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Closure of Turbulent Fluxes for the Transport of Momentum, Energy, and Mass

Marcelo Ferreira Alfradique and Affonso Silva Telles
Escola de Química, Universidade Federal do Rio de Janeiro, Caixa Postal 68542, RJ, Cep 21949 900, Brazil

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The methods of extended thermodynamics are employed to establish a set of closure equations for the turbulent fields. The main advantage of its use resides in the elimination of all arbitrariness in the selection of the constitutive variables and basic model for the average fields present in the various equations for the turbulent moments. In addition, the method provides a systematic way correcting observed improprieties. Starting with the equations for the fluctuations of the velocity and of passive scalar fields, it is possible to write successive equations for the moments of increasing orders in the form of balances in terms of a time derivative, a convective flux, and a source field. The unknown terms for each order are assumed to be determined by constitutive equations given as functions, exclusively, of the moments of lower order. The only free choice is on the level of description, as determined by the order of the highest moment considered. Equations required for the two first levels, pertaining to the moments of the fluctuations of velocity, and of temperature and concentrations are presented, discussed and compared to previous models and known results. Heat and mass-transfer effects are considered, and it is shown the existence of interference between these processes in a form analogous to the Dufour and Soret effects, with a marked anisotropy following the Reynolds stress. *AIChE J,* 52: 2684–2696, 2006
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Introduction

The proposed options for the closure of the equations for the average fields in turbulent flows are constantly under critical appraisal, reexamination and inclusion of correction factors of various forms and means of justification. This status reflects the inexistence of a sound and systematic method of achieving closure, and in part from the inadequacy of the concept of turbulent viscosity, introduced by Boussinesq[1] in analogy to the molecular viscosity

$$\overline{u_i u_j} \equiv R_{ij} = \frac{2}{3}\kappa\delta_{ij} + 2\nu^t[D_{ij} - \frac{1}{3}D_{kk}\delta_{ij}]$$

$$D_{ij} = \frac{1}{2}(L_{ij} + L_{ji}) \qquad (1)$$

where u_i is the velocity fluctuation, R_{ij} is the Reynolds stress, κ is the average value of the kinetic energy of the turbulent fluctuations per unit mass, and ν^t is the turbulent viscosity. Cartesian tensor notation is used with the summation convention in the repeated indices.

The mixing length theory of Prandlt[2] employs scales of length and time with which a workable form for the eddy viscosity is constructed. Subsequently, the kinetic energy of turbulence was chosen as a natural scale, a choice that gave rise to the family of "one equation models". This procedure has been transformed into complex schemes of multi-equations models, which despite their complexity require the use of wall corrections, determined as functions of position. These corrections are not expressed in terms of properties of the turbulent

Correspondence concerning this article should be addressed to A. S. Telles at affonso@eq.ufrj.br.

fluctuations, and, therefore, they are not constitutive, and are valid only for a single flow configuration.

It is important to mention that the basic relation for the Reynolds stress R_{ij}, as determined by the symmetric part of the velocity gradient is insufficient. It predicts, even, for simple shearing flows, an incorrect equipartition of the kinetic energy of the turbulent fluctuations between the three normal stresses. The addition of the Stokesian term in $\mathbf{D}^2$ does not improve predictions satisfactorily

$$R_{ij} = \frac{2}{3}\kappa\delta_{ij} + 2\nu^t[D_{ij} - (\tfrac{1}{3}D_{kk})\delta_{ij}] + \lambda^t[D_{ik}D_{kj} - (\tfrac{1}{3}D_{lk}D_{kl})\delta_{ij}] \tag{2}$$

This relation for the Reynolds stress and all its modifications by the long line of multi equation methods yield predictions about normal stresses in conflict with observations. This leads to an inability to properly predict secondary flows in noncircular pipes, and in all more complex flow configurations.

A different approach for the development of constitutive equations for the Reynolds stress was originally proposed by Pope[3], and termed second-closure model. Pope based on the work of Launder, Reece and Rodi[4], which rests on the transformation of the balance equation for the Reynolds stress into an algebraic nonlinear equation. Gatski and Speziale[5] extended the method to cases of three-dimensional flows and included the effects of rotations in noninertial reference frames.

All the above propositions can be summarized in the statement that the Reynolds stress is determined by the velocity gradient decomposed into its symmetric and antisymmetric parts

$$R_{ij} = R_{ij}(D_{ab}, W_{ab})$$

$$W_{ij} = \frac{1}{2}(L_{ij} - L_{ji}) \tag{3}$$

Noll[6] introduced in continuum mechanics the usage of frame indifference under the Euclidean group of transformations. The argument being that the Euclidean group corresponds to rigid body like motions, in which the material properties are preserved. Equation 3 $_1$ does not describe material properties, but average properties of a turbulent motion of a fluid with well established density and viscosity. Furthermore motions occur in contact with surfaces possibly in motion, providing a special frame with respect to which the velocity and spin are measured. Speziale[7] proposed the adoption of the group of Einstein, which allows arbitrary linear accelerations but no spin, as the group determining the invariance properties for the moments associated to turbulence. The use of isotropic functions that depend simultaneously on the two parts of the velocity gradient reduce the limitations pertinent to the erroneous prediction of the normal stresses, and dependence on the relative velocity between fluid and wall, may dispense with the use of the distance from the wall.

An alternative to the eddy viscosity hypothesis rests on the assumption that Reynolds stress in turbulent flows can be described by the constitutive equations of simple fluid as defined by Noll[6]. Constitutive equations describing second grade fluids have been applied to turbulence. Busuioc[8] has shown this to be equivalent to the Camassa-Holm equation (Camassa and Holm[9]) derived with the help of the "shallow water approximation". This effort can be generalized letting the Reynolds stress be given by an isotropic algebraic function of the Rivlin-Ericksen tensors (Rivlin and Ericksen[10]) of increasing grades with the flow complexity

$$R_{ij} = R_{ij}(A_{1ab}, A_{2ab}, \ldots)$$

$$A_{1ij} = 2D_{ij}, \quad A_{2ij} = \dot{A}_{1ij} + A_{1ik}L_{kj} + L_{jk}A_{1ki} \tag{4}$$

More complex models in which the material time derivative of the Reynolds stress is part of the model are similar to the equations proposed for hypoelastic materials defined by the assignment of a set of first-order differential equations of the type

$$\mathring{R}_{ij} = \mathring{R}_{ij}(D_{ab}, W_{ab}, R_{ab}) \tag{5}$$

where the superimposed circle designate one of the derivatives with the appropriate invariance properties as proposed by Oldroyd[11], or Jaumann[12], or Truesdell[13].

Maxwell model for viscoelastic fluids can be viewed as the fusion between Eqs. 4 and 5, resulting in

$$\mathring{R}_{ij} = \mathring{R}_{ij}(A_{1ab}, A_{2ab}, \ldots W_{ab}, R_{ab}) \tag{6}$$

Modeled balance equations for the Reynolds stress can lead to equations of the general type of Eqs. 5 or 6, in which the circle indicate a still different derivative which differ from the lower-convected Oldroyd derivative in the sign of some terms.

Systematic approaches for the proposition of constitutive equations, (not necessarily for the turbulent stresses), started with thermodynamics of irreversible processes. The application of this theory to the Reynolds stress results in a linear relation between that variable and the velocity gradient, the conjugate force in the equation for the entropy production. Since R_{ij} is symmetric the requisite of linearity eliminates dependence on the spin W_{ij}, resulting in an expression similar to the Boussinesq proposition.

Continuum thermodynamics developed by Coleman and Noll[14] allows nonlinear dependence on the constitutive variables, and these are selected independently of the entropy production inequality. The theory does not impose the restriction that the constitutive variables be selected as the thermodynamic forces appearing in the expression for the dissipation of energy. This freedom is a requisite of the observed deviations in the mechanical behavior of complex materials. Thus, the principle of equipresence as proposed by Truesdell (see Truesdell and Noll[15]) was extended to the chosen constitutive variables, not necessarily participating in the dissipation expression, and equally applied to thermodynamic equations for the internal energy, and entropy. Equipresence allows, in some cases, the rigorous demonstration of local equilibrium hypothesis.

A significant step toward the formulation of a systematic theory of constitutive equations has been called "extended thermodynamics". This discipline, developed initially by Liu and Muller[16], is an outgrown of the thermodynamics of irreversible processes whose main motivation was to replace the parabolic field equations, which results from the use of the constitutive assumptions of Navier-Stokes, Fourier, and Fick on the momentum, energy, and mass balances. The method is fully explained in the text by Muller and Ruggeri[17]. Additional references are presented by: Ruggeri and Strumia[18] and Boillat and Ruggeri[19].

From this effort, and beyond its original intention, there resulted a well-founded constitutive theory, which reduces the arbitrariness associated with the choice of independent variables for the constitutive equations. In some applications the balance equations are obtained for the moments of the velocity distribution derived from Boltzmann theory of gases. The state of the system is *a priori* defined, and no dubiousness remains in selecting the constitutive variables to be set as state functions. Equations of balance for the moments of progressive orders are derived, and constitutive equations are postulated for the unknown terms appearing in the equation of the highest order. The chain of interdependent equations can be simultaneously solved. Once the order of the highest moment is chosen, dependent and independent variables are forced by the method leaving no space for arbitrary choices.

The constitutive functions must satisfy the principle of material frame indifference with respect to the Galilean group of transformation. This is one of the tenets of extended thermodynamics, in flagrant opposition to the tenets of continuum thermodynamics as developed by Coleman and Noll[14] and Truesdell and Noll[15].

The constitutive and field equations must satisfy further, the second law in the form of the Clausius-Duhem inequality, and in addition a convexity hypothesis, which produce as consequence hyperbolic equations with finite pulse propagation velocity, for the velocity and passive scalars fields.

Presently, extended thermodynamics has surpassed its initial motif of overcoming the paradox of infinite pulse propagation velocities, and has become a predictive macroscopic theory, which is needed when steep gradients and rapid changes occur.

The first application of extended thermodynamics to the closure of turbulence was made by Huang and Rajagopal[20], motivated by the existence of similarities between the constitutive equations for the turbulent flow of a Newtonian fluid, and the laminar flow of a non-Newtonian fluid. The authors follow the methods without deviations and arrive at equations for a general nonlinear $\kappa-\varepsilon$ model. This effort has been criticized by Speziale[21] both in respect to its ability to predict turbulent stress relaxation, and with respect to the validity of the analogy between turbulence and non-Newtonian fluids, and to the adequacy of the Clausius-Duhem inequality to restrict the turbulent closure equations. The rebuttal by Rajagopal[22] ascertains its valid points in both aspects.

Our motivation in this respect is to adapt the theory in order to provide a system of equations circumventing the turbulence closure problem. It is well known that once it is assumed that the properties of turbulent flows are governed by the Navier-Stokes system, and the mass and energy balances it is possible to derive equations for the average values of all kinematic properties. However, these balance equations always contain higher order terms, and the set is insoluble. The set of average values of the moments of the velocity fluctuations of progressive orders can be arranged in a format analogous to the basic equations of extended thermodynamics, with the balance equations for the velocity, temperature, and concentrations fluctuations, assuming roles similar to Maxwell's equation. The similarity between velocity fluctuations on the molecular level responsible for the macroscopic observable fluxes of momentum and the turbulent velocity fluctuations responsible for the average Reynolds stress, the other turbulent fluxes permits the transposition of the methods of extended thermodynamics to the closure of the equations for the turbulent fields. The argument here stands on the point that we employ the set of traditional balances derived from the assumption that the instantaneous fields satisfy the well-established balances of momentum, heat and mass, and with these the balances for the moments of all orders can be derived. These are written under the standard form proposed by the theory, resulting in the definition of constitutive fluxes and source terms for each equation of the theory. The required constitutive equations are written as functions of the moments of all previous orders, and this procedure eliminates all arbitrariness in the selection of the constitutive variables. This point will become clearer when the set of balance equations is discussed.

Furthermore, in the region close to walls, about which the flow is taking place the gradients of time-averaged quantities are very steep, a fact that may signify the necessity of considering the effects of higher-order moments. This is related to the main claim of extended thermodynamics, which bases its methods on systems of multiple equations involving moments of increasing order.

Once this is ascertained it becomes possible to follow the dictates of the theory to arrive at progressive set of closure systems for the turbulence equations.

Preliminary definitions and turbulent fluctuations

Consider the turbulent motion of an incompressible, Newtonian fluid about a wall, possibly in motion. The wall is a two-dimensional (2-D) manifold described by a set of almost everywhere smooth maps from an open set of $\mathbb{R}^2$ into a set of the 3-D Euclidean space $\mathbb{E}$

$$x_i = \sigma_i(\xi_1, \xi_2, t), \quad i = 1, 2, 3 \tag{7}$$

The time dependence expresses the motion, and if the wall is rigid the motion combines a translation and a rigid rotation determined by a time-dependent orthogonal transformation Q_{ij}

$$x_i = Q_{ij}(t)\sigma_j(\xi_1, \xi_2) + d_i(t) \tag{8}$$

The field of wall velocities can be calculated as follows

$$\dot{x}_i = W^s_{ij}(t)[x_j - d_j] + \dot{d}_i(t)$$

$$W^s_{ij} = \dot{Q}_{ik}Q_{jk} \tag{9}$$

The superimposed dot signifies time derivative, and is the surface spin.

The importance and necessity of including surface properties on the constitutive equations associated to turbulent flows has been considered by Telles[23]. In this work stationary walls will be considered, and the kinematical description is relative to an inertial frame as required by the formalism of extended thermodynamics. This implies that changes of frame be restricted to the Galilean group of transformations. Thus a change of frame from coordinates $\mathbf{x} \rightarrow \mathbf{x}^*$ is determined by

$$x_i^* = Q_{ik}x_k + \dot{d}_i t \tag{10}$$

where Q_{ij} is an orthogonal transformation, and $\dot{d}_i$ is a constant velocity.

Velocity fluctuations

The instantaneous velocity, and pressure fields $\nu_i = v_i + u_i$, and $\mathbb{P} = P + p$ are divided into average values and the fluctuating parts. The mass and momentum balances for the fluctuating components are written in the following form, as presented in Hinze[24]

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{11}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_p}[v_i u_p + v_p u_i + (u_i u_p - R_{ip})] = \upsilon \nabla^2 u_i - \frac{\partial p/\rho}{\partial x_i} \tag{12}$$

where $R_{ij} = \overline{u_i u_j}$ are the Reynolds stresses, and the bar designate the ensemble averaging operator.

This equation is the basis for the calculation of the evolution equations for the moments, which play the role of the basic quantities of the theory. The form of Eq. 12 is not unique for either or both terms on the righthand side can be included onto the divergence term on the left. The form chosen is one in which the average values of all the moments of the fluctuating components of the velocity fields, of increasing order appear inside the divergence term which contains, in addition, lower order moments exclusively, and no physical property.

Balance equations for the following products may be required

$$u_i u_j;\ u_i u_j u_k;\ u_i u_j u_k u_l \ldots$$

The time derivatives of each of these moments can be calculated starting from Eq. 12 leading to equations that can be put under the form of Eqs. 13, 15, and 16, following

$$\frac{\partial u_i}{\partial t} + \frac{\partial J_{ip}}{\partial x_p} = K_i \tag{13}$$

In this equation

$$J_{ip} = v_i u_p + v_p u_i + (u_i u_p - R_{ip})$$

and

$$K_i = \upsilon \nabla^2 u_i - \frac{\partial p/\rho}{\partial x_i} \tag{14}$$

The products of the fluctuating velocities of various orders can be expressed as

$$\frac{\partial u_i u_j}{\partial t} + \frac{\partial J_{ijp}}{\partial x_p} = K_{ij}$$

where

$$J_{ijp} = u_j J_{ip} + u_i J_{jp} \tag{15}$$

$$\frac{\partial u_i u_j u_k}{\partial t} + \frac{\partial J_{ijkp}}{\partial x_p} = K_{ijk},$$

where

$$J_{ijkp} = u_j u_k J_{ip} + u_k u_j J_{ip} + u_k u_i J_{jp} \tag{16}$$

This method depends on the balance equations for the moments of these products

$$\overline{u_i} = 0; \quad \overline{u_i u_j} = R_{ij}; \quad \overline{u_i u_j u_k} = R_{ijk}$$

$$\overline{K_i} = 0; \quad \overline{K_{ij}} = S_{ij}; \quad \overline{K_{ijk}} = S_{ijk} \tag{17}$$

These lead to equations for the average values of the following: the velocity v_i, the Reynolds stress R_{ij}, and for all moments of increasing orders, as required to achieve accurate results. These are:

average velocity

$$\frac{\partial v_i}{\partial t} + \frac{\partial}{\partial x_p}[v_i v_p + R_{ip}] = \upsilon \nabla^2 v_i - \frac{\partial P/\rho}{\partial x_i} \tag{18}$$

double moment or Reynolds stress

$$\frac{\partial R_{ij}}{\partial t} + \frac{\partial}{\partial x_p}[R_{jp}v_i + R_{ip}v_j + R_{ij}v_p] + \frac{\partial R_{ijp}}{\partial x_p} = S_{ij}, \quad \text{or}$$

$$\dot{R}_{ij} + R_{jp}\frac{\partial v_i}{\partial x_p} + R_{ip}\frac{\partial v_j}{\partial x_p} + \frac{\partial R_{ijp}}{\partial x_p} = S_{ij} \tag{19}$$

triple moment

$$\frac{\partial R_{ijk}}{\partial t} + \frac{\partial}{\partial x_p}[R_{jkp}v_i + R_{ikp}v_j + R_{ijp}v_k + R_{ijk}v_p] + \frac{\partial}{\partial x_p}[-R_{ij}R_{kp} - R_{jk}R_{ip} - R_{ik}R_{jp} + R_{ijkp}] = S_{ijk} \tag{20}$$

The set of Eqs. 18 to 20 constitute the basis for the application of the methods of extended thermodynamics to the closure of turbulence. Clearly, additional terms for higher order moments can be incorporated as required. The structure of this set is characterized by the fact that the divergence term in each equation contain moments of increasing order, and the source term contain more complex moments involving the fluctuations in the velocity and pressure gradients. For future reference, Eq. 19 is rewritten in terms of the material time derivative.

The sequence of closure procedures follows the order:

- for the 0^{th} level the moments are the average velocity and the Reynolds stress, present in Eq. 18, thus, the appropriate constitutive equation for is $Rij = Rij\ (v_a)$.
- The 1^{st} level includes the balance of double moments appearing in Eq. 19, which include the triple moment $R_{ijk} = R_{ijk}(R_{ab},\ v_a)$ and source term $S_{ij} = S_{ij}(R_{ab},\ v_a)$. Their substitution into Eq. 19 yield a closed set of Eqs. 19 and 18 for the velocity and Reynolds stress fields.
- The same procedure is repeated for the 2^{nd} level, when constitutive equations for R_{ijkp} and S_{ijk} are written in terms of the previous moments $R_{ijkp} = R_{ijkp}(R_{abc},\ R_{ab},\ v_a)$, $S_{ijk} = S_{ijk}(R_{abc},\ R_{ab},\ v_a)$ and $S_{ij} = S_{ij}(R_{abc},\ R_{ab},\ v_a)$. Introducing these into Eqs. 20 and 19 results in a closed set of equations for $R_{ijk},\ R_{ij},\ v_i$.

Temperature and concentration fluctuations

The temperature, or the concentrations of chemical species, is assumed to be determined by equations with constant physical properties. A balance equation for the instantaneous temperature field θ, divided into an average value and a fluctuating component

$$\theta = \bar{\theta} + \theta' \tag{21}$$

is assumed to satisfy the following field equation

$$\frac{\partial \theta}{\partial t} + \frac{\partial \nu_p \theta}{\partial x_p} = \alpha \nabla^2 \theta + \sum_{\beta} \lambda_{q\beta} \nabla^2 c^{\beta} + \chi \tag{22}$$

where α is a thermal diffusivity, and χ the source term, and $\lambda_{q\beta}$ are the material coefficients responsible for the Dufour effects of the laminar heat flux associated to the concentration gradients.

Similarly the instantaneous solute concentrations obey balance equations of the same form ($c^{\alpha} = \bar{c}^{\alpha} + c'^{\alpha}$):

$$\frac{\partial c^{\alpha}}{\partial t} + \frac{\partial \nu_p c^{\alpha}}{\partial x_p} = \lambda_{\alpha\theta} \nabla^2 \theta + \sum_{\beta} D_{\alpha\beta} \nabla^2 c^{\beta} + \chi^{\alpha} \tag{23}$$

where $\lambda_{\alpha\theta}$ are the thermal diffusion coefficients determining the mass fluxes of each component due to the temperature gradient (Soret effect), and $D_{\alpha\alpha}$ is the self-diffusion coefficient, while $D_{\alpha\beta}$ ($\beta \neq \alpha$) give the coupling effects between the chemical components.

Substitution of the decomposition Eqs. 21 into 22, application of the averaging functional, and subsequent subtraction from the original Eq. 22 yield the balance equation for the fluctuating part of the temperature field, and the fluctuating part of the concentration fields

$$\frac{\partial \theta'}{\partial t} + \frac{\partial}{\partial x_p}[u_p \bar{\theta} + v_p \theta' + (u_p \theta' - q_p)] = k \tag{24}$$

$$\frac{\partial c'^{\alpha}}{\partial t} + \frac{\partial}{\partial x_p}[u_p \bar{c}^{\alpha} + v_p c'^{\alpha} + (u_p c'^{\alpha} - m_p)] = n^{\alpha} \tag{25}$$

Notice that these equations are independent of all transport coefficients for heat and mass. A fact that would seem to exclude the Soret and Dufour effects in association to turbulence.

The two equations, in conjunction with Eq. 12 allow the calculation of balance equations for the following products: $u_i\theta'$, $u_iu_j\theta'$, $u_iu_ju_k\theta'$ and $u_ic'^{\alpha}$, $u_iu_jc'^{\alpha}$, $u_iu_ju_kc'^{\alpha}$. They can be transformed into equations with the same structure and form as Eqs. 13 to 16

$$\frac{\partial \theta'}{\partial t} + \frac{\partial j_p}{\partial x_p} = k$$

$$j_p = u_p \bar{\theta} + v_p \theta' + (u_p \theta' - q_p) \tag{26}$$

$$\frac{\partial u_i \theta'}{\partial t} + \frac{\partial j_{ip}}{\partial x_p} = k_i,$$

$$j_{ip} = \theta' J_{ip} + u_i j_p \tag{27}$$

$$\frac{\partial u_i u_j \theta'}{\partial t} + \frac{\partial j_{ijp}}{\partial x_p} = k_{ij}$$

$$j_{ijp} = \theta' J_{ijp} + u_i u_j j_p \tag{28}$$

Similar equations apply to the moments of fluctuating velocities and the fluctuating concentration fields.

The average values of the products that must be considered in the closure equations in the presently proposed methodology are:

$$q_i = \overline{u_i \theta'}, \quad q_{ij} = \overline{u_i u_j \theta'}, \quad q_{ijk} = \overline{u_i u_j u_k \theta'} \tag{29}$$

and

$$m_i^{\alpha} = \overline{u_i c'^{\alpha}}, \quad m_{ij}^{\alpha} = \overline{u_i u_j c'^{\alpha}}, \quad m_{ijk}^{\alpha} = \overline{u_i u_j u_k c'^{\alpha}} \tag{30}$$

average temperature

$$\frac{\partial \bar{\theta}}{\partial t} + \frac{\partial}{\partial x_k}[v_k \bar{\theta} + q_k] = \alpha \nabla^2 \bar{\theta} + \sum_{\beta} \lambda_{q\beta} \nabla^2 \bar{c}^{\beta} + \bar{\chi} \tag{31}$$

double moment, or turbulent heat flux

$$\frac{\partial q_i}{\partial t} + \frac{\partial}{\partial x_p}[R_{ip} \bar{\theta} + q_i v_p + q_{ip}] = s_i \tag{32}$$

triple moment

$$\frac{\partial q_{ij}}{\partial t} + \frac{\partial}{\partial x_p}[R_{ijp}\bar{\theta} + q_{jp}v_i + q_{ip}v_j] + \frac{\partial}{\partial x_p}[q_{ij}v_p - R_{jp}q_i - R_{ip}q_j] - \frac{\partial}{\partial x_p}[R_{ij}v_p - q_{ijp}] = s_{ij} \quad (33)$$

Equations for the average concentration fields dissolved in the fluid can be written:

average concentration

$$\frac{\partial \bar{c}^\alpha}{\partial t} + \frac{\partial}{\partial x_p}[v_p\bar{c}^\alpha + m_p^\alpha] = \lambda_{\alpha\theta}\nabla^2\bar{\theta} + \sum_\beta D_{\alpha\beta}\nabla^2\bar{c}^\beta + \bar{\chi}^\alpha \quad (34)$$

double moment, or turbulent mass flux

$$\frac{\partial m_i^\alpha}{\partial t} + \frac{\partial}{\partial x_p}[R_{ip}\bar{c}^\alpha + m_i^\alpha v_p + m_{ip}^\alpha] = n_i^\alpha \quad (35)$$

triple moment

$$\frac{\partial m_{ij}^\alpha}{\partial t} + \frac{\partial}{\partial x_p}[R_{ijp}\bar{c}^\alpha + m_{ip}^\alpha v_j + m_{jp}^\alpha v_i] + \frac{\partial}{\partial x_p}[m_{ij}^\alpha v_p - R_{jp}m_i^\alpha - R_{ip}m_j^\alpha] - \frac{\partial}{\partial x_p}[+R_{ij}m_p^\alpha - m_{ijp}^\alpha] = n_{ij}^\alpha \quad (36)$$

Expressions for the turbulent heat and mass fluxes are usually postulated in analogy with Fourier and Fick's laws, and furthermore the turbulent diffusivities for heat and mass transport are assumed proportional to the turbulent viscosity, with recourse to the "turbulent Prandtl and Schmidt numbers"

$$q_i = \alpha^t \frac{\partial \theta}{\partial x_i} = \frac{1}{\mathrm{Pr}^t}\upsilon^t \frac{\partial \theta}{\partial x_i}, \quad (37)$$

$$m_i^\alpha = D_{\alpha\alpha}^t \frac{\partial c^\alpha}{\partial x_i} = \frac{1}{\mathrm{Sc}^t}\upsilon^t \frac{\partial c^\alpha}{\partial x_i}. \quad (38)$$

Substitution of these expressions into the equations for average temperature and average concentration, Eqs. 31 and 34 yield closed forms for the turbulent transport. This reduces the problem of turbulence closure to the determination of the turbulent viscosity. The isotropy proclaimed in these two expressions is difficult to sustain. The velocity fluctuations, which are responsible for the temperature and concentration fluctuations are not isotropic. The dampening of the velocity fluctuations due to the presence of a wall is strongly dependent on the direction. The transport of energy and mass is, in consequence anisotropic, and this anisotropy should manifest in Eqs. 37 and 38.

Extended Method in Turbulence

In turbulent flows one is interested in determining the average values of the velocity field and of the passive scalar; in the average values of kinematic variables for double, triple, and higher-order moments; and in properties composing the turbulent budget. The Reynolds stresses appearing in the averaged equation of motion is unknown and must be determined by a closure method.

This proposition does not deviate completely from the previous methods. To a certain extent it can be made to reproduce, at least partially, all the aforementioned methods. A progression of approximations to the correlation balances presented in previous section forms its basis.

The constitutive variables in all constitutive propositions will be:

- The average fluid velocity relative to the walls, average temperature and concentration,
- the Reynolds stress,
- the turbulent heat and mass fluxes,
- moments of progressive orders for the successive closure levels.

In writing the constitutive equations, and in view of the principle of material frame indifference the fluid velocity is considered relative to the instantaneous linear velocity of the wall about which the flow is taking place. Observance of the symmetry properties of the moments modeled by the constitutive equations is of equivalent importance. It is simple to observe that the moments yielding dependent variables are completely symmetric with respect to all indices.

The first closure level is obtained by considering Eq. 19 for the Reynolds stress, with the specification of constitutive equations for the third-order moment and for the source term

$$R_{ijk} = R_{ijk}(v_a, R_{ab}, q_a, m_a^\gamma), \quad R_{ijk} = R_{jki} = R_{kij}$$

$$S_{ij} = S_{ij}(v_a, R_{ab}, q_a, m_a^\gamma), \quad S_{ij} = S_{ji} \quad (39)$$

At this point equipresence is recalled to ascertain that the unknown terms in the Eqs. 23 and 35 for the double moments for the turbulent heat and mass fluxes are determined by the same set of variables, that is

$$q_{ij} = q_{ij}(v_a, R_{ab}, q_a, m_a^\gamma), \quad q_{ij} = q_{ji}$$

$$s_i = s_i(v_a, R_{ab}, q_a, m_a^\gamma) \quad (40)$$

$$m_{ij}^\alpha = m_{ij}^\alpha(v_a, R_{ab}, q_a, m_a^\gamma), \quad m_{ij}^\alpha = m_{ji}^\alpha$$

$$n_i^\alpha = n_i^\alpha(v_a, R_{ab}, q_a, m_a^\gamma) \quad (41)$$

The knowledge of Eqs. 39 to 41 represent closure of turbulence at the first level of description. Substitution of these expressions into Eqs. 18 and 19, 31, 32, 34, and 35, transforms them into a system of field equations for the average fields of velocity and Reynolds stresses; the average temperature and the turbulent heat flux; the average concentrations, and turbulent mass fluxes. The interdependence is a consequence of the equipresence independently of existence of analogous phenomena at the molecular level.

The second and each consecutive level of closure are obtained by the specification of constitutive equations for the moments of a given order and for the source terms in all the previous equations. All the lower order moments can, in principle, be determined, and in addition the average velocity, temperature, and concentration fields are determined.

Table 1. Moments and Constitutive Variables

Order	Balances For:	Moments	Constitutive Variables
0	v_i, θ, c	R_{ij}, q_i, m_i	v_i, θ, c
1	R_{ij}, q_i, m_i	R_{ijk}, q_{ij}, m_{ij}	v_i, θ, c, R_{ij}, q_i, m_i
2	R_{ijk}, q_{ij}, m_{ij}	R_{ijkp}, q_{ijk}, m_{ijk}	v_i, θ, c, R_{ij}, q_i, m_i, R_{ijk}, q_{ij}, m_{ij}

The second closure level is determined by

$$R_{ijkp} = R_{ijkp}(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma)$$

$$S_{ijk} = S_{ijk}(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma) \tag{42}$$

$$q_{ijk} = q_{ijk}(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma)$$

$$s_{ij} = s_{ij}(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma) \tag{43}$$

$$m_{ijk}^\alpha = m_{ijk}^\alpha(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma)$$

$$n_{ij}^\alpha = n_{ij}^\alpha(v_a, R_{ab}, q_a, m_a^\gamma, R_{abc}, q_{ab}, m_{ab}^\gamma) \tag{44}$$

It is clear that additional orders of turbulence description may be added if required by the dictates of the required accuracy. In this exploratory article only the first and second closure levels are considered, employing equations for R_{ijk}, R_{ijkp}, S_{ij}, S_{ijk}, as shown in Table 1.

All the constitutive equations must be made to satisfy the principle of material frame indifference, the complete symmetries of the various moments, and the entropy principle. The Galilean group should be used, and it allows the dependence on the spin $\mathbf{W}^s$, and it must be kept in mind that the fluid velocity appearing in Eq. 18 and 19 is relative to the linear velocity of the wall. If Q_{ai} is a orthogonal transformation defining a change of frame $x_a^* = Q_{ai}x_i + \dot{d}_a t$, then the velocities and moments in the new frame will be

$$v_a^* = Q_{ai}v_i, \quad R_{ab}^* = Q_{ai}Q_{bj}R_{ij}$$

$$R_{a..e}^* = Q_{ai}..Q_{el}R_{i..l}, \quad S_a^* = Q_{ai}S_i$$

$$S_{a..e}^* = Q_{ai}..Q_{el}S_{i..l} \tag{45}$$

Smith[25] has determined general representation theorems for isotropic functions of vectors, symmetric and skew-symmetric second-order tensors. Other representation theorems for higher order tensors are available. The testing of this method will be confined to flows about stationary surfaces, in which cases the state variables reduce to the velocity and Reynolds stress, and heat and mass turbulent fluxes.

Additional simplification is obtained if one assumes the temperature and concentration fields to be passive scalars, that is, the velocity fluctuations are insensitive to the fluctuation of the scalar temperature and concentration fields. Under this supposition the constitutive equations for the triple correlation and respective source term are independent of the turbulent heat and mass fluxes.

Momentum flux

For the momentum flux at the first level of closure one needs equations for the third-order moments, and supply term appearing in the equation for the Reynolds stress. Invariant forms satisfying the symmetries are given by

$$R_{ijp} = a_0^1[\delta_{ij}v_p + \delta_{jp}v_i + \delta_{pi}v_j] + a_1^1[R_{ij}v_p + R_{jp}v_i + R_{pi}v_j] + a_2^1[R_{il}R_{lj}v_p + R_{jl}R_{lp}v_i + R_{pl}R_{li}v_j]$$

$$S_{ij} = b_0^0\delta_{ij} + b_0^2 v_i v_j + b_1^0 R_{ij} + b_2^0 R_{il}R_{lj} + b_1^2[v_i R_{jl} v_l + R_{il} v_l v_j] + b_2^2[v_i R_{jp} R_{pl} v_l + R_{ip} R_{pl} v_l v_j] \tag{46}$$

the coefficients of the above expressions are functions of the combined invariants of R_{ij} and v_i, v_i, ($\|\boldsymbol{v}\|$, $\boldsymbol{v}\cdot\boldsymbol{R}\boldsymbol{v}$, $\boldsymbol{v}\cdot\boldsymbol{R}^2\boldsymbol{v}$).

Notice that for the determination of all moments up to the third-order there are nine constitutive coefficient functions $a_0^1, .. a_2^1, b_0^0, .. b_2^2$. This is to be compared to the four constants in the algebraic full closure expressions posed by Launder, Reece and Rodi[4]; Gibson, Spalding and Zinser[26]; and Speziale et al.[27]. These models employ, in addition, modeled equations for the kinetic energy and dissipation associated with the fluctuating velocities, Eq. 50, which contain additional constants. In some proposals the constants are replaced by functions of various parameters, including the distance from the wall. The linear form of Eqs. 46[1, 2] are

$$R_{ijp} = a_0^1[\delta_{ij}v_p + \delta_{jp}v_i + \delta_{pi}v_j],$$

$$S_{ij} = b_0^0\delta_{ij} + b_1^0 R_{ij}. \tag{47}$$

Introducing the linear forms into the balance equations for the Reynolds stress, Eq. 19, results in

$$\dot{R}_{ij} + R_{jp}\frac{\partial v_i}{\partial x_p} + R_{ip}\frac{\partial v_j}{\partial x_p} - b_1^0 R_{ij} - b_0^0\delta_{ij} = -\left(\frac{\partial a_0^1 v_i}{\partial x_j} + \frac{\partial a_0^1 v_j}{\partial x_i}\right). \tag{48}$$

This result allows the interpretation of correspondence to the full closure method sustained by 6 partial differential equations in **x**, and t. The arguments presented by Pope[3] can be employed to transform this into an algebraic system

$$\left(\frac{\wp - \varepsilon}{\kappa} - b_1^0\right)R_{ij} + R_{ip}\frac{\partial v_j}{\partial x_p} + R_{jp}\frac{\partial v_i}{\partial x_p} = b_0^0\delta_{ij} - \left(\frac{\partial a_0^1 v_i}{\partial x_j} + \frac{\partial a_0^1 v_j}{\partial x_i}\right), \tag{49}$$

where

$$\wp = -R_{ij}\frac{\partial v_i}{\partial x_j}, \quad \varepsilon = 2\nu\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}} \quad \text{and} \quad \kappa = \overline{u_k u_k} \tag{50}$$

are, respectively, the turbulence production, dissipation, and kinetic energy.

This is a linear equation for R_{ij} as a function of D_{ij}, and W_{ij}, whose solution is of the form

$$R_{ij} = \frac{2}{3}\kappa\delta_{ij} + 2l_1^1\left(D_{ij} - \frac{1}{3}D_{kk}\delta_{ij}\right) + l_W^1(D_{ik}W_{kj} - W_{ik}D_{kj}) + l_2^2\left(D_{ik}D_{kj} - \frac{1}{3}D_{lk}D_{kl}\delta_{ij}\right) \quad (51)$$

This is similar to the form employed in all the full closure equations. The inclusion of nonlinear terms into Eq. 49 will allow even closer resemblance. Notice, however, that the procedure based on the arguments of Pope[3], is not necessary. Equation 48 is a differential equation that can be solved in conjunction with the equations of motion, Eq. 18 yielding values for the velocity and Reynolds stress fields. Anticipating the necessity to include nonlinear terms one can first consider the coefficients of Eqs. 47 to be functions of $\|v_i\|$, the module of the velocity, and independent of the remaining invariants. The next step includes the addition of nonlinear terms into Eq. 48.

Heat and mass fluxes

At the first closure level one needs constitutive equations for the two moments appearing in the balance for the Reynolds stress and, in addition, equations for, q_{ij}, s_i, m_{ij}^{α}, n_i^{α}, determined as functions of the complete set of variables (v_a, R_{ab}, q_a, m_a^{γ}).

$$q_{ij} = e_0^0\delta_{ij} + e_1^0R_{ij} + e_2^0R_{il}R_{lj} + \sum_{\substack{\varpi,\omega=\\ v,q,m}} e_0^{\varpi\omega}\varpi_i\omega_j + e_1^{\varpi\omega}[\varpi_iR_{jl}\omega_l + R_{il}\varpi_l\omega_j] + e_2^{\varpi\omega}[\varpi_iR_{jp}R_{pl}\omega_l + R_{ip}R_{pl}\varpi_l\omega_j]$$

$$s_i = \sum_{\varpi=v,q,m} f_0^{\varpi}\varpi_i + f_1^{\varpi}R_{ij}\varpi_j + f_2^{\varpi}R_{ij}R_{jk}\varpi_k \quad (52)$$

$$m_{ij}^{\alpha} = g_0^{\alpha0}\delta_{ij} + g_1^{\alpha0}R_{ij} + g_2^{\alpha0}R_{il}R_{lj} + \sum_{\substack{\varpi,\omega=\\ v,q,m}} g_0^{\alpha\varpi}\varpi_i + g_1^{\alpha\varpi\omega}[\varpi_iR_{jl}\omega_l + R_{il}\varpi_l\omega_j] + g_2^{\alpha\varpi\omega}[\varpi_iR_{jp}R_{pl}\omega_l + R_{ip}R_{pl}\varpi_l\omega_j]$$

$$n_i^{\alpha} = \sum_{\varpi=v,q,m} h_0^{\alpha\varpi}\varpi_i + h_1^{\alpha\varpi}R_{ij}\varpi_j + h_2^{\alpha\varpi}R_{ij}R_{jk}\varpi_k \quad (53)$$

in which the summation is over the set of vector variables in the argument of the constitutive equations. Thus, for pure fluid where the mass fluxes are zero the equation for the source term s_i reduces to

$$s_i = f_0^vv_i + f_0^qq_i + f_1^vR_{ij}v_j + f_1^qR_{ij}q_j + f_2^vR_{ij}R_{jk}v_k + f_2^qR_{ij}R_{jk}q_k \quad (54)$$

It is important to explicit the above equations for the case of a single diffusing component of the fluid, in the presence of heat flux. In this case there are three vector variables v_i, q_i, and m_i, the velocity, and the turbulent heat and mass fluxes. Only the linear case will be considered

$$q_{ij} = e_0^0\delta_{ij} + e_1^0R_{ij},$$

$$s_i = f_0^vv_i + f_0^qq_i + f_0^mm_i, \quad (55)$$

$$m_{ij}^{\alpha} = g_0^{\alpha0}\delta_{ij} + g_1^{\alpha0}R_{ij},$$

$$n_i = h_0^vv_i + h_0^qq_i + h_0^{m\alpha}m_i, \quad (56)$$

$$\dot{q}_i - f_0^qq_i - f_0^mm_i = R_{ip}\frac{\partial\bar{\theta}}{\partial x_p} + (\bar{\theta} + e_1^0)\frac{\partial R_{ip}}{\partial x_p} + f_0^vv_i \quad (57)$$

$$\dot{m}_i - h_0^qq_i - h_0^mm_i = R_{ip}\frac{\partial\bar{c}}{\partial x_p} + (\bar{c} + g_1^m)\frac{\partial R_{ip}}{\partial x_p} + h_0^vv_i. \quad (58)$$

These are a set of linear partial differential equations for the components of the turbulent heat and mass fluxes. The matrix formed with the coefficients of the terms on the left side of the set is assumed to be invertible. Let its inverse be the matrix $\mathbf{\Lambda}$ with components

$$\begin{pmatrix} \mathbb{L}_{q\theta} & \mathbb{L}_{qc} \\ \mathbb{L}_{m\theta} & \mathbb{L}_{mc} \end{pmatrix} = \begin{pmatrix} f_0^q & f_0^m \\ h_0^q & h_0^m \end{pmatrix}^{-1} \quad (59)$$

representing relaxation times, to reach the limiting solution

$$q_i = \mathbb{L}_{q\theta}\left(R_{ip}\frac{\partial\bar{\theta}}{\partial x_p} + (\bar{\theta} + e_1^0)\frac{\partial R_{ip}}{\partial x_p} + f_0^vv_i\right) + \mathbb{L}_{qc}\left(R_{ip}\frac{\partial\bar{c}}{\partial x_p} + (\bar{c} + g_1^m)\frac{\partial R_{ip}}{\partial x_p} + h_0^vv_i\right) \quad (60)$$

$$m_i = \mathbb{L}_{m\theta}\left(R_{ip}\frac{\partial\bar{\theta}}{\partial x_p} + (\bar{\theta} + e_1^0)\frac{\partial R_{ip}}{\partial x_p} + f_0^vv_i\right) + \mathbb{L}_{mc}\left(R_{ip}\frac{\partial\bar{c}}{\partial x_p} + (\bar{c} + g_1^m)\frac{\partial R_{ip}}{\partial x_p} + h_0^vv_i\right) \quad (61)$$

These equations demonstrate the existence of Soret — Dufour effects in turbulent flows. That is, the turbulent heat and mass fluxes are dependent simultaneously on the temperature and concentration gradients. This dependence is nonisotropic following the anisotropy of the Reynolds stress. In each equation there appear a velocity dependent term, which is justifiable for wall turbulence, with velocity relative to that of the wall; otherwise the coefficients f_0^v and h_0^v must be zero. Both fluxes possess terms proportional to the divergence of the Reynolds stress, which presents itself as an additional driving force for the turbulent heat and mass fluxes. Eqs. 60 and 61 show, in addition, the inadequacy of the usual model employed to describe heat or mass diffusion with a coefficient proportional to the eddy viscosity. A more justifiable proposition results from Eqs. 60 and 61 in combination with a closure model for the Reynolds stress. Simplified versions of Eqs. 60 and 61 are

$$q_i = \mathbb{L}_{q\theta}R_{ip}\frac{\partial\bar{\theta}}{\partial x_p} + \mathbb{L}_{qc}R_{ip}\frac{\partial\bar{c}}{\partial x_p} \quad (62)$$

$$m_i = \mathbb{L}_{m\theta}R_{ip}\frac{\partial\bar{\theta}}{\partial x_p} + \mathbb{L}_{mc}R_{ip}\frac{\partial\bar{c}}{\partial x_p} \quad (63)$$

These guard a strong resemblance to the equations of linear theory of thermodynamics of irreversible processes, on an anisotropic medium, where the anisotropy is associated to the Reynolds stress, and not to the material structure.

Simple shearing flows

A simple test of the applicability of the proposed method in simple flow configurations will be confronted to direct numerical simulation (DNS) results. The fully developed flow between parallel plates is considered. All turbulent properties are functions only of the distance from the wall, and a single component of the average velocity differs from zero $v_1 = v_1(x_2)$, $v_2 = v_3 = 0$. All models based on the concept, introduced by Boussinesq, of turbulent viscosity rely on the following expression

$$\mathbf{R} = \tfrac{2}{3}\kappa\mathbf{1} + 2\nu^t\mathbf{D} \tag{64}$$

which for simple flows, independently of the proposed form for the calculation of ν^t, results in a inaccurate equipartition of the normal stresses $R_{11} = R_{22} = R_{33} = \frac{2}{3}\kappa$. All efforts are concentrated on the prediction of the shearing stresses, which for the case under examination reduces to $R_{12} = \nu^t(dv_1/dx_2)$. The algebraic, the one equation, or two equations models, including the κ, ε renormalization group of Yakhot and Orszag[28], they all present this well known imprecision. Inclusion of a Stokesian term

$$\mathbf{R} = \tfrac{2}{3}\kappa\mathbf{1} + 2\nu^t\mathbf{D} + \sigma^t\mathbf{D}^2 \tag{65}$$

improve results, but not sufficiently, because there remains the equality of two normal stresses

$$R_{11} = R_{22} = \tfrac{2}{3}\kappa - 2\sigma^t\left(\frac{dv_1}{dx_2}\right)^2; \quad R_{33} = \tfrac{2}{3}\kappa \tag{66}$$

For the first closure level the linear form of constitutive equations applied to the Reynolds stress balance yield Eq. 48 which for this case reduce to the set

$$(1,1) \quad -b_1^0 R_{11} - b_0^0 = 2R_{12}\frac{dv_1}{dx_2},$$

$$R_{11} = -b_0^0/b_1^0 + 2\nu^t\left(\frac{dv_1}{dx_2}\right)^2$$

$$(2,2) \quad -b_1^0 R_{22} - b_0^0 = 0, \quad \Rightarrow R_{22} = R_{33} = -b_0^0/b_1^0$$

$$(3,3) \quad -b_1^0 R_{33} - b_0^0 = 0$$

$$(1,2) \quad R_{22}\frac{dv_1}{dx_2} - b_1^0 R_{12} = -\frac{da_0^1 v_1}{dx_2} = -\left(\frac{\partial a_0^1 v_1}{\partial v_1}\right)\frac{dv_1}{dx_2} = \varphi\frac{dv_1}{dx_2}$$

$$(1,2) \quad R_{12} = \frac{R_{22} - \varphi}{b_1^0}\frac{dv_1}{dx_2} = \nu^t\frac{dv_1}{dx_2}, \quad \nu^t = \frac{R_{22} - \varphi}{b_1^0}$$

$$(1,3) \quad R_{23}\frac{dv_1}{dx_2} - b_1^0 R_{13} = 0$$

$$(2,3) \quad -b_1^0 R_{23} = 0 \Rightarrow R_{13} = R_{23} = 0 \tag{67}$$

The last two results are of general validity for simple shearing flows.

The coefficients of the constitutive equations must satisfy the following equations, with which they can be determined from experimental or DNS data:

$$\begin{pmatrix} 1 & \frac{1}{2}(R_{22} + R_{33}) & 0 \\ 1 & R_{11} & 0 \\ 0 & R_{12} & \dfrac{dv_1}{dx_2} \end{pmatrix} \begin{pmatrix} b_0^0 \\ b_0^1 \\ \varphi \end{pmatrix} = \begin{pmatrix} 0 \\ 2R_{12}\dfrac{dv_1}{dx_2} \\ R_{22}\dfrac{dv_1}{dx_2} \end{pmatrix}. \tag{68}$$

The determinant of this matrix is $[R_{11} - (1/2)(R_{22} + R_{33})](dv_1/dx_2)$, and differs from zero when there exist a difference in the normal stresses ($R_{11} \neq (1/2)(R_{22} + R_{33})$). Under this circumstance the constitutive coefficients can be exactly calculated from DNS data, and all the six equations (Eq. 67) are satisfied exactly. For every line of DNS results the coefficients can be expressed as functions of $\|\boldsymbol{v}\| = v_1$.

$$b_0^0(v_1) = \frac{2(R_{22} + R_{33})R_{12}}{(R_{22} + R_{33}) - 2R_{11}}\frac{dv_1}{dx_2},$$

$$b_0^1(v_1) = \frac{2R_{12}}{(R_{22} + R_{33}) - 2R_{11}}\frac{dv_1}{dx_2},$$

$$\varphi(v_1) = \frac{4R_{12}^2}{(2R_{11} - R_{22} - R_{33})} + R_{22}. \tag{69}$$

The use of DNS data[29] allows an exact calculation of the three parameters, from which values of R_{12} are reproduced; consequently, the average velocity profile follows.

The turbulent shear stress distribution inside the channel can be determined from the momentum balance, to be compared to the solution set of Eq. 69, written in terms of the wall variables $u^* = \sqrt{\tau_0/\rho}$, $u^+ = v_1/u^*$, $y^+ = x_2 u^*/\nu$, $R_{ij}^+ = R_{ij}/(u^*)^2$.

$$R_{12}^+ = 1 - y^+/y_{\max}^+ - \frac{du^+}{dy^+}, \quad R_{12}^+ = \frac{R_{22}^+ - \varphi}{b_1^0}\frac{du^+}{dy^+} \tag{70}$$

Calculated results are shown in the graph in Figure 1. The original data, the solution of the momentum balance, and the calculated value from Eq. 70_2 yield essentially the same curve.

Notice, however, that predicted identical values for and $R_{22} = R_{33}$ are not correct. In addition the predicted values for the triple moments satisfying Eq. 47 are also incorrect, they are

$$R_{111} = 3a_0^1 v_1, \quad R_{122} = R_{133} = a_0^1 v_1,$$

$$R_{112} = R_{113} = R_{123} = R_{222} = R_{333} = R_{223} = R_{233} = 0 \tag{71}$$

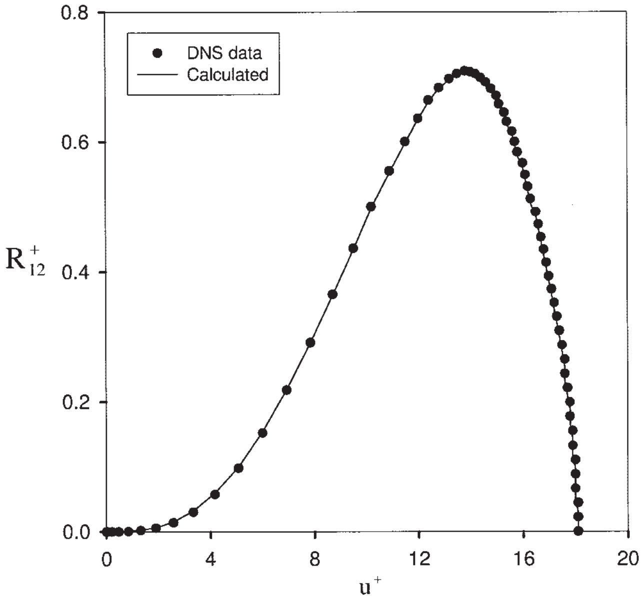

Figure 1. Turbulent shear stress distribution inside the channel: comparison with the DNS data.

The test of Eq. 47, against DNS data demonstrates the insufficiency of the first closure level. Results, except for the shear stress, do not conform to the data, indicating the need to employ higher closure levels. This is a special feature of the method that indicates how to improve its results.

The linear form of representation of the second level of closure equations is:

$$R_{ijkp} = R_{ijkl}(v_a, R_{ab}, R_{abc}) = d_0^0\delta_{ij}\delta_{kp} + d_1^0(\delta_{ij}R_{kp} + \delta_{jk}R_{pi} + \delta_{kp}R_{ij} + \delta_{pi}R_{jk}),$$

$$S_{ijk} = c_0^1[\delta_{ij}v_k + \delta_{jk}v_i + \delta_{ki}v_j] + eR_{ijk},$$

$$S_{ij} = b_0^0\delta_{ij} + b_1^0R_{ij}. \tag{72}$$

Inserting these into Eq. 19 and 20 yield the following set of balance equations for the triple moments

$$(1,1,1)\quad \frac{d}{dx_2}[3R_{112}v_1 - 3R_{11}R_{12} + 2d_1^0R_{12}] = 3c_0^1v_1 + eR_{111},$$

$$(1,1,2)\quad \frac{d}{dx_2}[2R_{122}v_1 - (R_{11}R_{22} + 2R_{12}^2) + d_0^0 + d_1^0(R_{11} + R_{22})] = eR_{112},$$

$$(1,1,3)\quad \frac{d}{dx_2}[2R_{123}v_1 - R_{11}R_{23} - 2R_{12}R_{13} + d_1^0R_{23}] = eR_{113},$$

$$(1,2,2)\quad \frac{d}{dx_2}[R_{222}v_1 - 3R_{12}R_{22} + 2d_1^0R_{12}] = c_0^1v_1 + eR_{122},$$

$$(1,2,3)\quad \frac{d}{dx_2}[R_{223}v_1 - 2R_{12}R_{23} - R_{13}R_{22}] = eR_{123},$$

$$(1,3,3)\quad \frac{d}{dx_2}[R_{233}v_1 - (2R_{13}R_{23} + R_{12}R_{33}) + d_1^0R_{12}] = c_0^1v_1 + eR_{133},$$

$$(2,2,2)\quad \frac{d}{dx_2}[-3R_{22}^2 + (d_0^0 + 4d_1^0R_{22})] = eR_{222},$$

$$(2,2,3)\quad \frac{d}{dx_2}[-3R_{22}R_{23} + 2d_1^0R_{23}] = eR_{223},$$

$$(2,3,3)\quad \frac{d}{dx_2}[-2R_{23}^2 - R_{22}R_{33} + d_1^0(R_{22} + R_{33})] = eR_{233},$$

$$(3,3,3)\quad \frac{d}{dx_2}[-3R_{23}R_{33} + 2d_1^0R_{23}] = eR_{333}. \tag{73}$$

A new set of equations for Reynolds stresses substitute Eqs. 67

$$(1,1)\quad b_0^0 + b_1^0R_{11} = \frac{d}{dx_2}[2R_{12}v_1 + R_{112}],$$

$$(2,2)\quad b_0^0 + b_1^0R_{22} = \frac{dR_{222}}{dx_2},$$

$$(3,3)\quad b_0^0 + b_1^0R_{33} = \frac{dR_{233}}{dx_2},$$

$$(1,2)\quad b_1^0R_{12} = \frac{d}{dx_2}[R_{22}v_1 + R_{122}],$$

$$(1,3)\quad \frac{d}{dx_2}[R_{23}v_1 + R_{123}] = b_1^0R_{13} = 0,$$

$$(2,3)\quad \frac{dR_{223}}{dx_2} = b_1^0R_{23} = 0. \tag{74}$$

The erroneous prediction of equality of the normal Reynolds stresses R_{22}, and R_{33} is properly corrected; the difference is given in the first three equations of the set (Eq. 74). The correction rests on the derivatives of triple moments, which are made to satisfy less trivial equations than Eq. 47. In fact, all the erroneous results for the triple moments listed with Eq. 71 seem to have been surpassed. Notice that the first four equations contain the derivatives of the four more important triple correlations, exactly those whose values are listed in the U. of Tokyo DNS data bank.

Least square solution of the 16 Eqs. 73 and 74 for the six constitutive coefficients b_0^0, b_0^1, c_0^1, d_0^0, d_0^1, e can be numerically obtained for every line of DNS data, and correlated to v_1. These will be discussed, elsewhere, in a future article, in which the complete system of DNS data for the Reynolds stresses, and for the triple moments R_{ijk} are compared to the predictions of the second level system of equations. For this problem, however, only four of the Reynolds stresses differ from zero, and in the four equations (Eq. 74) only four triple correlations are present R_{121}, R_{122}, R_{222}, and R_{233}.

An approximate solution is attempted setting to zero the coefficients in the righthand side of Eq. 73, and solving for the derivatives of the triple correlations present in the first four equations of Eq. 74. Only four adjustable functions remain, that is, the set of equations (Eq. 74) depend only upon adjustable constitutive functions $b_0^0(v_1)$, $b_1^0(v_1)$ and $d_0^0(v_1)$, $d_1^0(v_1)$. The expressions for the derivatives of the triple correlations obtained from the solution of Eqs. 73, can be inserted on Eqs. 74, yielding a set of four linear equations for the unknown constitutive functions. It is convenient to transform the two variables $d_0^0(v_1)$, $d_1^0(v_1)$ into new groupings defined by

$$f = \frac{d}{dx_2}\left[\frac{d_1^0 R_{12}}{v_1}\right], \quad \text{and} \quad g = \frac{d}{dx_2}\left[\frac{d_0^0 + d_1^0(R_{11}+R_{22})}{2v_1}\right]. \tag{75}$$

With these the set (Eq. 74)

$$(1,1) \quad b_0^0 + b_1^0 R_{11} + \frac{2}{3} f = \frac{d}{dx_2}[2R_{12}v_1 + R_{11}R_{12}/v_1],$$

$$(2,2) \quad b_0^0 + b_1^0 R_{22} + \frac{1}{2} f = 3\frac{d}{dx_2}[R_{12}R_{22}/v_1],$$

$$(3,3) \quad b_0^0 + b_1^0 R_{33} + f = 0,$$

$$(1,2) \quad b_1^0 R_{12} + g = \frac{d}{dx_2}[R_{22}v_1 + (R_{11}R_{22} + R_{12}^2)/v_1]. \tag{76}$$

Once again four equations for the unknown constitutive variables allow an exact solution, which should reproduce exactly the four Reynolds stresses. A solution for b_0^0, b_1^0, f, exists if the determinant whose value is $(1/3)R_{11} + (1/6)R_{22} - (1/2)R_{33}$ differs from zero. In that case, as in the first level, the set is exactly satisfied and the values for the normal and shearing stresses are exactly reproduced. This is viewed in Figure 2 where the three-dimensionless normal stresses are plotted and compared with the DNS data. Wall variables are employed.

A problem arises in using the calculated values of the constitutive parameters to determine the Reynolds stresses. For that it is necessary to solve the nonlinear system of four first-order ordinary differential (Eq. 76). A numerical procedure can be used or, more conveniently, a series solution employing the method of Adomian[30] (see also Abbaoui et al.[31]) is particularly suited for the case. With that objective we write Eq. 76 under the form

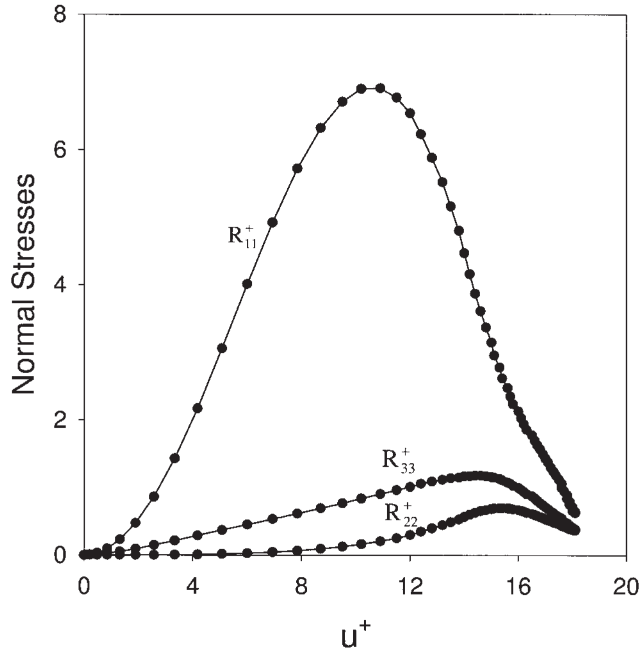

Figure 2. Dimensionless turbulent normal stresses: comparison with the DNS data.

(—) Normal stress and (●) DNS data.

$$R_{11} = -\frac{b_0^0 + 2/3f}{b_1^0} + \frac{1}{b_1^0}\frac{d}{dx_2}[2R_{12}v_1 + R_{11}R_{12}/v_1],$$

$$R_{22} = -\frac{b_0^0 + 1/2f}{b_1^0} + \frac{3}{b_1^0}\frac{d}{dx_2}[R_{12}R_{22}/v_1],$$

$$R_{33} = -\frac{b_0^0 + f}{b_1^0},$$

$$R_{12} = -\frac{g}{b_1^0} + \frac{1}{b_1^0}\frac{d}{dx_2}[R_{22}v_1 + (R_{11}R_{22} + 2R_{12}^2)/v_1]. \tag{77}$$

The first term of the series retain the linear part of Eq. 77, that is

$$R_{ij} = R_{ij}^0 + N_{ij}(R_{11}, R_{22}, R_{33}, R_{12}). \tag{78}$$

where the terms on the right side are

$$R_{11}^0 = -\frac{b_0^0 + 2/3f}{b_1^0} + \frac{2}{b_1^0}\frac{d}{dx_2}[R_{12}^0 v_1],$$

$$R_{22}^0 = -\frac{b_0^0 + 1/2f}{b_1^0},$$

$$R_{33}^0 = -\frac{b_0^0 + f}{b_1^0},$$

$$R_{12}^0 = -\frac{g}{b_1^0} + \frac{1}{b_1^0}\frac{d}{dx_2}[R_{22}^0 v_1]. \tag{79}$$

The method utilizes decomposition in series both for independent variables and the dependent nonlinear terms in Eq. 78 are expanded in the polynomials of Adomian A_{ij}^n

$$R_{ij} = R_{ij}^0 + \sum_{n=1}^{m} R_{ij}^n\Big|_{\varepsilon=1}, \quad N_{ij} = \sum_{n=0}^{m} A_{ij}^n,$$

$$A_{ij}^n = \frac{1}{n!}\frac{d^n}{d\varepsilon^n}\left[N_{ij}\left(\sum_{n=0}^{m}\varepsilon^n R_{ij}^n\Big|\right)\right]_{\varepsilon=0} \tag{80}$$

There follows from Eqs. 80

$$R_{ij}^1 = A_{ij}^0 = N_{ij}(R_{11}^0, R_{22}^0, R_{33}^0, R_{12}^0), \tag{81}$$

$$R_{ij}^2 = A_{ij}^1 = \frac{\partial N_{ij}}{\partial R_{11}}(R_{11}^0, R_{22}^0, R_{33}^0, R_{12}^0)R_{11}^1 + \frac{\partial N_{ij}}{\partial R_{22}}(R_{11}^0, R_{22}^0, R_{33}^0, R_{12}^0)R_{22}^1 + \frac{\partial N_{ij}}{\partial R_{33}}(R_{11}^0, R_{22}^0, R_{33}^0, R_{12}^0)R_{33}^1 + \frac{\partial N_{ij}}{\partial R_{12}}(R_{11}^0, R_{22}^0, R_{33}^0, R_{12}^0)R_{12}^1. \tag{82}$$

Concluding remarks

This report demonstrates the potentiality of the application of the methods of extended thermodynamics to the closure of turbulence properties. A close similarity between the moments of the velocity fluctuations in turbulent flows and the balance equations employed by extended thermodynamics is observed. This similarity is explored to generate field equations for the turbulent moments of increasing orders. The set of moments and the respective independent variables are shown in Table 1.

Only the first and second levels are presently considered. It is shown that these are already capable of predicting the correct distribution of the normal and shearing stresses. The functions present in the proposed constitutive equations need be determined with the use of experimental or obtained from DNS data. The constitutive coefficients are determined as a function of the fluid velocity in terms of the wall variables.

Balance equations for the passive scalars, as temperature and solute concentrations must be added to the set of Eqs. 18 through 20. These will give means of expressing the turbulent heat flux and mass fluxes with equations that are not simply determined by the turbulent Prandtl and Schmidt numbers. The existence of turbulent Soret and Dufour effects appear naturally as consequence of the balances and of expressions for the constitutive equations in terms of the velocity, Reynolds stress, and turbulent heat and diffusion fluxes. These result in expressions for the fluxes showing an anisotropic dependence on the thermodynamic forces, that is, on the temperature and concentration gradients. The anisotropy is determined by the Reynolds stress.

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Notation

a_i^j = constitutive coefficient in Eq. 46
$A_{n,ij}$ = Rivlin-Ericksen tensors of the n^th grade
b_i^j = constitutive coefficients in Eq. 46
c^α = solute concentration of component α
d_i = point in Euclidean space
$D_{\alpha\beta}$ = diffusion coefficients
$D_{\alpha\beta}^t$ = turbulent diffusion coefficients
D_{ij} = symmetric part of the mean velocity gradient
e_i^j = constitutive coefficients in Eq. 52
f_i^j = constitutive coefficients in Eq. 52
$g_i^{\alpha j}$ = constitutive coefficients in Eq. 53
$h_i^{\alpha j}$ = constitutive coefficients in Eq. 53
J_{ip} = flux term in Eq. 13
j_p = flux term in Eq. 26
k = source term in Eq. 24
K_i = source term in Eq. 13
L_{ij} = mean velocity gradient
l_i^j = constitutive coefficients in Eq. 51
m_i^α = turbulent mass flux of component α
n^α = source term in Eq. 25
p = pressure fluctuation
P = mean piezometric pressure
Pr^t = turbulent Prandtl number
Q_{ij} = orthogonal transformation
q_p = turbulent heat flux
R_{ij} = Reynolds stress
s_i = source term in Eq. 32
S_{ij} = source term in Eq. 17
Sc^t = turbulent Schmidt number
t = time
u_i = velocity fluctuation
v_i = mean velocity
W_{ij} = antisymmetric part of the mean velocity gradient
W_{ij}^s = surface spin
x_i = spatial coordinate

Greek letters

α, (α^t) = thermal diffusivity, (turbulent)
χ = source term in Eq. 22
δ_{ij} = Kronecker delta
ε = turbulent dissipation
η^t = turbulent viscosity
κ = average value of the kinetic energy of turbulent fluctuations
$\lambda_{q\beta}$ = material coefficients responsible for the Dufour effects
$\lambda_{\alpha\theta}$ = thermal diffusion coefficients responsible for the Soret effects
λ^t = Stokesian parameter in Eq. 2
ν_i = Instantaneous velocity
θ = Temperature
υ, (υ^t) = kinematic viscosity, turbulent
ρ = density
σ_i = function defining the wall surface
ξ_i = space coordinates on the wall surface

Additional symbols

$\wp$ = turbulent production
$\mathbb{R}$ = set of real numbers
$\mathbb{E}$ = Euclidean space
$\mathbb{L}_{\varpi\omega}$ = Phenomenological coefficients

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