

# Integrated model of double-diffusive convection: numerical stability

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**Abstract**—The double-diffusion effect is a known phenomenon in oceanography. In this paper a model of thermohaline field turbulent energy evolution caused by double-diffusion effects, is under consideration. The mathematical model itself is a system of three nonlinear partial differential equations for environment's temperature, salinity and turbulence kinetic energy, where unknown functions depend on time and on one only space variable. The discretisation and numerical implementation of the model is given, which bases on implicit difference method, on the uniform rectangular time-space grid and Newton iteration method. As the main result of paper the computational stability condition is obtained. The numerical stability criterion of the numerical algorithm for finding approximate solution is estimated by the maximum values of the solutions of system components and main parameters of the model.

**Keywords**— turbulence, double diffusion, Newton method, numerical stability

## I. INTRODUCTION

THE effect of double-diffusion is known already from 1857, when in Sydney, W.S. Jevons performed the first known laboratory experiments on heat-sugar fingers. Fundamental notion that convective fluid motions can arise as a result of different molecular diffusivities was forgotten for nearly 100 years. Rediscovery happened in 1956: Arnold Arons suggested that a pipe with heat-conducting walls would allow a self-sustaining flow to occur the "perpetual salt fountain" [23].

The layering of initially stable vertical profiles of hydrophysical fields into stair-like profiles is a well-known phenomenon from oceanographic observation and laboratory investigations [4], [5], [25], [27]. The physical reason of the process proceeds from the difference of coefficients of molecular diffusion for different environment constituents, for example in oceans - heat and salt, characterised by temperature and salinity fields. Two different scenarios of layering processes are possible called as salt-fingering and diffusive layering regimes.

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## II. STRATIFICATION MODELS AND DOUBLE-DIFFUSION

In nature, the air in the atmosphere and the water in the oceans, seas and lakes are usually stratified. A direct consequence of stratification is that natural synoptic-scale motions frequently have nontrivial vertical structure. However, analysis in [19] shows that this consequence can be partially avoided if the stratification becomes evident in the form of well-defined layers of practically homogeneous fluid. The two-layer model is applicable in cases when the vertical density distribution in the ocean or atmosphere has one well-defined layer of large density gradients, and the rest of the medium is much more weakly stratified. There are, however, cases when the water masses have significantly more complex structure. For example, at medium latitudes the seasonal thermocline creates a 3-layer structure (the Baltic Sea) [1].

The stratification of a water column frequently becomes evident in the form of a series of homogeneous layers alternating with high gradient interfaces. Such a vertical structure is known as a stepped staircase or a stepwise thermohaline structure. Steplike vertical profiles with the typical height of the steps from a few centimeters to tens and hundreds of meters occur in the oceans. Such structures can be found in many regions of the world's oceans, including tropical, Caribbean, arctic or mid-latitude waters, e.g. Tyrrhenian Sea in the Mediterranean [20], [12], [28]. A large number of experiments in the Red Sea, in the Arctic Ocean, the North Atlantic, in the Canada Basin etc. suggest that the staircase-like structures are a common feature in the ocean [24], [13], [14]. They seem to be present in all areas where the conditions for thermohaline layering are sufficient. Layered structures can be found in some lakes also, e.g. lake Nyos in Cameroon where the contribution of CO<sub>2</sub> to the stratification is much larger than that of temperature and dissolved salts [19].

In order to estimate the correctness of underlying assumptions of the layered model and for a reliable implementation of results from a multi-layer ocean model, it is important to know if, when and how the layers develop. In current paper an attempt is made to clarify under which conditions the layering process occurs in the typical ocean environment. The analysis is based on the description of this mechanism owing to interplay of double-diffusive processes and turbulent mixing in the framework of the theory of rotationally anisotropic turbulence [6]. The research presented serves as a first stage of the studies of this mechanism and has the goal to qualitatively understand, under which conditions the layered structure is generated and which sort of numerical methods can be used for its analysis. Further studies are

needed in order to establish what can be the thickness of the layers and how large can be the temperature, density and salinity jumps in between the layers. The results obtained so far suggest that these studies require extensive computational efforts and are outside of the scope of this paper.

Double-diffusion is a phenomenon that occurs during the mixing processes in fluids with two constituents of greatly different molecular diffusivities [18]. In the oceans, such constituents, which also affect the water density, are the temperature and salinity. The molecular diffusivity of temperature is by two orders of magnitude larger than the molecular diffusivity of salinity. Equivalently, on the molecular scale heat diffuses much more rapidly than salt. Many oceanographers expect that double-diffusion has major effects on oceanic water masses and circulation. Although double-diffusion becomes evident mostly in small scales, the common opinion of the experts is that double-diffusive fluxes produce significant effects on various large-scale features of the ocean, and it is the potential of such effects that has driven much of the active research in the field [19]. The scope of investigations of double-diffusion is not restricted with oceanography. The process is studied even in porous medium [2].

### III. MECHANISMS OF LAYER FORMATION

The basic source of stratification in the ocean is the energy submitted to the ocean by the Sun and wind. There exist a large number of studies of formation of a staircase-like structure. Its mathematical modelling both in general fluid mechanics and in oceanography is supported by many laboratory experiments and with a large amount of experimental data [4], [5], [8], [25]. Many aspects of the origin of such a structure, in spite of long history of its studies, are still unclear and are a subject for speculations.

There exist several mechanisms that can produce structures similar to those observed in the nature. A field of turbulence in a strongly stratified fluid, far from boundaries, being supported by a Reynolds stress and having a non-zero vertical flux of buoyancy or density, may be unstable to variations in the vertical density gradient [15]. The vertical diffusion of salt or heat is a strongly nonlinear process, and the relevant nonlinear differential equation has initially unstable solutions under certain conditions. The properties of such solutions have been analysed by E.S. Posmentier in [16] who numerically demonstrated the possibility of development of initially smooth salinity profiles into staircase-like structures. Thermohaline intrusions may also create such structures [3]. A simple one-dimensional numerical model demonstrates how intrusions generate inversions in temperature and salinity. Under normal conditions the density usually increases with depth. A reversal of the normal behavior of density in the ocean is, in which a layer of more dense water is overlaid by a less dense layer. The medium seems to evolve toward an equilibrium state in both finger- and diffusive type stratifications. The equilibrium states are characterised by convecting and thus well mixed layers between specific interfaces - layers in which either diffusive layering takes

place or salt fingers occur. The resulting structure has staircase-like vertical profiles of temperature, salinity and/or density.

In this study we explain a novel mechanism of the formation of the layered structure, triggered by the joint influence of double-diffusive and turbulent mixing processes. This mechanism can trigger one of the most likely scenarios for formation of layers and the step-like structure in the sea. It may become active practically always when double-diffusion processes are active. The relevant process can be modelled in the framework of the theory described in [6].

A well-defined layered structure means that large gradients appear in some areas below called interfaces. The formation of a layer is therefore accompanied by large gradients of certain parameters (temperature, salinity and/or density in the ocean) at the interface(s). In extreme cases, the behaviour of their derivatives resembles delta-like peaks. This feature makes the numerical studies of the formation of step-like stratification a particularly difficult problem since onset of numerical instability may be interpreted as a (non-realistic) layer in the modelling process. The stability and reliability of the numerical scheme is thus a central prerequisite in the relevant studies.

The described problem resembles well-known difficulties appearing in numerical solving of stiff systems characterised by extensive variation of the magnitude of different terms in the equations to be solved. On the one hand, the numerical scheme may become unstable. While modelling the situation where layering is expected, it is hard to determine if the computed result is a fake or real, without analyzing the physical process. On the contrary, making the numerical scheme "too stable" (for example, with the use of a sort of additional numerical viscosity), we can artificially damp the layer formation process. Therefore one has to employ a method that is able to reproduce the physical results and to damp the instabilities.

The central problem is the relevant choice of the model type and parameters for a reliable description of the layer formation owing to the joint influence of double-diffusive (called DD below) and turbulent mixing processes in the framework of the theory [6]. The qualitative analysis of the model equations and results of a variety of numerical experiments suggest that the formation of layering in a stratified medium is a generic process in the oceans. The above has shown that the analysis of the stability of the relevant numerical code is equally important. It is established that for a certain range of parameters the numerical scheme is stable and the results are correct although the process looks unstable.

### IV. TYPES OF INTERFACES IN DOUBLE DIFFUSION PROCESSES

Let us consider two water masses with different temperature and salinity above each other. There exist two options of initially stable stratification. First, the overall stratification is stable when the upper layer is cooler but much less saline compared to warmer and more salty lower layer. Second, the upper layer may be more saline but warm enough compared to relatively cool and somewhat more fresh lower layer.

The interface between the water masses has a different nature in these cases. When the interface is unstable with respect to the highly diffusive constituent (i.e. heat – the warmer water is in the lower layer), the changes of water properties in the vicinity of the interface occur by the molecular diffusion of both heat and salt. The molecular diffusion causes density inversions that lead to the corresponding release of potential energy within the inversion region and initiate the mixing process and formation of new (more or less uniformly mixed) layers. An interface of this kind is known as a diffusive layering (DL) interface.

On the opposite case when the interface is unstable with respect to a substance of lower diffusion (i.e. the more saline water is in the upper layer) long, narrow “finger-like” convection cells with rising and sinking fluid motions that carry buoyancy flux will be created. These interfaces are called (salt) finger (SF) interfaces [3], [5], [26], [27].

The mathematical model, setup of which is explained in [6], [9], starts from traditional approach in solving the turbulent problems, based on the classical semi-empirical theory of turbulence [11] and a theory explained in [6]. The model itself is a system of three nonlinear partial differential equations for environment’s temperature, salinity and turbulence kinetic energy, where unknown functions depend on time and on one only, vertical space state variable. The discretisation, using difference method, leads us to the algebraic system with block-structured matrix. When more then one spatial direction is taken into account, then the idea of introducing virtual voxels could be used for discretisation of the problem, in real monitoring also the Kalman filtering would be useful. These ideas are applied in [10]. Within the mathematical problems arising from the model the central question is the stability of numerical realisation of the model. Some examples from numerical results are given.

V. THE MATHEMATICAL MODEL

When describing the layering process in environment due to double diffusive effects the quantities under consideration are the non-dimensional turbulent energy  $K(z,t)$ , salinity  $S(z,t)$ , temperature  $T(z,t)$  and density  $\rho(z,t)$ . Assuming that the state equation  $\rho = 1 - \tilde{\alpha}(T - 1) + \tilde{\beta}(S - 1)$  is linear, the model equations read:

$$\frac{\partial K}{\partial t} = b \frac{\partial}{\partial z} \left( K \frac{\partial K}{\partial z} \right) - K \left[ 1 + rb \left( \beta \frac{\partial S}{\partial z} - \alpha \frac{\partial T}{\partial z} \right) \right], \quad (1)$$

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[ (a + bK) \frac{\partial T}{\partial z} \right], \quad (2)$$

$$\frac{\partial S}{\partial t} = \frac{\partial}{\partial z} \left[ (d + bK) \frac{\partial S}{\partial z} \right]. \quad (3)$$

where  $b = ct_K^2 K_0 z_0^{-2}$  has the meaning of the coefficient of turbulent diffusion,  $t$  is non-dimensional time,  $t_K$  and  $z_0$  are

the characteristic time and vertical scale, respectively,  $K_0$  is the characteristic scale of the turbulent energy,  $r = gz_0 K_0^{-1}$ ,  $a = k_T^{mol} t_K z_0^{-2}$ ,  $d = k_S^{mol} t_K z_0^{-2}$ ,  $k_T^{mol}$  and  $k_S^{mol}$  are the coefficients of molecular diffusion of heat and salt, respectively,  $\tilde{\alpha} = \alpha T_0 \rho_0^{-1}$ ,  $\tilde{\beta} = \beta S_0 \rho_0^{-1}$ , and  $\alpha$  and  $\beta$  are the coefficients of thermal expansion and salinity contraction, respectively. The model thus contains five physical constants  $\alpha$ ,  $\beta$ ,  $k_T^{mol}$ ,  $k_S^{mol}$  and  $g$ . The derivation and discussion of the equations is presented in [9] and the value of the semi-empirical constant  $c = 0.05$  is suggested based on theoretical considerations of [21].

Depending on the character of initial stratification, two different scenarios of layering processes are possible. For the mathematical model the choice between these variants brings out different initial and boundary conditions [9].

For the discretisation of the continuous model described by equations (1)-(3) we introduce the rectangular time-space grid, with the time step  $\tau$  and vertical step  $h$ . Denote  $(t_i, z_j)$  the grid points and  $K_{i,j}$ ,  $T_{i,j}$  and  $S_{i,j}$  the approximate values of  $K$ ,  $T$  and  $S$  respectively, in these points. Here  $t_i = i\tau$ ,  $z_j = z_0 + jh$ ,  $i=0,1,2,\dots, j=0,1,2,\dots,n$ .

If the approximate values of the system variables are known at  $t=t_i$ , then discretisation of initial set of equations leads to the following system of algebraic equations for values at  $t=t_{i+1}$ :

$$\begin{aligned} f_j^{(1)} &\equiv \frac{K_{i+1,j} - K_{i,j}}{\tau} - b \left[ \frac{K_{i+1,j+1} - K_{i+1,j-1}}{2h} \right] - bK_{i+1,j} \frac{K_{i+1,j+1} - 2K_{i+1,j} + K_{i+1,j-1}}{h^2} + \\ &+ K_{i+1,j} \left[ 1 + rb \left( \beta \frac{S_{i+1,j+1} - S_{i+1,j-1}}{2h} - \right. \right. \\ &\quad \left. \left. - \alpha \frac{T_{i+1,j+1} - T_{i+1,j-1}}{2h} \right) \right] \\ f_j^{(2)} &\equiv \frac{T_{i+1,j} - T_{i,j}}{\tau} - \left( b \frac{K_{i+1,j+1} - K_{i+1,j-1}}{2h} \right) \frac{T_{i+1,j+1} - T_{i+1,j-1}}{2h} - \\ &- (a + bK_{i+1,j}) \frac{T_{i+1,j+1} - 2T_{i+1,j} + T_{i+1,j-1}}{h^2} = 0 \\ f_j^{(3)} &\equiv \frac{S_{i+1,j} - S_{i,j}}{\tau} - \left( b \frac{K_{i+1,j+1} - K_{i+1,j-1}}{2h} \right) \frac{S_{i+1,j+1} - S_{i+1,j-1}}{2h} - \\ &- (d + bK_{i+1,j}) \frac{S_{i+1,j+1} - 2S_{i+1,j} + S_{i+1,j-1}}{h^2} = 0. \end{aligned} \quad (4)$$

Equations (4), where  $j = 0,1,\dots,n$ , present the non-linear algebraic system accompanied with the set of linear equations representing boundary conditions and allowing to eliminate values of unknown functions beyond the grid [9].

For fixed  $i$  the system (4) presents the approximation of system of model equations (1)-(3) in the following discrete form:

$$F(x) = \bar{0}, \tag{5}$$

where  $x$  denotes the vector of dimension  $N=3(n+3)$  of unknown approximate values,  $x=(K_{i+1,0}, \dots, K_{i+1,n}, T_{i+1,0}, \dots, T_{i+1,n}, S_{i+1,0}, \dots, S_{i+1,n})$ ;  $F$ - vector function determined by system of equations (4) complemented with relations from initial and boundary conditions, with components  $f_j^{(s)} = f_j^{(s)}(x)$ ,  $s=1,2,3, j=0,1, \dots, n$ ;  $\bar{0}$ - vector of zeroes of length  $N$ . Below we use also the notation  $F_p, x_p, p=0,1, \dots, N-1$ , for the components of  $F$  or  $x$ .

VI. NUMERICAL PROCESS

It is convenient to solve the nonlinear algebraic system (5) using the Newton iteration method. For given initial values  $x^0$  the iteration process will be:

$$F'(x^{m-1})(x^m - x^{m-1}) = F(x^{m-1}), \tag{6}$$

where  $m$  is iteration index and  $F'(x^m)$  denotes the Jacobian of  $F$  evaluated in  $x^m, m=1,2, \dots$ . In our case the Jacobian has the 3x3 block structure:

$$\begin{pmatrix} A & B & B \\ A & A & O \\ A & O & A \end{pmatrix}, \tag{7}$$

where  $A$  and  $B$  denote different 3-diagonal, 2-diagonal matrixes,  $O$  is zero matrix. The structure of  $A$  and  $B$  is as follows:

$$A = \begin{pmatrix} * & * & 0 & 0 & \dots & 0 & 0 & 0 \\ * & * & * & 0 & \dots & 0 & 0 & 0 \\ 0 & * & * & * & \dots & 0 & 0 & 0 \\ 0 & 0 & * & * & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & * & * & 0 \\ 0 & 0 & 0 & 0 & \dots & * & * & * \\ 0 & 0 & 0 & 0 & \dots & 0 & * & * \end{pmatrix}$$

and

$$B = \begin{pmatrix} 0 & * & 0 & 0 & \dots & 0 & 0 & 0 \\ * & 0 & * & 0 & \dots & 0 & 0 & 0 \\ 0 & * & 0 & * & \dots & 0 & 0 & 0 \\ 0 & 0 & * & 0 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 0 & * & 0 \\ 0 & 0 & 0 & 0 & \dots & * & 0 & * \\ 0 & 0 & 0 & 0 & \dots & 0 & * & 0 \end{pmatrix}.$$

Here the asterisks denote the locations of nonzero elements in matrices. Formulas (8)-(19) below show the computational rules of those.

In the following we investigate the conditions, under which the Jacobian  $F'(x^m)$ , (7), has dominating main diagonal - i.e. the problem of solvability of system (6). It is well-known (see e.g. [22]), that such domination ensures the uniqueness of solution of the system (4) and stability of elimination process for solving linear system (6).

Let's consider the equation (5),  $F(x) = \bar{0}$ , (here and afterwards we omit the upper iteration index). According to component form (4) we find the nonzero components of Jacobian (7) for  $j=0,1, \dots, n$  as follows:

$$f_{j,j} = \frac{1}{\tau} - b \frac{K_{i+1,j+1} - 2K_{i+1,j} + K_{i+1,j-1}}{h^2} + \frac{2b}{h^2} K_{i+1,j} + \left[ 1 + rb \left( -\alpha \frac{T_{i+1,j+1} - T_{i+1,j-1}}{2h} + \beta \frac{S_{i+1,j+1} - S_{i+1,j-1}}{2h} \right) \right], \tag{8}$$

$$f_{j,j \pm 1} = -b \frac{1}{h^2} K_{i+1,j} \mp b \frac{K_{i+1,j+1} - K_{i+1,j-1}}{2h^2}, \tag{9}$$

$$f_{j,j+n+3} = -f_{j,j+n+1} = -\alpha rb K_{i+1,j} \frac{1}{2h}, \tag{10}$$

$$f_{j,j+2n+4} = -f_{j,j+2n+2} = \beta rb K_{i+1,j} \frac{1}{2h}. \tag{11}$$

$$f_{j+n+2,j+1} = -f_{j+n+2,j-1} = -\frac{b}{2h} \frac{T_{i+1,j+1} - T_{i+1,j-1}}{2h}, \tag{12}$$

$$f_{j+n+2,j} = -b \frac{T_{i+1,j+1} - 2T_{i+1,j} + T_{i+1,j-1}}{h^2}, \tag{13}$$

$$f_{j+n+2,j+n+2 \pm 1} = -\frac{1}{h^2} (a + bK_{i+1,j}) \mp \frac{1}{2h} \left( b \frac{K_{i+1,j+1} - K_{i+1,j-1}}{2h} \right), \tag{14}$$

$$f_{j+n+2,j+n+2} = \frac{1}{\tau} + \frac{2}{h^2} (a + bK_{i+1,j}). \tag{15}$$

$$f_{j+2n+3,j+1} = -f_{j+2n+3,j-1} = -\frac{b}{2h} \frac{S_{i+1,j+1} - S_{i+1,j-1}}{2h}, \tag{16}$$

$$f_{j+2n+3, j} = -b \frac{S_{i+1, j+1} - 2S_{i+1, j} + S_{i+1, j-1}}{h^2}, \quad (17)$$

$$f_{j+2n+3, j+2n+3 \pm 1} = -\frac{1}{h^2} (d + bK_{i+1, j}) \mp \frac{1}{2h} \left( b \frac{K_{i+1, j+1} - K_{i+1, j-1}}{2h} \right), \quad (18)$$

$$f_{j+2n+3, j+2n+3} = \frac{1}{\tau} + \frac{2}{h^2} (d + bK_{i+1, j}). \quad (19)$$

During the numerical process it is necessary to compute the values of described components of Jacobian (7) on every iteration step. The sparse structure of the Jacobian makes it possible to apply a modification of the elimination method for solving this system to reduce the number of arithmetical operations. The method will be discussed elsewhere.

VII. STABILITY CRITERION

In the following we show that by the choice of the rate of grid steps  $h$  and  $\tau$  it is possible to reach the domination of the main diagonal of the Jacobian  $F'(x)$ . This in turn guarantees the uniqueness of the solution of the system (4) and the stability of the elimination process of solving of that system. Denote also

$$K = \max_j |K_{i+1, j}|, \quad T = \max_j |T_{i+1, j}| \quad \text{and} \quad S = \max_j |S_{i+1, j}|,$$

where  $j = 0, 1, \dots, n$ .

According to the formulae for the components of the Jacobian we analyse the estimations

$$\sum_{q \neq j} |f_{j, q}| < |f_{j, j}|, \quad j = 0, 1, \dots, N - 1. \quad (20)$$

We consider the estimations (20) separately in three cases: for  $j = 0, 1, \dots, n$  (case 1<sup>0</sup>),  $j = n + 1, n + 2, \dots, 2n + 2$  (case 2<sup>0</sup>), for  $j = 2n + 3, 2n + 4, \dots, N - 1$  (case 3<sup>0</sup>).

For case 1<sup>0</sup> from (8) we find

$$\begin{aligned} |f_{j, j}| &= \left| \frac{1}{\tau} - \frac{b}{h^2} (K_{i+1, j+1} - 2K_{i+1, j} + K_{i+1, j-1}) + \frac{2b}{h^2} K_{i+1, j} + \frac{c}{b} + \right. \\ &\left. + rb\beta \frac{1}{2h} (S_{i+1, j+1} - S_{i+1, j-1}) - rb\alpha \frac{1}{2h} (T_{i+1, j+1} - T_{i+1, j-1}) \right| \geq \end{aligned} \quad (21)$$

$$\begin{aligned} &\geq \left| \frac{1}{\tau} - \frac{b}{h^2} (K_{i+1, j+1} - 4K_{i+1, j} + K_{i+1, j-1}) + rb \left( \beta \frac{S_{i+1, j+1} - S_{i+1, j-1}}{2h} - \alpha \frac{T_{i+1, j+1} - T_{i+1, j-1}}{2h} \right) \right| \geq \\ &\geq \frac{1}{\tau} - \frac{6b}{h^2} K - \frac{rb\beta}{h} S - \frac{rb\alpha}{h} T. \end{aligned}$$

For the case 1<sup>0</sup> from (9)-(11) follows the estimation for secondary diagonals:

$$\sum_{q \neq j} |f_{j, q}| = \frac{b}{h^2} |K_{i+1, j+1} - K_{i+1, j-1}| + \frac{2b}{h^2} |K_{i+1, j+1}| + \frac{rb(\alpha + \beta)}{h} |K_{i+1, j}| \leq K \left( \frac{4b}{h^2} + \frac{rb(\alpha + \beta)}{2h} \right). \quad (22)$$

For the case 2<sup>0</sup> from (15) we find

$$|f_{j+2n+2, j+2n+2}| = \left| \frac{1}{\tau} + \frac{2}{h^2} (a + bK_{i+1, j}) \right| \geq \frac{1}{\tau} + \frac{2a}{h^2} - \frac{2b}{h^2} K. \quad (23)$$

From (12)-(14) for non-diagonal elements follows, that

$$\begin{aligned} \sum_{q \neq j+2n+2} |f_{j+2n+2, q}| &= \frac{b}{2h^2} |T_{i+1, j+1} - T_{i+1, j-1}| + \frac{b}{h^2} |T_{i+1, j+1} - 2T_{i+1, j} + T_{i+1, j-1}| + \frac{2}{h^2} |a + bK_{i+1, j}| + \\ &+ \frac{1}{2h} \left| a + b \frac{K_{i+1, j+1} - K_{i+1, j-1}}{2h} \right| \leq 3 \frac{b}{h^2} K + 7 \frac{b}{h^2} T + \frac{3a}{h^2}. \end{aligned} \quad (24)$$

For the case 3<sup>0</sup> from (19) we find for diagonal elements:

$$|f_{j+2n+3, j+2n+3}| = \left| \frac{1}{\tau} + \frac{2}{h^2} (d + bK_{i+1, j}) \right| \geq \frac{1}{\tau} - 2 \frac{b}{h^2} K, \quad (25)$$

and from (16)-(18), that

$$\begin{aligned} \sum_{q \neq j+2n+3} |f_{j+2n+3, q}| &= \frac{b}{2h^2} |S_{i+1, j+1} - S_{i+1, j-1}| + \frac{b}{h^2} |S_{i+1, j+1} - 2S_{i+1, j} + S_{i+1, j-1}| + \\ &+ 2 \max \left\{ \frac{1}{h^2} |d + bK_{i+1, j}|, \frac{1}{2h} \left| d + b \frac{K_{i+1, j+1} - K_{i+1, j-1}}{2h} \right| \right\} \leq \frac{7b}{h^2} S + \frac{3}{h^2} (d + bK). \end{aligned} \quad (26)$$

The estimations for non-diagonal elements hold due to some elementary relations for real numbers. For cases 2<sup>0</sup> and 3<sup>0</sup> the condition (20) leads to the inequalities:

$$\frac{1}{\tau} > \frac{7b}{h^2} T + \frac{5b}{h^2} K + \frac{a}{h^2}, \quad \frac{1}{\tau} > \frac{7b}{h^2} S + \frac{5b}{h^2} K + \frac{d}{h^2}.$$

Both of these are satisfied if

$$\frac{1}{\tau} > \frac{7b}{h^2} T + \frac{7b}{h^2} S + \frac{5b}{h^2} K + \frac{a+d}{h^2}. \quad (27)$$

In case 1<sup>0</sup> the condition (20) holds if

$$\frac{1}{\tau} > \frac{rb\beta}{h} S + \frac{rb\alpha}{h} T + \left( \frac{10b}{h^2} + \frac{rb(\alpha + \beta)}{h} \right) K. \quad (28)$$

If  $hr\beta < 7b$  and  $h r \alpha < 7b$  then the inequalities (27) and (28) are true for

$$\frac{h^2}{\tau} > 7bS + 7bT + (10b + hrb(\alpha + \beta))K, \quad (29)$$

which is the final estimation to the rate of grid steps to ensure the numerical stability of discrete model.

From the right-hand side of inequality (29) it follows, that variability in parameters ( $S, T, K$ ) cannot introduce bifurcation in stability criterion, as their estimations depend on essential parameters ( $b, r$ ) linearly.

VIII. NUMERICAL RESULTS

The qualitative evolution of vertical profiles of temperature, salinity, kinetic energy and density in the framework of equations (1) - (3) in the vicinity of the diffusive layering and the salt finger interfaces within a stably stratified fluid is

sketched on Figure 1 and Figure 2, respectively. At the outset, the water density monotonously increases with the depth. In the course of time density inversions at one or both sides of the interface may be formed due to the double diffusion process for a certain range of parameters. In the diffusive layering case, two layers with density inversions are formed. One of them is located above and the other below the original interface (Figure 1). In the salt finger case (Figure 2) only one area of density inversion, which embraces the original interface area, is occasionally formed. In the inversion regions, the potential energy starts to release, equivalently, the turbulent kinetic energy  $K$  increases. Unstable stratification in the area of the inversion(s) launches the turbulent mixing process in the(se) area(s), and results in formation of new mixed layer(s). After the new interface(s) and the new mixed layer(s) have been formed, the turbulence intensity decreases again, and the double diffusion apparently becomes the governing process after a while. Under favorable conditions, this scenario may be repeated many times and result in formation of a multi-layered structure.

This process can be easily tracked in the framework of equations (1) – (3). For simplicity let us denote

$$1 + rb \left( \beta \frac{\partial S}{\partial z} - \alpha \frac{\partial T}{\partial z} \right) = 1 + rb \frac{\partial \rho}{\partial z} \equiv B \quad (30)$$

and assume that at the outset the density linearly increases with depth. The term  $B$  in equation of turbulence energy (1) is positive in this case. The turbulent energy is thus damped by the stable stratification and, if initially small, it remains small until a certain time instant  $t_1$  when the quantity  $B$  becomes negative  $B < 0$ . During this stage the diffusion process has an almost purely molecular character. It generally results in changes of local gradients of the constituents  $S$  and/or  $T$ , and if it is intense enough, after some time it may change the sign of  $B$  for some range of depths.

The situation  $B < 0$  reflects an inversion in the density profile in which  $\partial K / \partial t$  appears to be roughly proportional to  $K$  and the turbulent energy exponentially increases starting from  $t = t_1$ . This process may resemble (numerical) instability but in fact it only reflects a fast increase of turbulent energy in a certain sublayer owing to displacement of water masses towards restoring a stable stratification. This process soon overrides molecular diffusion and is accompanied by a fast increase of both  $\partial T / \partial t$  and  $\partial S / \partial t$ , followed by a fast decrease of  $\partial T / \partial z$  and  $\partial S / \partial z$  in the area of intense mixing owing to Eqs. (2) and (3). Equation (30) then implies that the quantity  $B$  soon becomes positive again, say, at  $t = t_2$ . Starting from this time instant, equation (1) implies fast decrease of turbulent energy in layers with  $B > 0$ . The whole process can be interpreted as forming a new mixed layer (with generally finite thickness) in the vicinity of the former interface. This layer is separated from over- and underlying regions by new interfaces where the

buoyancy gradients are big enough to suppress the turbulence energy.

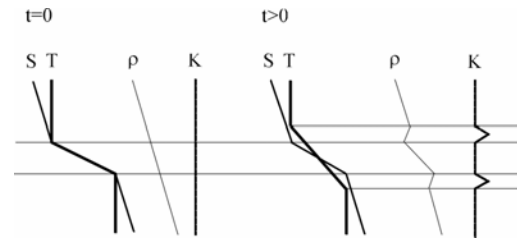


Figure 1. Evolution of the vertical profiles of temperature  $T$ , salinity  $S$ , density  $\rho = 1 - \alpha(T - 1) + \beta(S - 1)$ , and turbulent kinetic energy  $K$  in the case of the diffusive layering interface.

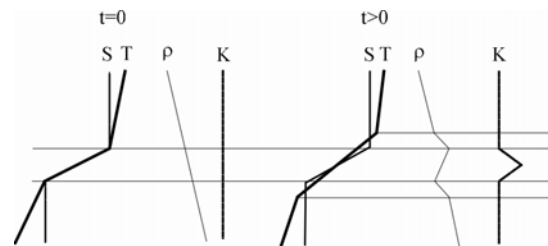


Figure 2. Evolution of the vertical profiles of temperature  $T$ , salinity  $S$ , density  $\rho$ , and turbulent kinetic energy  $K$  in the case of the salt finger interface.

The essence of the model requires that  $0 < d \ll a \ll bK_{\max}$ , where  $K_{\max}$  denotes the maximum value of the turbulent energy. New layers only can be generated if the turbulent energy is initially nonzero; however, this is normally the case in natural conditions. The initial profiles  $T(z, 0)$  and  $S(z, 0)$  were chosen so that the fluid density varied linearly in the vertical direction but a thin interface layer with relatively large temperature and salinity gradients was located at the mid-depth of the computational domain.

The domain of integration is  $\tilde{z} - D \leq z \leq \tilde{z} + D$ . The following initial and boundary conditions for equations (1) – (3) were adopted. The turbulent kinetic energy was set to a constant  $K(z, 0) = ab^{-1} \sim O(10^{-6})$ . The domain has an inner interface centered at  $z = \tilde{z}$  and with a thickness of  $2\delta$ , where  $\delta \ll D$ . The interface is determined as a thin layer with relative large temperature and salinity gradients compared to their gradients outside the interface area. The initial profiles  $T(z, 0)$  and  $S(z, 0)$  are chosen so that the fluid density varies linearly in the vertical direction at the outset. Its deviation from the nondimensional value  $\rho = 1$  at the centre of the interface is described by the state equation as

$\beta[S(z,0) - 1] - \alpha[T(z,0) - 1] = C(z - \tilde{z})$ , where  $C$  is jointly defined by  $\beta S(z,0)$  and  $\alpha T(z,0)$ .

The evolution of thermohaline field for diffusive layering is explained on Figures 3-5.

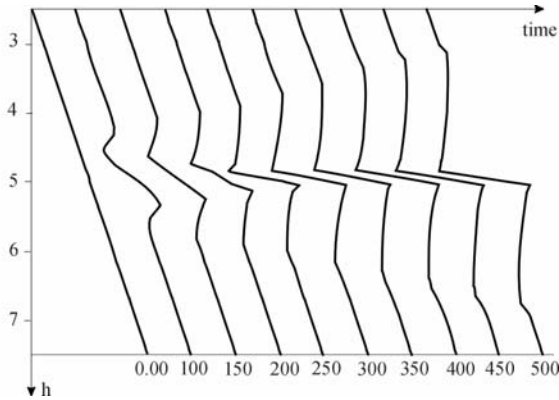


Figure 3. Temporal evolution of the vertical profile of water density

For the following values of the physical parameters:  
 $\tilde{\alpha} = 0.0003 \text{ K}^{-1}$ ,  $\tilde{\beta} = 0.0008 \text{ ‰}^{-1}$ ,  
 $k_T^{mol} = 1.3 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ ,  $k_S^{mol} = 1.7 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ ,  
 $D = \tilde{z} = 1$  and  $c = 0.05$ , the molecular diffusion has generated inversion regions (represented by negative gradients of the density profile, Fig. 3), large enough to launch the turbulent mixing at  $t=100$  s. For the realistic maximum values of the turbulent kinetic energy, temperature and salinity in the ocean, the ratio  $(\Delta h^2)/\Delta \tau > 0.01$  must hold, where  $\Delta h$  denotes the vertical step and  $\Delta \tau$  is the time step. In practical computations the time step has been taken as  $0.01 < \Delta \tau < 0.05$ . The resulting mixing process forms two new well-defined mixed layers by  $t=500$  s (Figure 5).

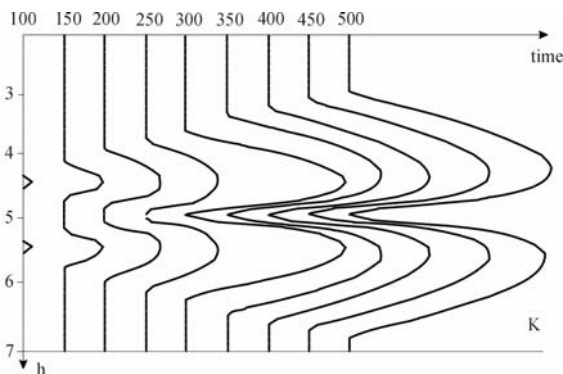


Figure 4. Temporal evolution of the vertical profile of the turbulent kinetic energy  $K$

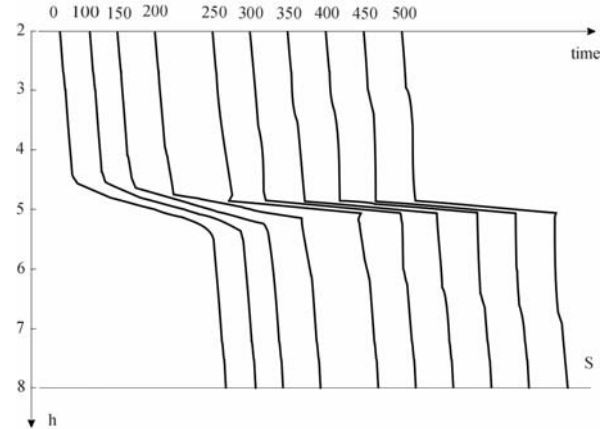


Figure 5. Temporal evolution of the vertical profile of water salinity

IX. CONCLUSION

The stability criteria for numerical realisation of the model of vertical structure of thermohaline fields, caused by double diffusion effects are discussed. The possibility to guarantee a numerical stability of discrete model based on the set of nonlinear differential equations (1) - (3) by a choice of suitable space and time step on the time-space grid is demonstrated. The estimated criterion is sufficient for numerical stability of formulated discrete model. The experience with various values of the parameters entered into equations (1) - (3) and into the initial and boundary conditions shows that the layering process apparently is only effective for a specific subset of the parameters, because of their many realistic combinations the layer-formation mechanism did not become evident within a reasonable computation time. However, in several cases it leads to quite fast forming of new layers and interfaces.

The experience with different sets of parameters and initial conditions suggests that the forming of such structures may have drastically different time scales in different regions, and that generally it is a long-term process and can be realized only in regions where the formation of stepwise structure has enough time to get formed. Research in this direction is clearly important, because as yet no modelling framework provides an integrated picture of DD-convection phenomena [7].

Although the example of double-diffusion in this article is taken from oceanography, the process itself (heat and mass transfer in a medium) is more and more investigated in non-oceanographic applications. Examples can be found in many engineering technological areas such as geothermal reservoirs, petroleum extraction, chemical catalytic reactors, prevention of water pollution, nuclear reactor, underground diffusion of nuclear wastes and other contaminants, and porous material regenerative heat exchangers [17].

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