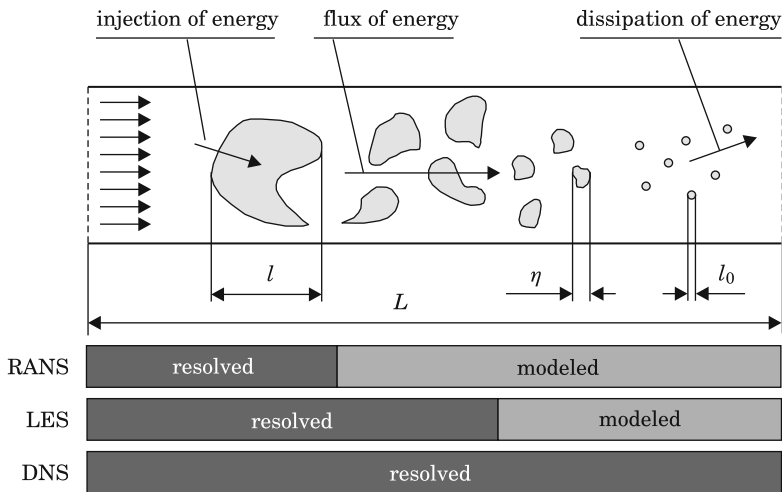


Fig 4. Scales of the eddies in turbulent flow

SAWICKI 2000), and next treating both scales separately. This concept follows from the observation that in flows with sufficiently high Reynolds number largest and smallest scales are well separated: the energy of the main flow passes through the mechanism of vortex-stretching and the decay of vortices to an ever smaller scale (Fig. 4). LES allows to obtain the explicitly result for

the large eddies in a calculation and implicitly solution for the small eddies by using a subgrid scale model (the principal operation in LES is low-pass filtering). For this reason, LES allows better fidelity than alternative approaches (RANS methods) that do not resolve any scales of the solution. This method requires greater computational resources than RANS methods, but is far cheaper than DNS.

Detached Eddy Simulations (DES) (SPALART et al. 2006). It is a mix of a RANS and LES models. Regions near solid boundaries and where the turbulent length scale is less than the maximum grid, dimensions are assigned the RANS mode of solution. As the turbulent length scale exceeds the grid dimension, the regions are solved using the LES mode. Therefore the grid resolution for DES is not as demanding as pure LES, thereby considerably cutting down the cost of the computation. The disadvantage of this method is that the grid generation is more complicated than for a simple RANS or LES.

Reynolds Averaged Navier-Stokes (RANS) models (EASOM 2000, FLUENT 6.3 User's Guide 2006). It is the oldest and most popular approach to the turbulence modeling in CFD area – for this reason, the approach is described here in more detail. In RANS concept, the conservation equations are time-averaged, according to the velocity decomposition proposed by Reynolds (CELIK 1999, ADRIAN et al. 2000, PUZYREWSKI, SAWICKI 2000). In this decomposition, the current value of velocity consists of an average velocity \bar{v} and a fluctuation v' (Fig. 5).

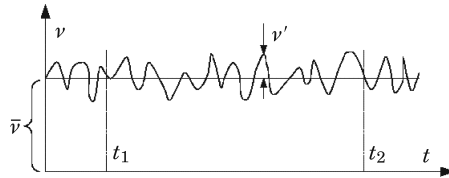


Fig 5. The idea of velocity decomposition

The velocity decomposition may be written as follow:

$$\bar{v} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} v dt \quad (21)$$

wherein

$$\frac{1}{t_2 - t_1} \int_{t_1}^{t_2} v' dt = 0 \quad (22)$$

and

$$\frac{1}{t_2 - t_1} \int_{t_1}^{t_2} v'v' dt = \overline{v'v'} \quad (23)$$

The decomposition idea can be introduced to the Navier-Stokes equation (i.e. to the momentum equation without the turbulence member), and therefore

$$\frac{\partial}{\partial t} (\rho(\bar{v} + v')) + \text{div}(\rho(\bar{v} + v')(\bar{v} + v') + \overset{\leftrightarrow}{p}I) = \text{div}(\overset{\leftrightarrow}{\tau}^m) + \rho s_b \quad (24)$$

or

$$\frac{\partial}{\partial t} (\rho(\bar{v} + v')) + \text{div}(\rho(\bar{v}\bar{v} + \bar{v}v' + v'\bar{v} + v'v') + \overset{\leftrightarrow}{p}I) = \text{div}(\overset{\leftrightarrow}{\tau}^m) + \rho s_b \quad (25)$$

Taking into account the relationships (22) and (23) in the above equations, receives a shorter form

$$\frac{\partial}{\partial t} (\rho\bar{v}) + \text{div}(\rho\bar{v}\bar{v} + \overset{\leftrightarrow}{p}I) = \text{div}(\overset{\leftrightarrow}{\tau}^m - \overline{\rho v'v'}) + \rho \vec{s}_b \quad (26)$$

where the member $\overline{\rho v'v'}$ (in equation (26) moved to the right side) is the general record of the turbulent stress tensor (DROBNIAK et al. 2008).

$$\overset{\leftrightarrow}{\tau}^R = \begin{vmatrix} -\rho v_x v_x & -\rho v_x v_y & -\rho v_x v_z \\ -\rho v_y v_x & -\rho v_y v_y & -\rho v_y v_z \\ -\rho v_z v_x & -\rho v_z v_y & -\rho v_z v_z \end{vmatrix} \quad (27)$$

In the current approach, the turbulent stress tensor is treated as a “correction” of viscous molecular stress tensor $\overset{\leftrightarrow}{\tau}^m$, which must be added into turbulent flows. This conception is often called the Boussinesq hypothesis or the Boussinesq approximation. The turbulent stress tensor has in this concept the same structure as the viscous molecular tensor

$$\overset{\leftrightarrow}{\tau}^R = 2\mu_t \overset{\leftrightarrow}{D} - \frac{2}{3}\mu_t \text{div}(\vec{v}) \overset{\leftrightarrow}{I} + \mu_t' \text{div}(\vec{v}) \overset{\leftrightarrow}{I} \quad (28)$$

but the dynamic viscosity μ_l is replaced by its turbulent counterpart μ_t . Now the total stress tensor may be noted as

$$\overleftrightarrow{\tau}^t = \overleftrightarrow{\tau}^m + \overleftrightarrow{\tau}^R = 2\mu_{eff} \overleftrightarrow{D} - \frac{2}{3}\mu_{eff} \text{div}(\vec{v}) \overleftrightarrow{I} + \mu'_{eff} \text{div}(\vec{v}) \overleftrightarrow{I} \quad (29)$$

where effective viscosity is defined as

$$\mu_{eff} = \mu_l + \mu_t \quad (30)$$

It is important, that μ_t is not a physical quantity, only a correction factor of μ_l . Usually it is assumed that this ratio depends on the kinetic energy of turbulence

$$k = \frac{1}{2} \overline{v_i v_i} \quad (31)$$

and its dissipation (denoted often as ε or ω). In the RANS approach, very often it is assumed that the turbulent viscosity depends on the distance of the wall. Another value is assumed in the boundary layer and another in the rest of the flow (KACZYŃSKI 1997).

Most popular models from the RANS group are shown in Fig. 6 (KACZYŃSKI 1997, VOIGT et al. 2003, ABDOL-HAMID et al. 2006, KARVINEN, AHLSTEDT 2008). On this figure, the linear models are divided due to the number of evolution equations needed to determine the value of μ_t , which must be added to the main set of equation (1) and which have the same mathematical structure, matched to the vector form of the balance equations. It is worth mentioning that in the literature are known models with a much larger number of evolution equations.

The equation (1) – and all derivation, which was shown in work (SOBIESKI 2011) – has the form typical for RANS methods. Using other methods require additional mathematic transformations of the set (1). In RANS methods, the members associated with turbulence are there treated as correction factors of parts describing laminar flows. After this adjusting, the results of calculations agree better with experiments, but only if the turbulence model is chosen correctly.

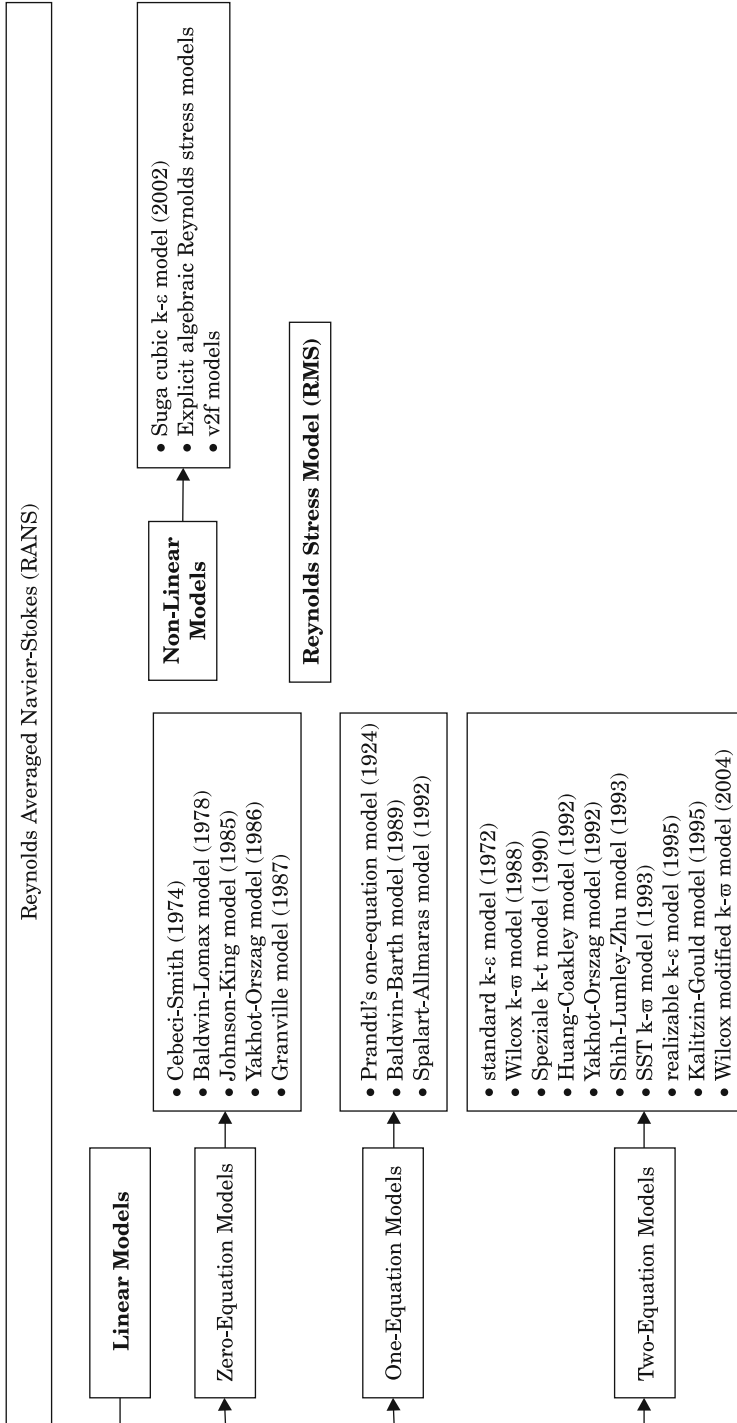


Fig. 6. The most popular models from the RANS group

Molecular and turbulent heat flux

The molecular heat flux in set of equations (1) can be calculated on basis the Fourier Law (MAGAGNATO 1998, STANISZEWSKI 1998, WRÓBLEWSKI 2008).

$$\vec{q}^m = -\lambda_l \cdot \text{grad}(T) \quad (32)$$

where:

λ_l – is the material's conductivity appropriate for laminar flows [W/(m · K)].

In the literature, it is assumed that a positive sign applies to the effluent stream from the volume, hence the negative sign in the formula. In the case of turbulent flow, one can exploit the concept of a correction factor (analogy like in the formula (29)), then

$$\vec{q}^t = \vec{q}^m + \vec{q}^R = \lambda_{eff} \cdot \text{grad}(T) \quad (33)$$

where effective material's conductivity is defined as

$$\lambda_{eff} = \lambda_l + \lambda_t \quad (34)$$

In this formula, λ_t is the material's conductivity appropriate for turbulent flows.

Momentum and energy sources

In case of one phase flow, the source vector is very simple. The momentum inside a control volume can be change only by the force of gravity, wherein this is important in principle, only for liquid flows. Effect of gravity, in the case of gas, is small and in most cases it can be neglected. The momentum source can therefore have a form

$$s_b = \pm g \quad (35)$$

where the sign depends on the orientation of the adopted coordinate system. The g is equal to the acceleration of objects under influence of the gravitational field [m/s²].

In case of flows without chemical reaction and phase change (which would require the existence in flow of several phases), the source of energy is always equal to zero.

Summary

This article presents basic information on the closures of balance equations, mass, momentum and energy in the form characteristic for the FVM and one phase flows. This information is very general in nature, but should orient the reader to the basic aspects of CFD. Unfortunately, the correct selection of the closures is a matter of a relatively difficult concept, requiring considerable knowledge and experience. Particularly troublesome is the determination of closure on the viscous stress tensor of non-Newtonian fluids and the closure describing the turbulence. It may indeed happen that laminar flow is analyzed, or those where the turbulence does not significantly affect the course of the modeled phenomenon, but in many cases, the choice of appropriate turbulence model is a key issue if we want to obtain quantitative agreement of calculation results with the experiment. Examples are flows in diffusers, ducts with plenty of walls or any type of flows around an object.

The issue relating to the closures is more complicated in cases with multiphase flows. It should then determine again the viscous and turbulent stress tensors of such a medium (we're talking about RANS approach), as well as numerous closures, describing interactions between phases: the exchange of mass, momentum and energy. These closures are dependent on many factors so that the final models describing two different situations of flow can be quite dissimilar to each other.

Translated by WOJCIECH SOBIESKI

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