FLOW AND TRANSPORT EQUATIONS IN SURFACE WATERS

CI 71Q HIDRODINAMICA AMBIENTAL Profs. Y. Niño & A. Tamburrino
Sem. Otoño 2004

1 Navier-Stokes Equations

The equations governing the motion of an incompressible Newtonian fluid are known as Navier-Stokes equations. For homogeneous fluid, they can be written in vector notation as:

$$\rho \, \frac{D\vec{v}}{Dt} = \rho \, \{ \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} \} = -\nabla \hat{p} + \mu \, \nabla^2 \vec{v} \tag{1}$$

where D/Dt denotes material or total derivative. It is decomposed into a local or temporal derivative, related to local acceleration, and an advective component, related to spatial changes of velocity. In (1), ρ and μ are fluid properties denoting density and dynamic viscosity, respectively, $\vec{v}$ denotes the velocity vector and $\hat{p}$ denotes piezometric pressure, including pressure and gravitational force terms:

$$\hat{p} = p + \rho \, g \, h \tag{2}$$

where p is the thermodynamic pressure, g denotes gravity acceleration and h is a vertical axis defined positive upwards, against the direction of gravity.

All terms in (1) are linear, with the exception of the advective acceleration. The first two terms in the right hand side represent the balance between mass forces and normal surface forces associated with the thermodynamic pressure. The last term of the right hand side represents the effect of viscous forces and, since it is linear, is valid only for Newtonian fluid. This term represents the diffusion of momentum due to the molecular action of viscosity.

The left hand side of (1), and the advective acceleration in particular, gives the equation a hyperbolic character, while the viscous term corresponds to a parabolic character. The definite character of the equation depends on which term is more relevant in a particular situation. Generally, in laminar flows the dominant character is parabolic (or even elliptic, if the flow is steady), because viscous diffusion dominates over the non-linear term associated to the advective acceleration. On the contrary, in turbulent flows the advective term becomes dominant as it is able to generate a generalized flow instability against the stabilizing effect of viscosity.

Equation (1) contains four unknowns, one for each velocity component of $\vec{v}$ and an additional one corresponding to the thermodynamic pressure p. To close the number of equations required to solve a given flow problem, the continuity equation derived from the mass conservation principle needs also to be considered. For an incompressible fluid, the continuity equation reduces to a condition expressing that $\vec{v}$ is solenoidal:

$$\nabla \cdot \vec{v} = 0 \tag{3}$$

This is a linear equation.

Tensor notation is conveniently used to better visualize the different terms composing the governing equations. Three coordinates are considered: (x_1, x_2, x_3), such that the velocity vector has three components: (u_1, u_2, u_3). The component of equation (1) in direction x_i, for homogeneous fluid, can be written as:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \hat{p}}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{4}$$

where $\nu = \mu/\rho$ denotes kinematic viscosity.

In tensor notation, the continuity equation reduces to:

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{5}$$

In (4) and (5) the repeated subindex j implies summation over $j = 1, 2, 3$.

2 Reynolds averaged equations

Navier-Stokes equations, including the continuity equation, are valid in both laminar and turbulent flows. It is known, however, that in the case of turbulent flow the velocity becomes unstable, presenting quasi-random characteristics, with significant variations of flow properties in time, even in the case of a steady flow, that is, one with constant discharge. The unsteady fluctuations of flow velocity are driven mainly by the non-linear terms of the equations of motion, that is, those associated to the advective acceleration. It is known that the flow velocity fluctuations arise due to the presence of eddies or vortices in the flow, which have a variety of sizes. In general, the largest eddies have a size that scales with the dimensions of the conduit that contains the flow. In the case of river flow, for instance, the largest eddies have a size that is commensurate with the flow depth. Due to the action of the non-linear terms, these large eddies transfer their energy to smaller eddies, and these, in turn, transfer their energy to even smaller eddies. This energy transfer mechanism occurs effectively, on average, from the large to the small scales, and is very efficient, in the sense that very little energy is lost or dissipated in the process. This energy transfer from the large to the small eddies is called *turbulent energy cascade*.

The energy dissipation is negligible at the largest scales, nonetheless, at sufficiently small ones the fluid viscosity dominates the energy dissipation process, transforming the turbulent kinetic energy of the flow into heat. This energy dissipation occurs at the *Kolmogorov's scale*, which represents the smallest eddy size in a turbulent flow. Kolmogorov's scale decreases as the Reynolds number of the flow increases and can be easily smaller than 1 mm in environmental surface water flows.

There exists a theorem, called *Nyquist criterion*, stating that to unequivocally resolve a wave of length L, it is necessary to know at least three points of it. This implies that to adequately resolve a wavelength L with a discretization grid of size Δx, then it is required that $\Delta x < L/2$. This requirement, in terms of the numerical modeling of a turbulent flow using Navier-Stokes equations, imposes a very strong restriction on the discretization grid to be used in the numerical simulation:

the grid size must be smaller than half of Kolmogorov's scale, which, as discussed, is already very small, much smaller than the dimensions of the conduit that contains the flow. In practice, this restriction makes it impossible to numerically solve the complete Navier-Stokes equations for turbulent flow modeling, a method known as *Direct Numerical Simulation* (DNS), given the present computing power, except in cases of flows of rather small dimensions. This, because of two reasons. Firstly, because in order to simulate turbulent flows, an unsteady problem in three dimensions must be solved; secondly because the dimensions of the flow system relevant to any engineering problem are much larger than Kolmogorov's scale, and therefore the three dimensional discretization grid of the spatial domain required to adequately solve the problem implies computer memory requirements that easily exceeds those of today's more advanced computers. Presently, DNS is successfully used to study turbulent flows, however the possible solutions are limited to rather low Reynolds number flows in small spatial domains, comparable, at most, with certain laboratory situations.

Because of the above reasons, many other simulation models for turbulent flows have been developed. A method less restrictive than DNS, in terms of computer memory requirements, is that known as *Large Eddy Simulation* (LES). This method is based in the following idea. Since the largest flow scales have dimensions comparable to those of the spatial domain in which the flow occurs, they are modulated by the boundary conditions specific to such spatial domain. They are not universal. On the contrary, the smallest flow scales, eddies with sizes close to or even larger than the Kolmogorov scale, because of their size, tend to be independent of the boundary conditions of the flow. Their behavior is, or at least tends to be, universal. In fact, it has been shown empirically that the smallest scales of any turbulent flow have an universal behavior that is independent of the particular flow situation analyzed. From this point of view, it seems appropriate to try to model the small scales based on empirical information, since they behave similarly in any flow. On the other hand, it does not seem to be a good idea to model the large scales based on empirical information, as those models would be valid only for the particular conditions for which they were derived. Taking into account these arguments, the LES method was developed to numerically resolve the behavior of the large scales of the flow (the large eddies), using empirical models of universal validity to simulate the behavior of the unresolved scales (the small eddies). Since the spatial scales that must be resolved in this case are larger than Kolmogorov's, the discretization grid of the spatial domain does not result to be as expensive, in terms of memory requirements, as in the case of DNS. In spite of this, the computational requirements are still large, as the problem to be solved is still three dimensional and unsteady. The LES method is currently being applied to the analysis of several different engineering problems, however its use is not yet generalized.

An alternative method to DNS and LES is that called RANS or *Reynolds averaged Navier-Stokes equations*. This method is based on the idea that a turbulent flow undergoes quasi- or pseudo-random fluctuations that can be analyzed statistically. In fact, it is always possible to distinguish between the behavior of the mean flow and that of the velocity fluctuations about the mean flow. Since, in general, the fluctuations are a minor fraction of the mean flow velocity (for instance, the standard deviation of velocity fluctuations of a turbulent open channel flow is about 15 % of the mean flow velocity), then it can be argued that it is more interesting to know the behavior of the mean flow rather than that of the fluctuations. This leads to the need for a method to average the Navier-Stokes equations over the turbulence, in order to extract the behavior of the mean flow velocities, eliminating the turbulent fluctuations from the computation. To perform this average, a statistical procedure known as *ensemble averaging* is followed. The repetition of a large number of realizations of a given turbulent flow, subject to the same initial and boundary conditions is considered, in order to average flow properties over all realizations, for every time instant considered.

Taking into account the ensemble averaging procedure, the instantaneous flow velocity in the x_i direction can be decomposed into a mean value, $\bar{u}_i$, where the overbar denotes ensemble average, plus a fluctuation, u'_i:

$$u_i = \bar{u}_i + u'_i \tag{6}$$

Similarly, for the pressure:

$$\hat{p} = \bar{\hat{p}} + \hat{p}' \tag{7}$$

The idea is to introduce this decomposition into the Navier-Stokes equations and then to ensemble average them over the turbulence. For that, it is convenient to modify (4), multiplying (5) by u_i and adding the resulting equation to (4). This results in:

$$\frac{\partial(\bar{u}_i + u'_i)}{\partial t} + \frac{\partial((\bar{u}_j + u'_j)\ (\bar{u}_i + u'_i))}{\partial x_j} = -\frac{1}{\rho}\ \frac{\partial(\bar{\hat{p}} + \hat{p}')}{\partial x_i} + \nu\ \frac{\partial^2(\bar{u}_i + u'_i)}{\partial x_j \partial x_j} \tag{8}$$

Then, taking the ensemble average of this equation, considering that: $\bar{\bar{a}} = \bar{a}$ and $\bar{a'} = 0$, for any variable a, yields:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial(\bar{u}_j \bar{u}_i + \overline{u'_j u'_i})}{\partial x_j} = -\frac{1}{\rho}\ \frac{\partial \bar{\hat{p}}}{\partial x_i} + \nu\ \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} \tag{9}$$

On the other hand, the ensemble averaged continuity equation results to be:

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \tag{10}$$

such that multiplying this equation by $\bar{u}_i$ and adding the result to (9) it finally yields:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j\ \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho}\ \frac{\partial \bar{\hat{p}}}{\partial x_i} + \nu\ \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \overline{u'_i u'_j}}{\partial x_j} \tag{11}$$

Note that the term $\overline{u'_i u'_j}$ is not zero, since, in general, the velocity fluctuations are correlated. In particular, the fact that the cross-correlations, $\overline{u'_i u'_j}$, with $i \neq j$, are different from zero implies that turbulence is not totally random, but it has structure. These correlations represent turbulent fluxes of momentum, hence they are associated to effective flow stresses. They are known as *turbulent or Reynolds stresses*:

$$\tau_{tij} = -\rho\ \overline{u'_i u'_j} \tag{12}$$

Since the viscous stresses of the mean flow, according to Stokes law for Newtonian fluid, are given by:

$$\tau_{vij} = 2\mu\ \epsilon_{ij} = \mu\ (\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}) \tag{13}$$

where ϵ_{ij} represents the deformation tensor, then it is possible to express the total stress in a turbulent flow as:

$$\tau_{ij} = \tau_{vij} + \tau_{tij} = \mu \, (\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}) - \rho \, \overline{u'_i u'_j} \tag{14}$$

Thus, (11) can also be written as:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \, \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \, \frac{\partial \bar{\bar{p}}}{\partial x_i} + \frac{1}{\rho} \, \frac{\partial \tau_{ij}}{\partial x_j} \tag{15}$$

It can be concluded, from this result, that averaging Navier-Stokes equations over the turbulence does not really solve the problem of the fluctuations, as they continue to appear in the resulting RANS equations in the form of Reynolds stresses. The attempt to obtain one set of equations describing the behavior only of the mean flow fails, as unknowns other than mean flow properties appear in the RANS equations, exceeding the number of available equations. This is the well known *turbulence closure problem.* It is relatively easy to show that further averaging the Navier-Stokes equations in order to obtain equations governing higher order moments of flow properties, always yields new unknowns in the form of even higher order moments, and the problem never closes.

The RANS method thus requires introducing additional (external) equations to close the problem. This closure consists of models for the Reynolds stresses. One of the most used hypothesis is to assume that they follow a behavior similar to that of the viscous stresses. That is, it is assumed that the turbulent fluxes of momentum (i.e., the Reynolds stresses) are proportional to the rate of deformation of the mean flow, just as the molecular flux of momentum is proportional to such rate. The proportionality factor, in analogy to viscous stresses, is called *eddy viscosity.* This is known as *Boussinesq hypothesis* and can be expressed as:

$$\tau_{tij} = 2\mu_t \, \epsilon_{ij} = \mu_t \, (\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}) \tag{16}$$

where μ_t denotes eddy viscosity.

It is important to note that μ_t, is not a fluid property, such as the dynamic viscosity μ, but a property of the flow, and therefore it is a variable that depends on the flow velocity. Defining $\nu_t = \mu_t/\rho$ as the kinematic eddy viscosity, it is possible to rewrite RANS equations as:

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \, \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \, \frac{\partial \bar{\bar{p}}}{\partial x_i} + \frac{\partial}{\partial x_j}\{(\nu + \nu_t) \, (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})\} \tag{17}$$

This result does not really contribute to solve the turbulence closure problem, since it is necessary to specify how the eddy viscosity ν_t is estimated. Nonetheless, the Boussinesq hypothesis has proved adequate to solve a large number of practical problems, despite the fact that there exist many cases for which the gradient hypothesis is simply not valid.

There exist several different methods to model ν_t. They are termed zero-, one- and two-equation models, depending on the number of differential equations used to estimate the eddy viscosity. All of them consider that this variable can be expressed as the product of a velocity scale, v, and a length scale, l, both representing turbulence:

$$\nu_t = v \, l \tag{18}$$

Different models determine v and l in different ways. For instance, the most basic model considers v and l as constants, which yields a constant value of ν_t. A less basic model is that known as *mixing length model*, which assumes that the length scale l corresponds to a mixing length that determines the amplitude of the displacements of fluid parcels driven by turbulent velocity fluctuations. For example, for a one-dimensional flow in the x_1 direction, with mean velocity $\bar{u_1}(x_2)$, the mixing length hypothesis gives:

$$v = |\frac{\partial \bar{u_1}}{\partial x_2}|\; l \tag{19}$$

and therefore:

$$\nu_t = |\frac{\partial \bar{u_1}}{\partial x_2}|\; l^2 \tag{20}$$

In wall bounded flows, it is generally assumed that the mixing length increases linearly with the distance from the wall, such that:

$$l = \kappa\; x_2 \tag{21}$$

where x_2 represents a normal coordinate with origin on the wall. In this equation, κ is a coefficient called *von Karman's constant*. Generally, it is considered that l reaches a maximum value at a certain distance from the wall and remains constant in the outer region of the flow.

The mixing length model is also termed *zero-equation model*, because the eddy viscosity is estimated from an algebraic equation, and no differential equation is invoked with this aim. More sophisticated models are one- and two-equation models, which make use of one or two differential equations, respectively, on top of the RANS equations, to determine the eddy viscosity.

In one-equation models, the length scale, l, is estimated from an algebraic equation, for instance, using a model such as that given by (21). However, the turbulence velocity scale, v, is determined from the turbulent kinetic energy of the flow, K, defined as:

$$K = \frac{1}{2}\; \overline{u_i' u_i'} \tag{22}$$

such that:

$$v \approx \sqrt{K} \tag{23}$$

and with this assumption:

$$\nu_t = \alpha\; \sqrt{K}\; l \tag{24}$$

where α is a coefficient.

To determine the eddy viscosity, a differential equation for K must be solved. This equation is obtained from the Navier-Stokes equations. For that, consider the equation for the velocity fluctuations, which results from the difference between the instantaneous equations (8) and the RANS equations (9):

$$\frac{\partial u_i'}{\partial t} + \frac{\partial}{\partial x_j}(u_i' u_j' + u_i' \bar{u}_j + \bar{u}_i u_j' - \overline{u_i' u_j'}) = -\frac{1}{\rho}\, \frac{\partial \hat{p}'}{\partial x_i} + \nu\, \frac{\partial^2 u_i'}{\partial x_j \partial x_j} \tag{25}$$

Multiplying the equation by u_i' and ensemble averaging over the turbulence, a transport equation for K is obtained, which is given by:

$$\frac{\partial K}{\partial t} + \bar{u_j}\ \frac{\partial K}{\partial x_j} = -\frac{\partial}{\partial x_j}\{\frac{1}{\rho}\ \overline{u'_j \hat{p}'} + \frac{1}{2}\ \overline{u'_i u'_i u'_j} - 2\nu\ \overline{u'_i \epsilon'_{ij}}\} - \overline{u'_i u'_j}\ \epsilon_{ij} - 2\nu\ \overline{\epsilon'_{ij}\epsilon'_{ij}} \tag{26}$$

where:

$$\epsilon'_{ij} = \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \tag{27}$$

denotes the deformation tensor associated to the velocity fluctuations.

The last term in the right hand side of equation (26), represents the rate of dissipation of turbulent kinetic energy, ϵ:

$$\epsilon = 2\nu\ \overline{\epsilon'_{ij}\epsilon'_{ij}} \tag{28}$$

The previous to last term in the right hand side of equation (26), represents the rate of production of turbulent kinetic energy from the mean flow due to its interaction with the Reynolds stresses, P:

$$P = -\overline{u'_i u'_j}\ \epsilon_{ij} \tag{29}$$

Introducing the eddy viscosity concept, and considering equations (12) and (16), the production term can be rewritten as:

$$P = 2\ \nu_t\ (\epsilon_{ij})^2 = \nu_t\ (\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i})^2 \tag{30}$$

The three first terms in the right hand side of equation (26) are related to molecular and turbulent diffusion of turbulent kinetic energy and with the contribution of the pressure fluctuations to the transfer of such energy. The following, simplified, transport equation for K is usually used:

$$\frac{\partial K}{\partial t} + \bar{u_j}\ \frac{\partial K}{\partial x_j} = \frac{\partial}{\partial x_j}\{\frac{\nu_t}{\sigma_K}\ \frac{\partial K}{\partial x_j}\} + P - \epsilon \tag{31}$$

where σ_K is the *Schmidt coefficient*, relating the turbulent diffusivity of K with the eddy viscosity ν_t. In this equation, molecular diffusion has been neglected, and the pressure term has been somehow included in the turbulent diffusion term.

In one-equation models, the dissipation rate of turbulent kinetic energy is modeled as:

$$\epsilon = C_D\ \frac{K^{3/2}}{l} \tag{32}$$

where C_D represents an empirical constant.

In two-equation models, v is determined from K just as in (23), and l is related to ϵ. It can be shown that the latter is determined by v and l, such that:

$$\epsilon \propto \frac{v^3}{l} \tag{33}$$

which yields:

$$l \propto \frac{(\sqrt{K})^3}{\epsilon} \tag{34}$$

and then:

$$\nu_t = \alpha \, \frac{K^2}{\epsilon} \tag{35}$$

where α is a coefficient. Just as in the case of the one-equation model, K is determined from equation (26), however in the case of two-equation models an extra equation for ϵ is needed. It is not possible to formally obtain such equation from Navier-Stokes equations, as it was done for K. However, it is accepted that the following model transport equation for ϵ is valid:

$$\frac{\partial \epsilon}{\partial t} + \bar{u_j} \, \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\{\frac{\nu_t}{\sigma_\epsilon} \, \frac{\partial \epsilon}{\partial x_j}\} + c_{1\epsilon} \, \frac{\epsilon}{K} \, P - c_{2\epsilon} \, \frac{\epsilon^2}{K} \tag{36}$$

where $c_{1\epsilon}$ and $c_{2\epsilon}$ are empirical constants.

The two-equation model resulting from (31), (35) and (36) is called $K-\epsilon$ *model.* The coefficients in the model have been calibrated using empirical data and are assumed to be rather universal. This is not the only two-equation model that exists, but it is one of the best known and, despite its limitations, it has produced good results when compared with experimental observations in several engineering applications.

The problems to be solved using the $K - \epsilon$ model can be steady or unsteady in one, two or three dimensions. Due to the complexity of the resulting equations, it is common, in the majority of the engineering applications, to introduce a number of approximations in order to simplify the system of equations to solve. Among them, the boundary layer approximation is usually invoked in the case of environmental flows, in which vertical gradients of the flow properties are much larger than the corresponding longitudinal gradients. This means that longitudinal diffusion terms can be neglected in comparison to vertical diffusion terms and, at the same time, vertical advection terms can be neglected in comparison to longitudinal advection terms.

In the case of flows in water bodies of large dimensions, usually denoted as geophysical flows, it is necessary to include the effect of Coriolis force, associated with the rotation of the earth, into the mass force terms of Navier-Stokes equations.

3 Transport equations

These equations govern the transport of dissolved or suspended species in water flows and are based on the principle of mass conservation. One of the basic transport processes of dissolved mass in fluids corresponds to molecular diffusion, which can be modeled by means of *Fick's law.* This law states that the diffusive mass flux in a fluid is proportional to the mass concentration gradient.

Calling C the concentration, expressed as the ratio between the solute mass and the total mass, then Fick's law can be written as:

$$\vec{f_m} = -\rho \, D \, \nabla C \tag{37}$$

where $\vec{f_m}$ denotes the diffusive mass flux vector, expressed as mass per unit area per unit time, ρ denotes fluid density, D denotes the coefficient of molecular diffusion of mass in the fluid (with dimensions of length squared over time) and the negative sign indicates that the flow of mass is from zones of large mass concentration towards zones of lower mass concentration.

The solute mass conservation equation applied onto a control volume of a constant density fluid, considering both advective fluxes due to the instantaneous velocity field and diffusive fluxes due to molecular action, can be written in vector form as:

$$\rho\,(\frac{\partial C}{\partial t} + (\vec{v}\cdot\nabla)C) = -\nabla\cdot\vec{f}_m \tag{38}$$

or, invoking Fick's law:

$$\frac{\partial C}{\partial t} + (\vec{v}\cdot\nabla)C = D\ \nabla^2\ C \tag{39}$$

This equation expressed in tensor notation is:

$$\frac{\partial C}{\partial t} + u_j\ \frac{\partial C}{\partial x_j} = D\ \frac{\partial^2\ C}{\partial x_j \partial x_j} \tag{40}$$

The conservative form of the mass conservation equation is obtained by taking the fluid continuity equation (5) multiplied by C and adding the result to equation (40):

$$\frac{\partial C}{\partial t} + \frac{\partial(u_j\ C)}{\partial x_j} = D\ \frac{\partial^2\ C}{\partial x_j \partial x_j} \tag{41}$$

This equation is valid for instantaneous conditions, in both laminar and turbulent flows. To analyze the turbulent flow case, Reynolds decomposition of flow velocities (6) is introduced. This is also applied to the instantaneous concentration, such that it can also be expressed as the sum of a mean value and a fluctuation:

$$C = \bar{C} + C' \tag{42}$$

Introducing these decompositions in (41) and taking the ensemble average over the turbulence yields:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial(\bar{u}_j\ \bar{C})}{\partial x_j} = D\ \frac{\partial^2\ \bar{C}}{\partial x_j \partial x_j} - \frac{\partial(\overline{u'_j\ C'})}{\partial x_j} \tag{43}$$

The last term of the right hand side represents turbulent mass fluxes, associated to the so called *turbulent diffusion* process. This process is analogous to molecular diffusion, but much more effective in terms of mass transport, since length scales of turbulent motion are much larger than those associated to molecular motion.

As with the Navier-Stokes equations, the ensemble averaging process to eliminate fluctuating terms from the analysis leads to a closure problem, this time for the turbulent mass fluxes. Just as in the case of the Reynolds stresses, an external model is required to close the turbulent fluxes. By analogy with Fick's law, a gradient model can be used, based on coefficients for turbulent diffusion, D_{tj}. Such coefficients are analogous to molecular diffusion coefficients, but of larger magnitude, since turbulent diffusion is much more effective than molecular diffusion, as already discussed. The molecular diffusivity D is independent of direction, since molecular activity is isotropic. Turbulent diffusivities, D_{tj}, on the other hand, are direction dependent, as turbulent flows are typically anisotropic. The gradient model for turbulent mass fluxes is:

$$\overline{u_j'\, C'} = -D_{tj}\, \frac{\partial \bar{C}}{\partial x_j} \tag{44}$$

where, in this particular case, the repeated subindex in the right hand side of the equation does not imply summation.

Replacing this model in (43) yields:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial (\bar{u}_j\, \bar{C})}{\partial x_j} = D\, \frac{\partial^2\, \bar{C}}{\partial x_j \partial x_j} + \frac{\partial}{\partial x_j}\{D_{tj}\, \frac{\partial \bar{C}}{\partial x_j}\} \tag{45}$$

or:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial (\bar{u}_j\, \bar{C})}{\partial x_j} = \frac{\partial}{\partial x_j}\{(D + D_{tj})\, \frac{\partial \bar{C}}{\partial x_j}\} \tag{46}$$

where D can be neglected in comparison with D_{tj}.

The so called *Schmidt coefficient*, σ, is defined as the ratio between the kinematic viscosity of the fluid, ν, and the molecular diffusion coefficient, D. Similarly, a turbulent Schmidt number, σ_t can be introduced in (46) to represent the ratio between the kinematic eddy viscosity, ν_t, and the turbulent diffusivity, D_t:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial (\bar{u}_j\, \bar{C})}{\partial x_j} = \frac{\partial}{\partial x_j}\{(\frac{\nu}{\sigma} + \frac{\nu_t}{\sigma_t})\, \frac{\partial \bar{C}}{\partial x_j}\} \tag{47}$$

where ν_t can be estimated using any of the zero-, one-, or two-equation models described in the previous section. It is worth noting that the turbulent diffusivities resulting from this procedure are isotropic. This points out an important feature of the eddy viscosity models discussed so far, they all consider ν_t as an isotropic property. It is left to the reader to investigate about non-isotropic eddy viscosity models.

4 Saint-Venant equations

As already discussed, several approximations to the Navier-Stokes equations are usually introduced to overcome their complexity in typical engineering applications. One of those approximations leads to what is known as *Saint-Venant equations* or *shallow water wave equations*. These equations can be used to analyze one- or two-dimensional flow situations. Open-channel and river flows are typically one-dimensional and in this case the main interest usually is to determine the longitudinal variation of flow properties in the longitudinal direction. The one-dimensional version of Saint-Venant equations is obtained by integrating Navier-Stokes and continuity equations in the flow cross-section, assuming hydrostatic pressure in the direction normal to the bottom wall. The two-dimensional version of these equations is obtained by depth averaging Navier-Stokes and continuity equations, such that the resulting equations describe the fluid motion in a plane parallel to the bottom wall.

Information regarding the vertical structure of the flow is lost when the cross-section averaging or depth averaging procedures are applied. This is not important, in as much as such information is less relevant than longitudinal (1-D case) or transverse variations (2-D case) of flow properties in a given flow situation. Saint-Venant equations are used in many engineering applications, since flow and transport phenomena in rivers, estuaries and shallow water bodies are usually resolved by them with sufficient accuracy.

Consider the two-dimensional case first. Integrating the Reynolds averaged continuity equation in the direction normal to the bottom wall, z, between the bottom ($z = \eta$) and the free surface ($z = \eta + H$), yields:

$$\int_{\eta}^{\eta+H} \{\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z}\}\, dz = 0 \tag{48}$$

where H is the local flow depth.

According to *Leibnitz's integration rule*:

$$\frac{\partial}{\partial r}\{\int_{a}^{b} f\, ds\} = \int_{a}^{b} \frac{\partial f}{\partial r}\, ds + f(b)\, \frac{\partial b}{\partial r} - f(a)\, \frac{\partial a}{\partial r} \tag{49}$$

equation (48) can be rewritten as:

$$\begin{aligned} &\frac{\partial}{\partial x}\{\int_{\eta}^{\eta+H} \bar{u}\, dz\} - \bar{u}(\eta+H)\, \frac{\partial(\eta+H)}{\partial x} + \bar{u}(\eta)\, \frac{\partial \eta}{\partial x} + \\ &\frac{\partial}{\partial y}\{\int_{\eta}^{\eta+H} \bar{v}\, dz\} - \bar{v}(\eta+H)\, \frac{\partial(\eta+H)}{\partial y} + \bar{v}(\eta)\, \frac{\partial \eta}{\partial y} + \\ &\bar{w}(\eta+H) - \bar{w}(\eta) = 0 \end{aligned} \tag{50}$$

The kinematic boundary condition is invoked now, which states that if $F(x, y, z, t)$ is a function that describes the free surface, then:

$$\frac{\partial F}{\partial t} + (\vec{v} \cdot \nabla)F = 0 \tag{51}$$

where $\vec{v}$ represents, in this case, the velocity vector at the free surface.

Describing the free surface with the equation:

$$F(x, y, z, t) = z - (\eta(x, y) + H(x, y, t)) = 0 \tag{52}$$

and using (51) yields:

$$\frac{\partial H}{\partial t} + \bar{u}(\eta+H)\, \frac{\partial(\eta+H)}{\partial x} + \bar{v}(\eta+H)\, \frac{\partial(\eta+H)}{\partial y} - \bar{w}(\eta+H) = 0 \tag{53}$$

The no-slip and no-penetration boundary conditions at the bottom wall are: $\bar{u}(\eta) = \bar{v}(\eta) = \bar{w}(\eta) = 0$. Replacing these conditions and equation (53) in (50), finally yields:

$$\frac{\partial(<\bar{u}>H)}{\partial x} + \frac{\partial(<\bar{v}>H)}{\partial y} + \frac{\partial H}{\partial t} = 0 \tag{54}$$

which represents the depth averaged continuity equation. Here, the following definitions have been introduced:

$$\int_{\eta}^{\eta+H} \bar{u}\, dz = <\bar{u}> H \tag{55}$$

$$\int_{\eta}^{\eta+H} \bar{v} \ dz =< \bar{v} > H \tag{56}$$

where the triangular brackets denote depth-average. In this way, $< \bar{u} >$ and $< \bar{v} >$ denote the depth-averaged velocities, parallel to the bottom wall, in the x and y directions, respectively.

Following similar procedures it is possible to obtain the depth-averaged version of Reynolds equations in the x and y directions, for which the momentum equation in the z direction must be replaced by the hydrostatic law:

$$\bar{\bar{p}} = \bar{p} + \rho \ g \ z = constant \ in \ z \tag{57}$$

Evaluating this equation at the free surface ($z = \eta + H$) where the relative pressure $\bar{p}$ vanishes, yields:

$$\bar{\bar{p}} = \rho \ g \ (\eta + H) \tag{58}$$

With these considerations, it is easy to obtain:

$$\frac{\partial(< \bar{u} > H)}{\partial t} + \frac{\partial(\beta_x \ < \bar{u} >^2 H)}{\partial x} + \frac{\partial(\beta_{xy} \ < \bar{u} >< \bar{v} > H)}{\partial y} =$$

$$-g \ H \ \frac{\partial(\eta + H)}{\partial x} + \frac{1}{\rho} \{ \frac{\partial(< \tau_{xx} > H)}{\partial x} + \frac{\partial(< \tau_{xy} > H)}{\partial y} + \tau_{xz}(\eta + H) - \tau_{xz}(\eta) \} \tag{59}$$

$$\frac{\partial(< \bar{v} > H)}{\partial t} + \frac{\partial(\beta_{xy} \ < \bar{u} >< \bar{v} > H)}{\partial x} + \frac{\partial(\beta_y \ < \bar{v} >^2 H)}{\partial y} =$$

$$-g \ H \ \frac{\partial(\eta + H)}{\partial y} + \frac{1}{\rho} \{ \frac{\partial(< \tau_{xy} > H)}{\partial x} + \frac{\partial(< \tau_{yy} > H)}{\partial y} + \tau_{yz}(\eta + H) - \tau_{yz}(\eta) \} \tag{60}$$

Equations (54), (59) and (60) constitute the Saint-Venant two-dimensional equations. The following definitions have been used in (59) and (60):

$$\int_{\eta}^{\eta+H} (\bar{u})^2 \ dz = \beta_x \ < \bar{u} >^2 H \tag{61}$$

$$\int_{\eta}^{\eta+H} (\bar{v})^2 \ dz = \beta_y \ < \bar{v} >^2 H \tag{62}$$

$$\int_{\eta}^{\eta+H} \bar{u} \ \bar{v} \ dz = \beta_{xy} \ < \bar{u} >< \bar{v} > H \tag{63}$$

where β_x, β_y and β_{xy} are *Boussinesq coefficients*, which have values that depend on the vertical structure of the flow velocities. It is usually assumed that these coefficients can be set to a value of 1.0 without much error, so they disappear from the formulation.

Equations (59) and (60) can take different forms depending on the assumptions and closures used for the terms in their right hand side. For instance, the terms $\tau_{xz}(\eta + H)$ and $\tau_{yz}(\eta + H)$ correspond to surface shear stresses in the x and y directions, respectively, which are determined by the wind velocity blowing over the free surface. On the other hand, the terms $\tau_{xz}(\eta)$ and $\tau_{yz}(\eta)$ correspond to the bed shear stresses in the x and y directions, respectively. To estimate them it is necessary to introduce a closure for resistance, relating shear stress with depth-averaged velocity. Using the friction slopes in the x and y directions, J_x and J_y, respectively, yields:

$$\tau_{xz}(\eta) = \rho\ g\ H\ J_x \tag{64}$$

$$\tau_{yz}(\eta) = \rho\ g\ H\ J_y \tag{65}$$

Manning's equation can be used as resistance closure:

$$J_x = (\frac{< \bar{u} >\ n}{H^{2/3}})^2 \tag{66}$$

$$J_y = (\frac{< \bar{v} >\ n}{H^{2/3}})^2 \tag{67}$$

where n denotes Manning's coefficient, to obtain a simple estimation of the bed shear stresses.

The terms $< \tau_{xx} >$, $< \tau_{xy} >$ and $< \tau_{yy} >$, which represent different components of the total depth-averaged stress (viscous and turbulent), also need closures. They can be obtained by depth-averaging the zero-, one-, or two-equation models discussed previously.

To close this discussion, the one-dimensional version of the Saint-Venant equations are derived next. This is probably the most well known version of these equations, and has been extensively used in flood routing applications, both in open channel and river flows, for which the one-dimensional approximation is appropriate. In this case, the Reynolds equations are averaged over the cross section of the flow.

A more direct way to obtain the one-dimensional Saint-Venant equations is to consider a mass and momentum balance over an infinitesimal control volume of length dx and cross sectional area Ω, which can vary both in time and space. Here x represents a longitudinal coordinate in the direction of the flow discharge, Q.

For an incompressible liquid, mass conservation requires that a net volume inflow must be balanced by a corresponding increase of volume:

$$\frac{\partial \Omega}{\partial t} + \frac{\partial Q}{\partial x} = q \tag{68}$$

where q represents a lateral inflow discharge per unit length in the x direction.

In the case of conservation of longitudinal momentum, the net variation of momentum (considering both the unsteady and spatial variations), must be balanced by the total external force acting on the control volume. The total force is composed of: gravity, hydrostatic pressure forces acting on the upstream and downstream flow cross sections, surface shear stress acting on the surface area (of width B and length dx) and bottom shear stress acting on the wetted perimeter, χ, over the whole length of the control volume. The momentum balance can be written as:

$$\frac{\partial Q}{\partial t} + \frac{\partial(\beta\, Q^2/\Omega)}{\partial x} = -g\ \Omega\ \frac{\partial(\eta + H)}{\partial x} + \frac{1}{\rho}\ \{\tau_{xz}(\eta + H)\ B - \tau_{xz}(\eta)\ \chi\} \tag{69}$$

where β denotes the Boussinesq coefficient, which depends on the velocity structure within the flow cross section (usually taking values close to unity), $\tau_{xz}(\eta + H)$ denotes the wind shear stress acting on the free surface and $\tau_{xz}(\eta)$ denotes the bottom shear stress. Here $z = \eta$ is the local bottom elevation and $z = \eta + H$ is the local elevation of the free surface, where H is the flow depth and z a coordinate normal to the bottom wall.

To estimate $\tau_{xz}(\eta)$ a resistance closure is needed, just as in the two-dimensional case. For that the following equation can be used:

$$\tau_{xz}(\eta) = \rho\ g\ R_h\ J \tag{70}$$

where $R_h = \Omega/\chi$ denotes the hydraulic radius of the flow cross section and J is the friction slope, which can be estimated using Manning's equation:

$$J = (\frac{Q\ n}{\Omega R_h^{2/3}})^2 \tag{71}$$

where n is Manning's coefficient.

The momentum transfer of the lateral inflow, q, has been neglected in equation (69), assuming that this discharge is small enough, or that the inflow is perpendicular to the x direction. It is easy to incorporate an additional term in (69) to take into account the momentum transfer from the lateral flow, in case it becomes important.

5 The case of Heterogeneous fluid

Environmental flows usually exhibit density variations in the water column as well as in the longitudinal direction. Flows in lakes and reservoirs, estuaries and coastal zones are typically stratified due to temperature variations, salinity, or both. In these cases, density differences are typically small, and the *Boussinesq approximation* is usually introduced, which neglects density variations in the inertial terms of the momentum equations, while keeping them in the mass force terms. In these cases, production or reduction of turbulent kinetic energy due to density differences in the flow must be included as extra source terms in the equations for K and ϵ.

A common assumption regarding heterogeneous fluids is that of incompressibility. Considering the complete continuity equation:

$$\frac{D\rho}{Dt} + \rho\ (\nabla \cdot \vec{v}) = 0 \tag{72}$$

and imposing the incompressibility condition: $\nabla \cdot \vec{v} = 0$, an equation governing the density variations is obtained:

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + (\vec{v} \cdot \nabla)\rho = 0 \tag{73}$$

Consider again Navier-Stokes equation (1), but this time with a variable density, ρ:

$$\rho\ \frac{D\vec{v}}{Dt} = -\nabla p + \rho\ \vec{g} + \mu\ \nabla^2 \vec{v} \tag{74}$$

where $\vec{g}$ denotes the gravity acceleration vector. If ρ is expanded about a constant reference value ρ_0, such that:

$$\rho = \rho_0 + \tilde{\rho} \tag{75}$$

where $\tilde{\rho}$ is a small density variation, and it is assumed that this variation is associated with a small deviation of the pressure, $\tilde{p}$, with respect to a reference state of hydrostatic equilibrium represented by a pressure p_0, such that:

$$p = p_0 + \tilde{p} \tag{76}$$

then, for the reference hydrostatic state: $\nabla p_0 = \rho_0 \, \vec{g}$, and equation (74) can be rewritten as:

$$(1 + \frac{\tilde{\rho}}{\rho_0}) \, \frac{D\vec{v}}{Dt} = -\frac{1}{\rho_0} \, \nabla \tilde{p} + \frac{\tilde{\rho}}{\rho_0} \, \vec{g} + \nu \, \nabla^2 \vec{v} \tag{77}$$

where $\nu = \mu/\rho_0$ represents the kinematic viscosity. It is interesting to note that only density differences with respect to a reference value are relevant in determining the effect of gravity in an heterogeneous fluid. The overall effect is that of a reduced gravity: $g' = (\tilde{\rho}/\rho_0) \, g$.

If $\tilde{\rho}$ is indeed small compared to ρ_0, then the term $\tilde{\rho}/\rho_0$ can be neglected in the left hand side of the equation, since it produces only a small correction to the inertia compared to a fluid of density ρ_0. On the contrary, the density variation is of primary importance in the gravity term, also called *buoyancy term* in this context. Boussinesq approximation consists of neglecting variations in density in so far as they affect inertia, but retaining them in the buoyancy terms. Variations in fluid properties due to $\tilde{\rho}$ are also neglected in this approximation. Equation (77) then reduces to:

$$\frac{D\vec{v}}{Dt} = -\frac{1}{\rho_0} \, \nabla \tilde{p} + \frac{\tilde{\rho}}{\rho_0} \, \vec{g} + \nu \, \nabla^2 \vec{v} \tag{78}$$

Consider again Navier-Stokes equation with variable density (74). Taking the curl of this equation leads to an equation for the vorticity, $\vec{\omega} = \nabla \times \vec{v}$:

$$\frac{D\vec{\omega}}{Dt} = \vec{\omega} \cdot \nabla \vec{v} + \nu \, \nabla^2 \vec{\omega} + \nabla p \times \nabla(\frac{1}{\rho}) \tag{79}$$

Again, $\nu = \mu/\rho \approx \mu/\rho_0$ is the kinematic viscosity, which is taken to be a constant, neglecting the effect of $\tilde{\rho}$ on this property. The last term of the right hand side vanishes in the case of a fluid of constant density. In such a case, vorticity is produced by vortex stretching (first term of the right hand side) or by molecular diffusion of vorticity from the boundaries of the flow, where the no-slip boundary condition applies (second term of the right hand side). In a heterogeneous fluid, vorticity will also be produced whenever the fluid is displaced from a state in which ∇p and $\nabla \rho$ are parallel (condition for which the vector product is zero). In the simple case of a stably stratified fluid in hydrostatic equilibrium, vorticity can be produced by displacement of density surfaces away from the horizontal. The vorticity will oscillate in magnitude and direction with the density surfaces, so that internal waves are in fact rotational flow (in the sense that $\vec{\omega} \neq 0$). In the case of unstable stratification, the last term of the right hand side of equation (79) will cause the vorticity to increase monotonically during the development of convection.

The production of vorticity also implies the production of circulation Γ:

$$\Gamma = \int_C \vec{v} \cdot d\vec{l} = \int_S \vec{\omega} \cdot d\vec{S} \tag{80}$$

where $d\vec{l}$ is a line element of a closed curve in fluid space C, and $d\vec{S}$ is a surface element of the corresponding surface S bounded by C. Considering the simple case of an inviscid fluid (so that the second term of the right hand side of (79) vanishes) then :

$$\frac{D\Gamma}{Dt} = -\int_C \frac{1}{\rho} \, \nabla p \cdot d\vec{l} = \int_S (\nabla p \times \nabla(\frac{1}{\rho})) \cdot d\vec{S} \tag{81}$$

In the case of a homogeneous fluid, the right hand side of this equation vanishes and *Kelvin's theorem* is obtained, which states that in an inviscid fluid of constant density the circulation is conserved. When ρ is variable along the path of integration, circulation is generated unless density and pressure iso-surfaces coincide.

When vorticity and circulation are generated due to variable density effects ($\nabla p \times \nabla(1/\rho) \neq 0$) the resulting flow is called *baroclinic*, as opposed to a *barotropic flow*, which is driven by pressure gradients.

6 References

- Chow, Maidment and Mays. Applied Hydrology. McGraw-Hill. 1988.
- Fisher, List, Koh, Imberger and Brooks. Mixing in Inland and Coastal Waters. Academic Press. 1979.
- Martin and McCutcheon. Hydrodynamics and Transport for Water Quality Modeling. Lewis Publishers. 1999.
- Rodi. Turbulence Models and their Application in Hydraulics. IAHR Monograph. 1984.
- Tennekes and Lumley. A First Course in Turbulence. The MIT Press. 1972.
- Turner. Buoyancy effects in Fluids. Cambridge University Press. 1973.