Investigation of Buoyant Parameters of k-ε Turbulence Model in Gravity Stratified Flows

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Abstract—Different variants for buoyancy-affected terms in k-ε turbulence model have been utilized to predict the flow parameters more accurately, and investigate applicability of alternative k-ε turbulence buoyant closures in numerical simulation of a horizontal gravity current. The additional non-isotropic turbulent stress due to buoyancy has been considered in production term, based on Algebraic Stress Model (ASM). In order to account for turbulent scalar fluxes, general gradient diffusion hypothesis has been used along with Boussinesq gradient diffusion hypothesis with a variable turbulent Schmidt number and additional empirical constant $c_{3\varepsilon}$.To simulate buoyant flow domain a 2D vertical numerical model (WISE, Width Integrated Stratified Environments), based on Reynolds-Averaged Navier-Stokes (RANS) equations, has been deployed and the model has been further developed for different k-ε turbulence closures. Results are compared against measured laboratory values of a saline gravity current to explore the efficient turbulence model.

Keywords—Buoyant flows, Buoyant k-ε turbulence model, Saline gravity current.

I. Introduction

GRAVITY stratified and buoyancy-affected flows are very dominant in many flow domains in different fields of engineering in hydraulics and fluid mechanics; transient stratification in estuaries and coastal zones due to salt intrusion, gravity currents in lakes and dam reservoirs as result of heat gradient, pollutant dispersion, and thermal plumes are some cases of non-homogeneous (i.e. variable density) gravity stratified flow fields [1]. Since most flows in nature and industry are almost always turbulent, and buoyancy has an important role in production and dissipation of turbulent kinetic energy, the accuracy of numerical simulation of turbulent buoyant flows is largely dependent on how well the buoyancy effects in turbulence are considered and modeled [2], [3].

Because of complexity of turbulence phenomenon and its modeling, turbulence has been the subject of diverse studies in different fields of engineering and science. Many turbulence models for different purposes and applicability have been proposed ranging from zero and one-equation models, the two-equation k-ε, k-ω and k-kl Mellor and Yamada model [4], Reynolds Stress Model (RSM), algebraic Stress Model (ASM) to more recent ones such as the Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS) models. However, DNS and LES are less practical because of difficulty in numerical simulations, especially in complex flows, and the vast required computer resources [5].

Among the turbulence models, the Boussinesq based two-equation models have been able to satisfy engineering needs proportional to an acceptable accuracy [2], [3], [5]. In particular, the *k-ε* turbulence model is possibly the most extensively used because of its almost simplicity, stability in numerical methods, and less computing capacity, comparing to other complex models such as RSM and ASM or DNS and LES [3], [5]. However, the standard *k-ε* model with buoyancy terms needs especial modification to improve the prediction and consideration of buoyancy effects on production and destruction of turbulence in different turbulent buoyant flows [3], [5]–[7].

ASM and RSM use specific algebraic or partial differential equations to solve each individual Reynolds stress; therefore, ASM and RSM will be able to account for the buoyancy effects automatically and more realistically [5], [8]. However, they demand much more computational time and consequently are more costly. Beside the numerical difficulty, the model might suffer from a higher risk of instability in complex flow conditions [5]. Initial turbulence model developments utilized the Standard Boussinesq Gradient Diffusion Hypothesis (SGDH) to represent buoyancy induced turbulence generation. The mean deficiency of these models, like the *k-ε* model, is the isotropic eddy viscosity assumption, which does not take into account the non-isotropic behavior of turbulence due to buoyancy forces [7], [9], [10]. Moreover, in simulation of each specific turbulent buoyant flow, a suitable level of turbulent mixing with calibrated values for coefficients, as well as appropriate production and destruction terms are required; for example, in thermal simulations, the standard buoyancy modified *k-ε* model tends to under-predict the spreading rate of vertical buoyant plumes, and over-predict the spreading rate of horizontal, stably-stratified flows [5], [11], [12].

As RSM and ASM turbulence models solve transport equations for individual $\overline{u_i'u_j'}$ stress and $\overline{u_i'\phi'}$ flux components, they are able to take direct account of transport and history effects on these components and also of the anisotropy of the turbulent transport in complex flows; moreover, they

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introduce terms accounting for the effect of buoyancy automatically [8]. Therefore, the main attempts of previous researchers, related to buoyancy effects, have been to modify the simple two equation *k-ε* model on the basis of employing some relations from ASM or RSM models to consider direct effect of buoyancy on turbulence components. Thus, the relations for Reynolds stresses and turbulent scalar fluxes have been modified by this consideration. Daly and Harlow [13] proposed general gradient diffusion hypothesis (GGDH) for accounting turbulent scalar fluxes. Yan and Holmstedt [5] and Worthy et al. [6] in their studies on thermal plumes found that generalized diffusion hypothesis gives more realistic results. Davidson [9] combined ASM and *k-ε* formulas for Reynolds stress, and proposed a second closure correction method for accounting Reynolds stress components. Bonnet et al. [10] and Kun et al. [7] used this hybrid model in their studies respectively on coastal circulations modeling and vertical planar buoyant jets and came to more realistic results.

In this study we have implemented different considerations of computing turbulent scalar (e.g. salinity) fluxes and Reynolds stresses (i.e. turbulent stresses or turbulent momentum fluxes) in terms *P* and *G* in the *k-ε* equations on the basis of general gradient diffusion hypothesis of Daly and Harlow [13] for turbulent scalar fluxes and hybrid expression of Davidson [9] for Reynolds stresses. Along with these implementations, Henkes's [14] suggestion for controversial empirical constant, $c_{3\varepsilon}$, in ε equation has been used with a variable turbulent Schmidt number. To investigate the applicability of these solutions for gravity currents the experimental study of Gerber [15] on a horizontal saline gravity current has been simulated numerically and results have been compared to explore the most suitable turbulence model.

II. Buoyant $k-\varepsilon$ Models

A. The Standard k-ε Model with Buoyancy Terms

The standard buoyancy-modified *k-ε* model is based on the eddy- viscosity/diffusivity concept of Boussinesq, which uses an isotropic eddy-viscosity/diffusivity to relate the Reynolds stresses $\overline{u'_i u'_j}$ and turbulent flux $\overline{u'_i \phi'}$ of concentration or heat to the mean fields:

$$-\overline{u'_i u'_j} = \nu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{i,j} \tag{1}$$

$$\overline{u'_i \phi'} = -\Gamma \frac{\partial \phi}{\partial x_i} = -\frac{\nu_t}{\sigma_t} \frac{\partial \phi}{\partial x_i} \tag{2}$$

where U_i and $u_i^{'}$ are respectively the mean and fluctuating velocity components in x_i direction, φ and $\varphi^{'}$ are the mean and fluctuating of either temperature or concentration (e.g., of salinity), ν_t is the turbulent or eddy viscosity, Γ is turbulent diffusivity of heat or concentration, and σ_t is the turbulent Schmidt number which relates eddy viscosity to the eddy diffusivity and its value can be an indication of the level of turbulent mixing. The production and dissipation of turbulent kinetic energy is subject to transport process, thus to describe the evolution of turbulence, two transport equations for *k* and ε are written in tensorial form as follows:

$$\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + P + G - \varepsilon \tag{3}$$

$$\frac{\partial \varepsilon}{\partial t} + U_i \frac{\partial \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\nu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_i} \right) + c_{1\varepsilon} \frac{\varepsilon}{k} (P + G)(1 + c_{3\varepsilon} R_f) - c_{2\varepsilon} \frac{\varepsilon^2}{k} \tag{4}$$

where *P* represents the production of *k* by interaction of Reynolds stresses and mean-velocity gradient, and *G* represents the production/destruction of turbulence by buoyancy [16]:

$$P = -\overline{u'_i u'_j} \left(\frac{\partial U_i}{\partial x_j} \right) = \nu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \tag{5}$$

$$G = -\beta g_i \overline{u'_i \phi'} = \beta g_i \frac{\nu_t}{\sigma_t} \frac{\partial \phi}{\partial x_i} \tag{6}$$

In the *k-ε* model the eddy viscosity ν_t, relates to *k* and ε via (7), which is obtained from a dimensional analysis and eddy viscosity concept [8].

$$\nu_t = c_\mu \frac{k^2}{\varepsilon} \tag{7}$$

In above equations $c_{1\varepsilon}$, $c_{2\varepsilon}$, $c_{3\varepsilon}$, β, and c_μ are empirical constants, g_i acceleration in x_i direction, and R_f is flux Richardson number. The R_f term is the ratio of the buoyancy production or dissipation of *k* to its production by the shear, $R_f = -G/P$ [16]. By this definition of R_f, in accordance with Rodi's argument [16], $c_{3\varepsilon}$ should be close to unity for vertical buoyant shear layers and close to zero for horizontal layers. To simplify this difficulty Rodi suggested an alternative definition of R_f, as $R_f = -G/(G+P)$. By this definition of R_f, miscellaneous value of $c_{3\varepsilon}$ has been proposed as optimized amounts. Another approach for $c_{3\varepsilon}$ is the suggestion of Henkes et al. [14] as follows:

$$c_{3\varepsilon} = \tanh|v / u| \tag{8}$$

Equation (8) expresses that in vertical shear layers and unstable stratifications which lateral component of velocity (v) has much greater value than horizontal component (u), the value of $c_{3\varepsilon}$ is close to unity, and in contrary, in horizontal shear layers it adopts a value almost equal to zero; therefore, the contribution ratio of buoyancy in turbulence is adjusted automatically.

For the other empirical constants the following standard values are specified [16]:

$$c_\mu = 0.09,\ c_{1\varepsilon} = 1.4,\ c_{2\varepsilon} = 1.92,\ \sigma_k = 1.0,\ \sigma_\varepsilon = 1.3 \quad (9)$$

The turbulent transport is inversely proportional to the Schmidt number σ_t; its value, according to Rodi [16], is about 0.90 in near-wall flows, 0.50 in plane jets and mixing layers, and 0.70 in round jets. However, as σ_t can directly affect the level of turbulence, and buoyancy is one of the production/dissipation source terms of turbulence, its value should be modified by the effect of buoyancy force. One relation to account for this is the Munk-Anderson formula [16] as follows:

$$\sigma_t / \sigma_{t_0} = \frac{(1+3.33Ri)^{1.5}}{(1+10Ri)^{0.5}} \quad (10)$$

$$Ri = -\frac{g}{\rho}\frac{\partial\rho/\partial z}{(\partial u/\partial z)^2} \quad (11)$$

ρ is the density and Ri is the gradient Richardson number which is the ratio of gravity to internal forces and characterizes the importance of buoyancy effects. One may be able to fit definite experimental data by simply adjusting the constant σ_t as has been demonstrated by Gerber [15], and Nam and Bill [17], although, this may seems to vanished the generality of turbulence model [5]. In this paper $\sigma_t = 0.90$ has been used and is updated in each time step by (10).

B. The $k-\varepsilon$ Model with General Gradient Diffusion

The term G in k and ε equations represents an exchange between the turbulent kinetic energy and potential energy. In stable stratification it is negative and acts as a sink term which damps turbulence, while it is positive in unstable flows and acts as a source term that amplifies turbulence [16]. Thus, it can be understood that there is a direct relation between intensity of production/dissipation of turbulence by buoyancy and shear layer situation; it means that the greater stable stratification, the less turbulence production. It implies that in accounting for term G the direct effects of Reynolds stresses should be considered on prediction of turbulent scalar fluxes. A particular advantage of ASM is that terms accounting for buoyancy effect are in close correlation with turbulent stresses, so as an alternative to the standard gradient diffusion hypothesis of Boussinesq in accounting term G, the ASM relation of turbulent scalar fluxes (Φ) can be used as follows:

$$\overline{u_i'\Phi'} = \frac{k}{c_1\varepsilon}\left(-\overline{u_i'u_j'}\frac{\partial\Phi}{\partial x_j} - (1-c_2)\overline{u_j'\Phi'}\frac{\partial U_i}{\partial x_j} - (1-c_3)\beta a_{gi}\overline{\Phi'^2}\right) \quad (12)$$

where $\overline{\Phi'^2} = -2R(k/\varepsilon)\overline{u_i'\Phi'}.\partial\Phi/\partial x_i$, and c_1, c_2, c_3, and R are constants [8].

Shabbir and Taulbee [12] in their study on buoyant plumes found that the magnitude of G predicted by (12) agrees well with measured data, while it is likely to be under-estimated, using standard gradient diffusion hypothesis. Yan and Holmestedt [5] tried to implement above expression to compute turbulent scalar (i.e. heat) flux in their study; however, they encountered problem to reach convergence. Daly and Harlow [13] proposed the so-called generalized gradient diffusion hypothesis, which is simpler than above ASM formula but retains its basic features:

$$\overline{u_i'\phi'} = -\tfrac{3}{2}\frac{c_\mu}{\sigma_t}\frac{k}{\varepsilon}.\overline{u_i'u_j'}\frac{\partial\phi}{\partial x_j} \quad (13)$$

using above expression, the term G becomes:

$$G = \beta g_i \tfrac{3}{2}\frac{c_\mu}{\sigma_t}\frac{k}{\varepsilon}.\overline{u_i'u_j'}\frac{\partial\phi}{\partial x_i} \quad (14)$$

Therefore, according to this and recommendations of Gerber [15] in his experimental study of same field of interest, saline gravity current, We used (14) in accounting for term G in the second turbulence closure.

C. The k-ε Model with Davidson's Second-order Correction for Term P.

A particular limitation of turbulence models based on the eddy-viscosity/diffusivity concept, concerning buoyant flows, is that they cannot describe non-isotropic behavior of turbulence. This non-isotropy which is due to Buoyancy force or Earth rotation in geophysical flows is characterized by amplification of the turbulent fluctuations in one direction and damping it in the other one [10]. Second-order closure schemes which employ transport equations for each $\overline{u_i'u_j'}$ and $\overline{u_i'\phi'}$ components have been developed to hinder this deficiency. However, these models like RSM and ASM give complex relations which need large amount of time and cost for practical use. In ASM turbulent stresses are computed through (15) [5], [7], [8]:

$$\overline{u_i'u_j'} = \frac{2}{3}\delta_{ij}k + \frac{k}{\varepsilon}\frac{(1-c_2)(P_{ij} - 2/3\,\delta_{ij}P)}{c_1 + (P+G)/\varepsilon - 1} + \frac{k}{\varepsilon}\frac{(1-c_3)(G_{ij} - 2/3\,\delta_{ij}G)}{c_1 + (P+G)/\varepsilon - 1} \quad (15)$$

where

$$P_{ij} = -\overline{u_i'u_l'}\frac{\partial U_i}{\partial x_l} - \overline{u_j'u_l'}\frac{\partial U_i}{\partial x_l} \quad (16)$$

$$G_{ij} = -\beta\overline{u_i'\phi'}g_j - \beta\overline{u_j'\phi'}g_i \quad (17)$$

Davidson [9] proposed a second closure correction method to simplify above relation while it preserves its advantages. In this method Reynolds stresses consist of two parts: the non-isotropic turbulence stresses due to buoyancy force and isotropic turbulence part due to shear production; the first part will be calculated through ASM model and the second part is as given by standard k-ε model on the basis of Boussinesq assumption, that is:

$$\overline{u_i'u_j'} = (\overline{u_i'u_j'})_{ASM} + (\overline{u_i'u_j'})_{k-\varepsilon} \tag{18}$$

where

$$(\overline{u_i'u_j'})_{ASM} = \frac{k}{\varepsilon}\frac{(1-c_3)(G_{ij} - 2/3\,\delta_{ij}G)}{c_1+(P+G)/\varepsilon - 1} \tag{19}$$

$$(\overline{u_i'u_j'})_{k-\varepsilon} = -\nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{2}{3}k\delta_{i,j} \tag{20}$$

$$G_{ij} = -\beta\overline{u_i'\phi'}g_j - \beta\overline{u_j'\phi'}g_i \tag{21}$$

therefore the total production term, P becomes:

$$P = P_{ASM} + P_{k-\varepsilon} = -\left(\frac{k}{\varepsilon}\frac{(1-c_3)(G_{ij} - 2/3\,\delta_{ij}G)}{c_1+(P+G)/\varepsilon - 1}\right)\frac{\partial U_i}{\partial x_j} + \nu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\frac{\partial U_i}{\partial x_j} \tag{22}$$

Equation (18) can also be used for accounting term G in (14); however, Yan and Holmestedt [5] found that utilizing this equation simultaneously for both G and P can cause numerical difficulty. In the present study this relation has only been used for term P. Regarding local equilibrium assumption according to the Rodi [16], the term "$(P+G)/\varepsilon - 1$" in (22) will be omitted; Rodi demonstrated that equilibrium assumption does not affect the accuracy of the ASM model. We have used this assumption herein.

III. Numerical Modeling

An arbitrary Lagrangian-Eulerian (ALE) 2D vertical hydrodynamic numerical model has been deployed, based on time dependent Reynolds-averaged Navier-Stokes equations to simulate saline gravity currents. The model is further refined and developed for different k-ε turbulence closures. A structured non-orthogonal curvilinear staggered mesh is used for computational domain. To discrete flow and transport equations of velocities and scalar quantities like salinity, concentration, k and ε, finite volume method was utilized, providing flexibility for defining control volumes in a staggered grid system, especially near the bed and water surface, where rapid changes of bathymetry and free surface may have significant effect on the prediction of the flow flied. Moreover, the finite volume method provides the assurance of global conservation.

A. Governing Equations in ALE

In the ALE method the mesh motion can be chosen arbitrarily; the newly updated free surface is determined purely by Lagrangian method, by the velocity of fluid particles at the free surface. Therefore, in horizontal direction the grids are fixed while they move in vertical direction. The grid geometry is computed and redistributed after completion of each time step. With this consideration, an additional grid velocity w_g, appears in the the Navier-Stokes and species concentration equations. The set of equations of continuity, momentum and species concentration (C) in two directions is written as follows:

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0 \tag{23}$$

$$\frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial x} + \frac{\partial uw}{\partial z} - w_g\frac{\partial u}{\partial z} = -\frac{1}{\rho_r}\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left((\nu_t+\nu)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial z}\left((\nu_t+\nu)\frac{\partial u}{\partial z}\right) \tag{24}$$

$$\frac{\partial w}{\partial t} + \frac{\partial wu}{\partial x} + \frac{\partial w^2}{\partial z} - w_g\frac{\partial w}{\partial z} = -\frac{1}{\rho_r}\frac{\partial p}{\partial z} + \frac{\partial}{\partial x}\left((\nu_t+\nu)\frac{\partial w}{\partial x}\right) + \frac{\partial}{\partial z}\left((\nu_t+\nu)\frac{\partial w}{\partial z}\right) - g\frac{\rho-\rho_r}{\rho_r} \tag{25}$$

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial wC}{\partial z} - w_g\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left((\nu_t+\nu)\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}\left((\nu_t+\nu)\frac{\partial C}{\partial z}\right) \tag{26}$$

where u and w are velocity components in x and z directions respectively, ρ is the local density and ρ_r a reference density, ν is kinematic viscosity, and g is the gravitational acceleration.

B. Solution Method

The projection (fractional-step) method, proposed by Chorin [18] and Temam [19], has been adopted. The method generally is accomplished in two steps; the pressure gradient terms are omitted from the momentum equations in the first step. The transport part of Navier-Stokes equations including advection and diffusion are advanced in time to obtain a provisional velocity field U^*. In the second step, the provisional velocity is corrected by accounting for the pressure gradient and continuity equation as follows:

$$\frac{U^{n+1} - U^*}{\Delta t} + \nabla P^{n+1} = 0 \tag{27}$$

Subject to the continuity constraint:

$$divU^{n+1} = 0 \tag{28}$$

by taking the divergence of (27), the continuity equation will be exerted and the Possion equation is obtained:

$$\nabla^2 P^{n+1} = \frac{divU^*}{\Delta t} \tag{29}$$

From the above equations the pressure distribution is obtained and velocity quantities are then updated. Advection