10th International Research/Expert Conference
"Trends in the Development of Machinery and Associated Technology"
TMT 2006, Barcelona-Lloret de Mar, Spain, 11-15 September, 2006

APPLICATION OF *T-RANS* NEW APPROACH TO DOUBLE-DIFFUSIVE PHENOMENA

Rajfa Musemić
Mechanical Engineering Faculty University of Sarajevo
71000 Sarajevo, Vilsonovo šetalište 9, Bosnia and Herzegovina

Goran Krstović
Bosna-S Co.
71000 Sarajevo, Nova 26, Bosnia and Herzegovina

ABSTRACT
Solutions of mass and heat transport within the variety of industrial and environmental flows are usually provided using Computational Fluid Dynamics (CFD). Calculation of transport processes relies on mathematical engineering methods which have been developed by using averaged transport equations closed with models of turbulence. This paper presents the application of mathematical modeling and numerical simulation of unsteady turbulence to problems of double-diffusive flows. Time-dependent Reynolds-averaged Navier-Stockes (T-RANS) technique serves as a suitable tool for simulating turbulent flows with dominant large transport structures. T-RANS model has been incorporated into a finite solver for three-dimensional non-orthogonal domains, using Cartesian vector and tensor components and collocated variable arrangement. The approach has been validated in a number of test cases and applied in a couple of numerical cases, simulating real-time field component movement, driven by the dominant buoyancy mechanism, and providing very good numerical results. Double-diffusion/convection processes (heat and mass) are often found in thermal applications and energy conversion systems, particularly for energy storage (salt solar ponds), as well as in other engineering areas, in environment, astrophysics and geology. Recently, T-RANS tool has been developed for solving momentum and heat transport equations. Only some simple models for mass transport have been treated so far. Since the mass transport was modeled as a passive scalar without direct interaction with heat transport equation, it couldn't have provided satisfactory accuracy for calculated results. The scope of this work was to implement comprehensive equations for mass transfer into the T-RANS tool making it capable of solving double-diffusive problems. The mass transport equations were adapted to the model and the results tested on different test cases. This paper shows the technique we used and some results provided from the calculation.
Keywords: thermal and mass stratification, double diffusive (D-D) convection, turbulence modeling

1. INTRODUCTION
In the focus is the fluid flow in which the change to density is caused by the changes of temperature and specific mass concentration, with dominant buoyancy effects. These two components (temperature T and salt concentration S) diffuse at different levels. Should convection motions be generated when scalar components are making opposite contributions to the vertical density gradient, then the phenomena known as *double diffusive convection* are created. The results of such movements depend on the vertical distribution of scalar components, where one component is always of an unstable pattern, so it can provide energy for movement, and where the other one is always stabile in order to maintain the general stabile stratification of density.

Double diffusive phenomena occur in various engineering systems and in the nature. They are distinctive to ocean's staircase structures, where the great saline water masses stratify and start to move due to violation of stabile stratification of a scalar field. A solar salt pond is a typical example of D-D system, found in nature (oceans and salty lakes) and in many areas of engineering, in which strong density stratification dominates the transport processes (metal solidification and crystal growth, heavy gas storage, handling, etc.) [3]. The stratification is usually expressed in terms of density increment, where β_T , β_S denote the volume expansion coefficients caused by unit temperature and concentration changes, respectively. D-D system can be characterized by two or more layers of fluid with different densities, separated by interface, as shown in Figure 1. Special of interest here is the situation shown in Fig. 1b), 1c), where both layers are well mixed because of convection or mechanical turbulence production /e.g. wind shear/ locally or elsewhere in the layer.

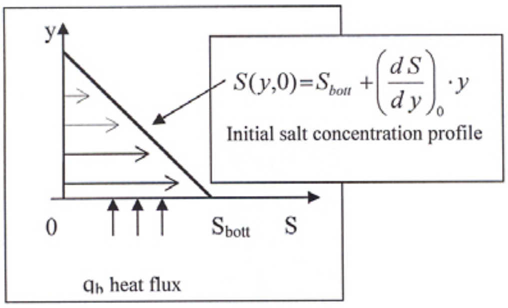
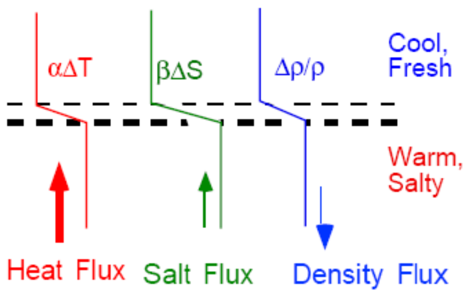
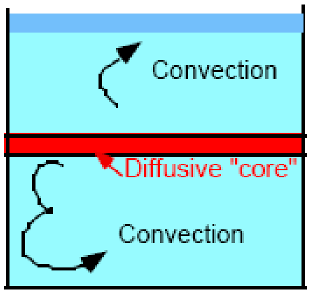


Figure 1.(a) Schetch of a D-D system with the initial profile of salinity and uniform vertical initial temperature distribution through whole accumulation heated from below

(b)



(c)



(b) Background stratification for a D-D convection experiment, with a diffusive interface and well-mixed layers above and below.(c) Sketch of tank showing convective layers and diffusive interface.

2. AN APPROACH TO D-D PHENOMENA MODELING

Natural motion in convective mixed layer is turbulent. It is necessary to choose a proper turbulent model for quantitative research of the D-D system. In the case of buoyancy-driven turbulent motion, there are several phenomena originating from the strong coupling and mutual interaction between the temperature, concentration and velocity fields that must be considered. A special challenge arises in modeling turbulent transport in mixed layers such as those in solar ponds, where the mean temperature and concentration fields are almost uniform. Here, the conventional gradient hypothesis, by which the turbulent fluxes are modeled in terms of the mean property gradients, fails to produce sensible results, because it yields very small or negligible vertical turbulent fluxes. It should be pointed out that these fluxes, generated by buoyancy, are significant in magnitude, representing the major cause of upward turbulent convection and mixing, so that the almost uniform T and S distributions are the consequence, not the cause, of the vertical turbulent fluxes. A proper mathematical treatment should employ a higher-order modeling approach, like rational second moment closure, SCM level of modeling. In D-D systems, molecular interactions within the diffusive interface and in its vicinity have significant influence, regardless of the intensity of turbulence in the mixed layers. Therefore, in all turbulence equations the molecular effects should be included.

The SMC model, completely introduced and discussed in Ref. [4] can serve as a basis for deriving algebraic models, which do not require solutions of different transport equations for each stress and flux component, but can still capture important physical processes. By suitable elimination of differential terms, differential equations for the second moments can be truncated to yield algebraic expressions for turbulent fluxes, e.g. Dol at al.[2]. The truncation of heat and mass flux seems very justified for buoyancy-dominated flows, such as D-D also, because of a strong coupling velocity and temperature/concentration fields through the buoyancy forces. The model used here solves the mean energy (in terms of temperature <T>), and mean concentration (<S>)) equations

$$\rho\frac{\partial\langle T\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\sigma_T}\frac{\partial\langle T\rangle}{\partial x_j}\right)-\frac{\partial\left(\rho\tau_{\theta_i}\right)}{\partial x_j} \quad (1) \qquad \rho\frac{\partial\langle S\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu}{\sigma_S}\frac{\partial\langle S\rangle}{\partial x_j}\right)-\frac{\partial\left(\rho\tau_{s_i}\right)}{\partial x_j} \quad (2)$$

where $\mu_{ef}=\mu+\mu_t$, $\mu_t=C_\mu f_\mu\rho\frac{\langle k^2\rangle}{\langle\varepsilon\rangle}$, $f_\mu=\exp\left(-3,4/(1+0,02\,\mathrm{Re}_t)^2\right)$ is correction for low Re.

A full SCM model use differential equations for temperature $\left\langle\overline{\theta^2}\right\rangle$, and variance of turbulent concentration fluctuations, $\left\langle\overline{s^2}\right\rangle$, and for double single-point correlation of T-S fluctuations, $\left\langle\overline{\theta s}\right\rangle$:

$$\rho\frac{\partial\left\langle\overline{\theta^2}\right\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu_{ef}}{\sigma_{\overline{\theta^2}}}\frac{\partial\left\langle\overline{\theta^2}\right\rangle}{\partial x_j}\right)-2\rho\tau_{\theta_i}\frac{\partial\langle T\rangle}{\partial x_j}-\frac{1}{C_{T'}}\rho\frac{\langle\varepsilon\rangle}{\langle k\rangle}\left\langle\overline{\theta^2}\right\rangle \;;\; \rho\frac{\partial\left\langle\overline{s^2}\right\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu_{ef}}{\sigma_{\overline{s^2}}}\frac{\partial\left\langle\overline{s^2}\right\rangle}{\partial x_j}\right)-2\rho\tau_{s_i}\frac{\partial\langle S\rangle}{\partial x_j}-\frac{1}{C_{S'}}\rho\frac{\langle\varepsilon\rangle}{\langle k\rangle}\left\langle\overline{s^2}\right\rangle$$

$$\rho\frac{\partial\left\langle\overline{\theta s}\right\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu_{ef}}{\sigma_{\overline{\theta s}}}\frac{\partial\left\langle\overline{\theta s}\right\rangle}{\partial x_j}\right)-\rho\left(\tau_{s_i}\frac{\partial\langle T\rangle}{\partial x_j}-\tau_{\theta_i}\frac{\partial\langle S\rangle}{\partial x_j}\right)-\frac{1}{C_{TS'}}\rho\frac{\langle\varepsilon\rangle}{\langle k\rangle}\left\langle\overline{\theta s}\right\rangle \quad (3)$$

The closure of equations above requires solution of an additional set of transport equations for turbulence properties, such as the turbulence kinetic energy *k* and its dissipation rate *ε*.

$$\rho\frac{\partial\langle k\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu_{ef}}{\sigma_k}\frac{\partial\langle k\rangle}{\partial x_j}\right)+\rho g\left(\beta_T\tau_{\theta_i}+\beta_S\tau_{s_i}\right)-\rho\langle\varepsilon\rangle \quad (4)$$

$$\rho\frac{\partial\langle\varepsilon\rangle}{\partial t}=\frac{\partial}{\partial x_j}\left(\frac{\mu_{ef}}{\sigma_\varepsilon}\frac{\partial\langle\varepsilon\rangle}{\partial x_j}\right)+\rho g\frac{\langle\varepsilon\rangle}{\langle k\rangle}\left(C_{\varepsilon_3}\beta_T\tau_{\theta_i}+C_{\varepsilon_4}\beta_4\tau_{s_i}\right)-C_{\varepsilon_2}f_\varepsilon\rho\frac{\langle\varepsilon\rangle\tilde{\varepsilon}}{\langle k\rangle} \quad (5)$$

The first truncation of equations for *k*, $\left\langle\overline{\theta^2}\right\rangle$ and $\left\langle\overline{s^2}\right\rangle$ is performed by assuming the weak equilibrium hypothesis, after which the following algebraic expressions for turbulent fluxes are derived:

$$\tau_{\theta_i}=\frac{\tau_{ij}\frac{\partial\langle T\rangle}{\partial x_j}+\varsigma\tau_{\theta_j}\frac{\partial\langle U_i\rangle}{\partial x_j}+\eta g_i\left(\beta_T\left\langle\overline{\theta^2}\right\rangle-\beta_S\left\langle\overline{\theta s}\right\rangle\right)}{-C_{T_1}\frac{\langle\varepsilon\rangle}{\langle k\rangle}+\frac{1}{2\left\langle\overline{\theta^2}\right\rangle}\left(2\tau_{\theta_j}\frac{\partial\langle T\rangle}{\partial x_j}+\left\langle\varepsilon_{\theta^2}\right\rangle\right)+\frac{1}{2\langle k\rangle}\left(\tau_{ij}\frac{\partial\langle U_i\rangle}{\partial x_j}+\beta_T g_i\tau_{\theta_i}-\beta_S g_i\tau_{s_i}+\langle\varepsilon\rangle\right)} \quad (6)$$

$$\tau_{s_i}=\frac{\tau_{ij}\frac{\partial\langle S\rangle}{\partial x_j}+\varsigma_1\tau_{s_j}\frac{\partial\langle U_i\rangle}{\partial x_j}+\eta_1 g_i\left(\beta_T\left\langle\overline{\theta s}\right\rangle-\beta_S\left\langle\overline{s^2}\right\rangle\right)}{-C_{S_1}\frac{\langle\varepsilon\rangle}{\langle k\rangle}+\frac{1}{2\left\langle\overline{s^2}\right\rangle}\left(2\tau_{s_j}\frac{\partial\langle S\rangle}{\partial x_j}+\left\langle\varepsilon_{s^2}\right\rangle\right)+\frac{1}{2\langle k\rangle}\left(\tau_{ij}\frac{\partial\langle U_i\rangle}{\partial x_j}+\beta_T g_i\tau_{\theta_i}-\beta_S g_i\tau_{s_i}+\langle\varepsilon\rangle\right)} \quad (7)$$

Set of equation from (1) to (7) was solved numerically using general finite-volume N-S code adapted for 1D and 2D unsteady computation. A collocated numerical grid was used for all variables with typically 100 grid points clustered around interface and close to bottom wall and free surface. So, the adopted model solves **7** differential equations, but for turbulent heat and mass fluxes uses the algebraic form given with equations (6) and (7).

3. SOME OF RESULTS AND CONCLUSIONS

The applicability of derived turbulence model for simultanous transport of salt and heat in D-D system of salt stratified water accumulation heated from below, as shows Fig. 1(a) where upper layer is unmixed, and the system of two highly turbulent mixed layers from Fig. 1(b) (see [1]) was tested. When a cold fresh water layer is deposited over a layer of warm salty water with sharp border area between them, the system completely can become unstable, even if the density differences $\beta_S \, \Delta S$ on account of the salinity are much greater then density differences caused by the temperature changes $\beta_T \, \Delta T$. The convective motion is arising in both layers. The computations, carried out for a series of different initial density differences between two layers, showed expected behavior, as can be seen from a sample of results presented in Figures 2. to 5., where profiles of temperature, double T-S correlation**,** salinity and turbulent kinetic energy at different time instant, are plotted.

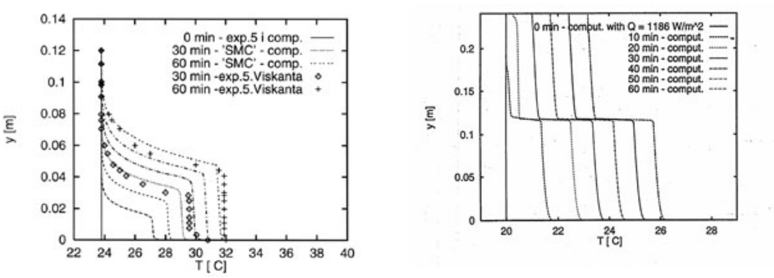


Figure 2(a) and (b) Time-evolution of T for both cases

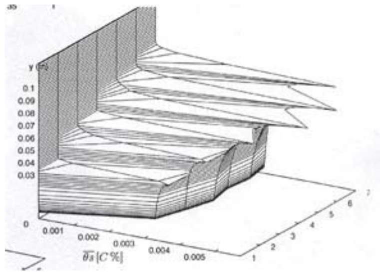


Figure 3 Predicted distribution of double T-S correlation

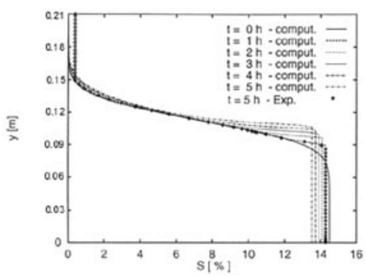


Figure 4 Time-evolution of S field in two mixed convective layer system

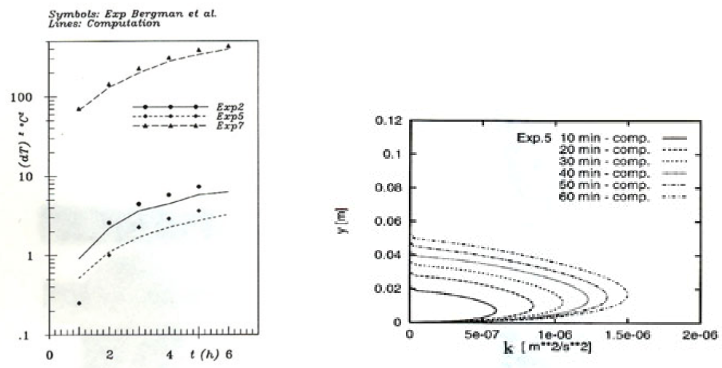


Figure 5:Time evolution of T in bottom mixed layer compared with experiments, and vertikal distribution of kinetic energy profiles

There is a reasonable agreement between the predicted and measured correlation, especially at small stratification. It means that adopted turbulent model can simulate described phenomenon quite well.

4. REFFERENCES

[1] Turner, J. S.: The coupled turbulent transport of salt and heat across a sharp density interface, Int. J. Heat and Mass Transfer 8, 759-767, 1985

[2] Dol, H.S., Hanjalić, K and Kenjereš, S.: A coparative assessment of the second moment differential and algebraic models in turbulent natural convection, Proc. Int. Turbulent Heat Transfer Conf., San Diego, USA, 1996

[3] Turner, J.S., G. Veronis, 2000. Laboratory studies of double-diffusive sources in closed regions, J. Fluid Mech., 405, 269-304.

[4] Musemić, R: Contribution to the Development of Mathematical Models of the Penetrative Turbulent Double Diffusion, Ph Dissertation, Faculty of Mechanical Engineering University of Ljubljana, Ljubljana, Slovenia, 1996