CHAPTER 191

ALGORITHM FOR VERTICAL DIFFUSION

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ABSTRACT

A. mathematical method and a computer algorithm is developed for the case of one-dimensional vertical mixing for an estuary with rather small advection. In the case under consideration varies the diffusion coefficients both with time and depth, and the case is therefore closer to actual estuaries than earlier computing methods that applies constant coefficients. Model experiments with a small grid oscilliationg with high frequecies in two fluids with different densities were performed to test the algorithm. Reynolds number for turbulence was near $1.6 \cdot 10^4$.

The results showed that the ratio between the stabilizing Brunt-Väisälä frequency and the agitating cyclic frequency was a governing parameter for the system, and dimensionless diffusion coefficients could be expressed as a function of this parameter.

INTRODUCTION

Pollution problems in the sea and in the adjacent estuaries play an important role in coastal engineering and demands more and more sophisticated computational technique to be solved in a satisfactory way.

This paper deals with the case where two fluids with different densities are found in an estuary, with very small advection. After initial mixing in outlets and jets has occurred a more calm phase will be found where a light fluid is overlying a more dense fluid, and vertical mixing is due only to local turbulence.

This situation is common in many cases where the coastal engineer is involved such as:

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1) Thermal power plants with density differences between heated water and cooler recipient water.

2) Water power plants with density differences between fresh water in the mountains and salt water in the recipient.

3) Outlets that belong to the municipal sewage system.

4) Outlets and rivers containing different kinds of sediments in suspension.

Figure 1 shows a typical Norwegian fjord. The advection that occurs here is mainly wind driven. (See H. Rye, 1973 [1]). The algorithm presented here can also be extended to include advection and treat a case like this, as outlined below.

Figure 1. Site for collection of field data. Romsdalsfjord, Norway.

MATHEMATICAL ANALYSIS

Let us now consider the one-dimensional case without advection. The problem under consideration is shown in Figure 2. A salinity profile varying with depth is slowly mixed due to local turbulence. In the case under consideration no current is acting and all diffusion is vertical.

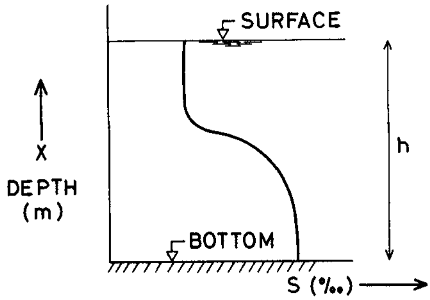

Figure 2. Definition of the problem.

The general equation for this situation is:

$$\frac{\partial s}{\partial t} = \frac{\partial}{\partial x} (D \cdot \frac{\partial s}{\partial x}) \tag{1}$$

D is the diffusion coefficient varying both with time and depth, x is the vertical co-ordinate, t is the time co-ordinate and s is the concentration of substance; here salinity (in other cases this could be heat or concentration of particles in suspension).

The boundary conditions for this situation are that the salt flux through the surface is zero, and that the time derivative of salinity integrated over the whole volume is zero as no material is transferred to the system from outside the control volume. (Eq. (2) and (3).)

$$FLUX_{x=h} = D \cdot \frac{\partial s}{\partial x} = 0 \tag{2}$$

$$\int_o^h \frac{\partial s}{\partial t} \cdot dx = 0 \tag{3}$$

Integration of the general equation with respect to x for a certain time kept constant gives

$$\int_o^x \frac{\partial s}{\partial t} \cdot dx = D \cdot \frac{\partial s}{\partial x} + CONSTANT \tag{4}$$

An integration constant appears here on the right side. This constant can be determined as shown in eq. (5) where the integration is taken over the whole volume.

$$CONSTANT = \int_o^h \frac{\partial s}{\partial t} \cdot dx - [D \cdot \frac{\partial s}{\partial x}]_{x=h} = 0 \tag{5}$$

The last term is the flux through the surface which is known to be zero, and the first term is also zero due to continuity. Thus the integration constant in eq. (4) is determined to be zero. The diffusion coefficient can then be found as the integral on the left hand side divided with the salinity gradient. Eq. (6) thus shows the determination of the diffusion coefficient for a certain time t_1 and a certain depth x_1.

$$[D]_{\substack{x=x_1\\t=t_1}} = \frac{\left[\int_0^{x_1} \frac{\partial s}{\partial t} \cdot dx\right]_{t=t_1}}{\left[\frac{\partial s}{\partial x}\right]_{\substack{x=x_1\\t=t_1}}} \tag{6}$$

This result is now transferred to an algorithm for computer work.

Figure 3 shows the **flow sheet** of the computer version of the algorithm. The input is recorded density profiles. They are written out for each series or test.

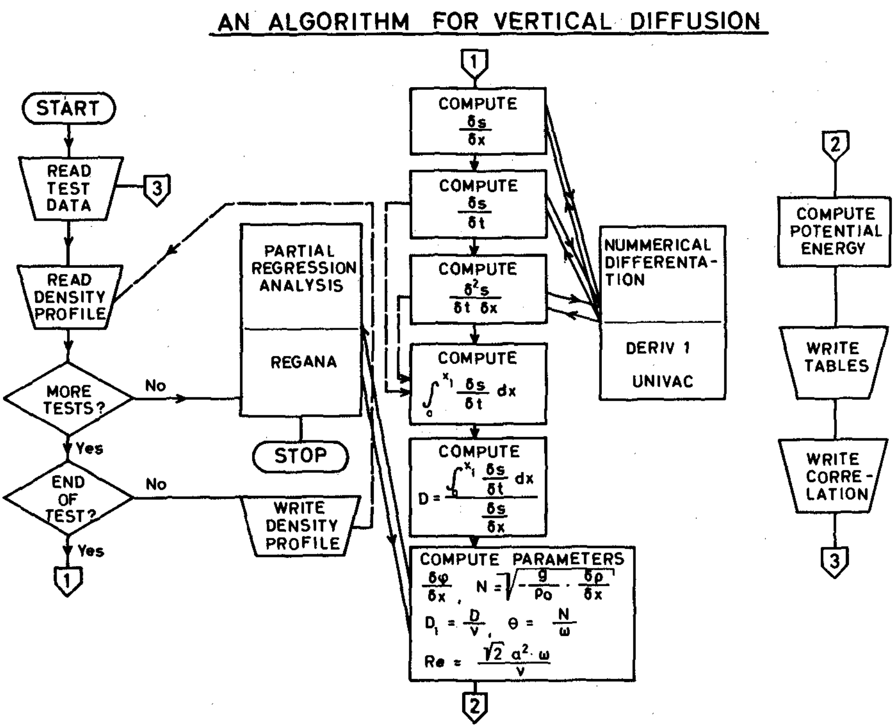

Figure 3. Flow diagram for algorithm.

A vital part of the programme is shown in two boxes, viz. a routine for numerical differentiation and a routine for a partial regression analysis. When a series of recordings is ended the computational part of the programme is called. This computes all the derivatives shown. Further, the programme uses a routine for numerical integration in which the input is both the salinity gradient with respect to time and the second derivative of salinity with respect to time and depth. From this the integral is found, and division with the local salinity gradient then gives the diffusion coefficients. Further, a special part of the programme computes all parameters that are considered necessary for the analysis of diffusion, such as density gradient, Brunt-Väisälä frequency, dimensionless diffusion coefficient, and Reynolds number for turbulence. The programme then goes on and computes potential energy and writes all parameters in tables.

Finally the regression analysis is called and it is then possible to investigate if there is any correlation between diffusion coefficients and selected density or turbulence parameters. This programme gives the final correlations directly. It takes density profiles as input and it gives the final correlation between diffusion coefficients and selected parameters immediately as output. It should, therefore, be an effective tool for research work in this field.

MODEL EXPERIMENTS

Experimental laboratory data for vertical mixing were used to test the algorithm. These were obtained in a small test tank that contained a layer of fresh water overlying a layer of salt water. A fine mesh grid was installed in the test tank and this could oscillate with different frequencies and amplitudes and thus generate the necessary turbulence. Two types of fine mesh grid were used, one with horizontal nets and one with vertical nets. Water samples could be extracted from the test tank through small tubes and the salinity was then determined with a conductivity meter. The temperature was kept constant during the tests. The test arrangement is shown in Figure 4.

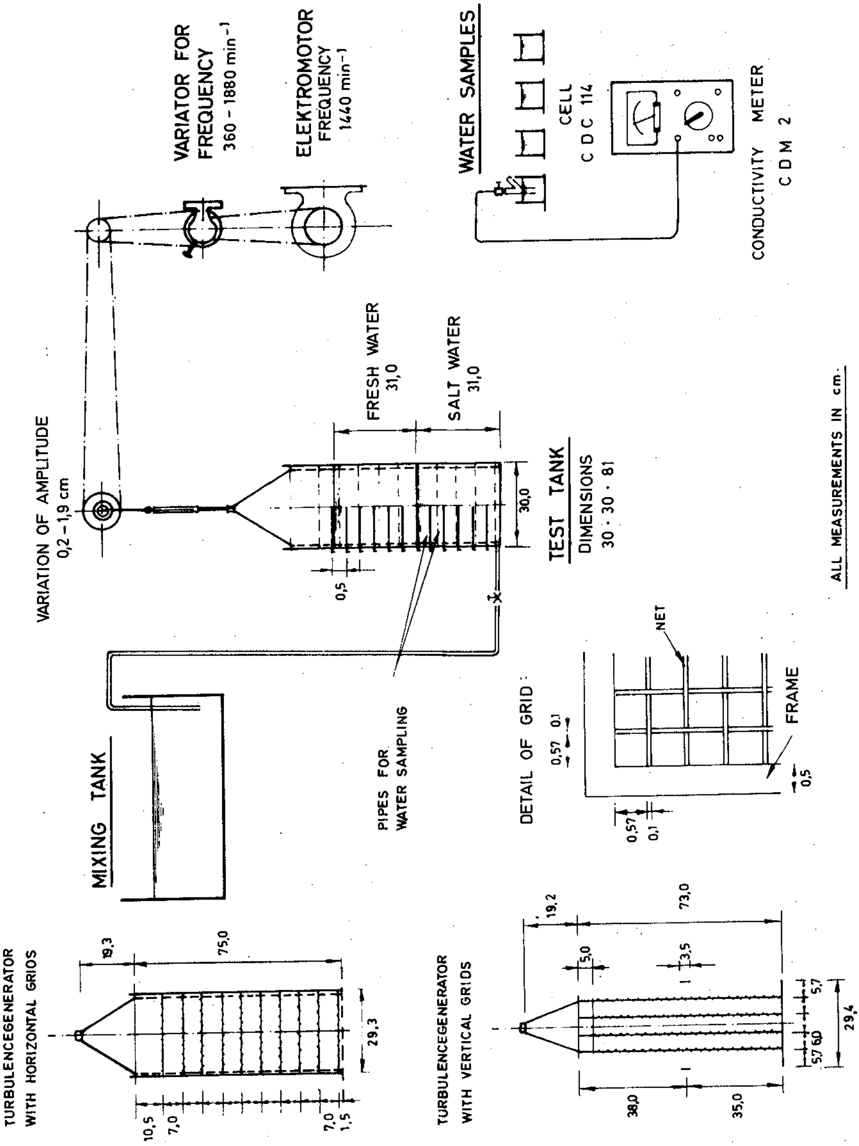

FIG. 4. MODEL ARRANGEMENT

RESULTS

Figure 5 shows a typical test result, after 2 minutes testing. The density profile is mixed to some extent. The Brunt-Väisälä frequency is the reference parameter for the density profile that is considered most important. It is defined by the equation:

$$N = \sqrt{-\frac{g}{\rho_o} \cdot \frac{\partial \rho}{\partial x}} \tag{7}$$

where g is the acceleration of gravity, ρ_o is the local density and $\partial\rho/\partial x$ the density gradient. It can be derived from the density profile. It shows a clear maximum in a certain level. 2π divided by this frequency is the lowest period with which internal waves can exist, and the distribution of the Brunt-Väisälä frequency is thus one of the most important dynamical characteristics of an estuary. Corresponding with this we can here see the computed vertical diffusion coefficient from the algorithm. It has a local minimum where the Brunt-Väisälä frequency has its maximum, and it has two local tops. This illustrates the inverse proportionality between these two parameters.

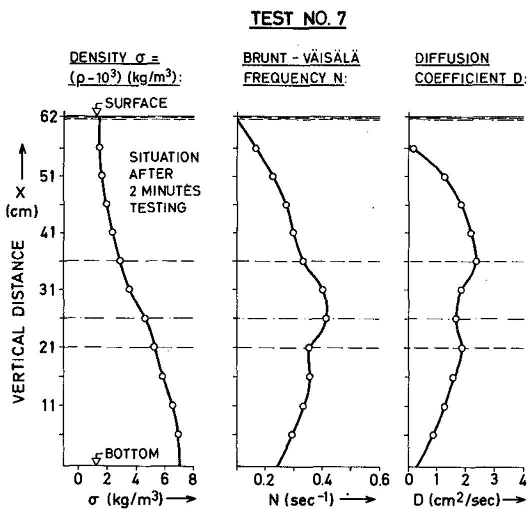

Figure 5. Test result after 2 minutes mixing.

Figure 6 shows a correlation between the diffusion coefficient and the squared Brunt-Väisälä frequency in one of the tests. The figure contains 154 points taken at different times during the 6 minutes test period. There is a considereable scatter. Still the partial regression analysis showed an inverse proportionality between the two parameters with a multiple correlation coefficient 0.94.

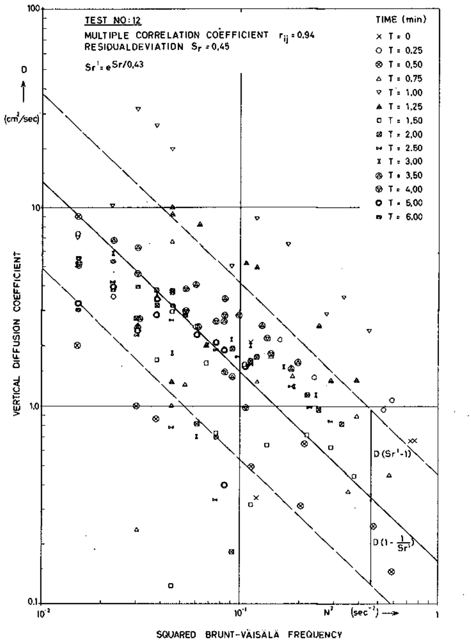

Fig. 6. Diffusion coefficient as a function of Brunt-Väisälä frequency.

Table 1 gives the equations for similar obtained correlations for all five performed tests.

TABLE 1

REGRESSION ANALYSIS NO 2

Level of significance to enter variable : 4.0
Level of significance to delete variable : 4.0
Minimum (residual variance/observed variance): 10^{-4}

Run	Correlation between D and N^2	Number of observations	Multiple corr. coefficient	Residual error	Anti-log residual error
No	Equation	m	r_{ij}	S_r	$S_r' = e^{S_r/0.4343}$
7	$D = \frac{8.989 \cdot 10^{-2}}{(N^2)^{0.9928}}$	66	0.9535	0.5147	3.271
8	$D = \frac{4.957 \cdot 10^{-1}}{(N^2)^{0.9852}}$	33	0.9924	0.2886	1.944
9	$D = \frac{1.247 \cdot 10^{-1}}{(N^2)^{0.9551}}$	66	0.9630	0.4035	2.532
11	$D = \frac{2.572 \cdot 10^{-1}}{(N^2)^{0.9008}}$	66	0.9423	0.5620	3.648
12	$D = \frac{1.597 \cdot 10^{-1}}{(N^2)^{0.9604}}$	154	0.9414	0.4525	2.834

D = cm^2/sec
N = sec^{-1}

The power in the equation for the squared Brunt-Väisälä frequency is in the first test 0.99 obtained for 66 points. In the second test the power was 0.99 obtained for 33 points. In the following tests the power was 0.96 for 66 points and 0.90 for 66 points respectively, and in the last test the power was 0.96 for 154 points. Altogether 385 points were recorded and correlation coefficients varied between 0.94 and 0.99 as shown in the table.

The power for the squared Brunt-Väisälä frequency was thus in all cases found to be a little less than one.

Fig. 7 further illustrates that and shows the calculated best fit obtained from the regression analysis for all 5 tests performed, and the correlation coefficients. Further it is indicated that two types of grids, one horizontal and one vertical are used with different oscillating frequencies, and it is observed that the diffusion coefficient for both types of grids increases with increasing oscillation frequency.

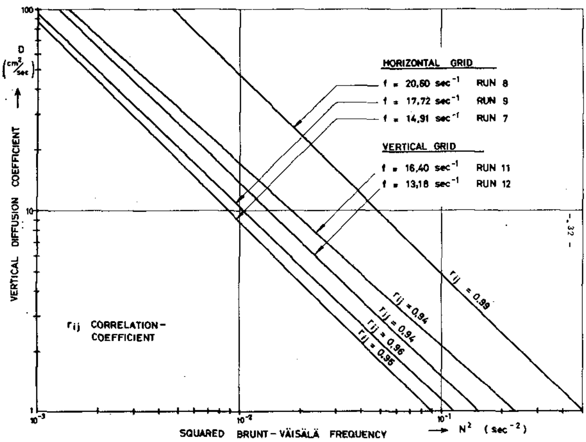

Fig. 7. Results of regression analysis. Diffusion coefficients as functions of Brunt-Väisälä frequencies.

The next step is then to relate the obtained results to the turbulence that acted in the test tank.

DESCRIPTION OF TURBULENCE

It is well known that if u denotes the velocity fluctuation in the turbulence then the scalar energy spectrum is given by equation (8), where κ is the wave number.

$$\overline{u^2} = 2 \int_0^\infty E(\kappa)\, d\kappa \qquad (8)$$

We can then form a Reynolds number consisting of the root-mean-square of the velocity fluctuations multiplied by a characteristic length scale for the eddies l and divided by the kinematic viscosity (Eq. (8)).

$$Re = \frac{(\overline{u^2})^{\frac{1}{2}} \cdot l}{\nu} \qquad (9)$$

Unfortunately it was not possible to make direct measurements of the turbulence when the tests were performed. A first estimate of the turbulence parameters is therefore extracted from the sinusoidal oscillation of the agitating grid. In

Fig. 8 one of the bars in the grid is shown in the mean position and in positions with maximum amplitudes, where the velocity is zero. The streamlines according to potential flow theory are also shown for the case where the oscillating velocity is maximum.

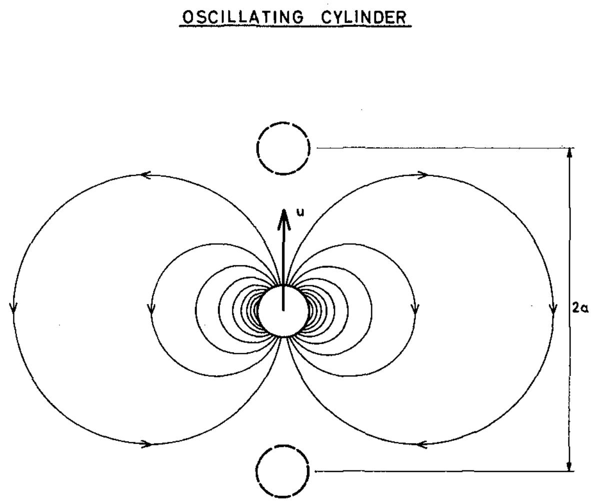

Fig. 8. Oscillating cylinder.

It is believed that it is the streamlines in this situation that dominate the flow pattern, as the velocity becomes smaller and the circles decrease near the amplitude maximum. Therefore as a first estimate the characteristic length of the eddies l is taken to twice the amplitude, a.

$$l = 2a \tag{10}$$

The validity of this approach to the macro-length scale is dependent on the Reynolds numbers for the oscillating cylinder. It will not be possible to obtain a better estimate without access to experimental data. Eddie shedding will occur from the back-side of the cylinder, but l is defined as the maximum length in which velocities can be correlated and it is therefore equation (10) and not the scale of the smaller eddies that is the best approximation for the scale of turbulence.

Further as a first approximation to the root mean square of the turbulent fluctuations the root mean square of grid velocity is taken as outlined in equation (11). ω is here the cyclic frequency in the oscillation. This is a reasonable first estimation as the added mass coefficient for an accelerated cylinder is near to one.

$$(\overline{u^2})^{\frac{1}{2}} = [\frac{1}{T} \int_0^T a^2 \omega^2 \sin^2(\omega t)\, dt]^{\frac{1}{2}} = \frac{\sqrt{2}}{2} a\omega \qquad (11)$$

It is now possible to form the characteristic Reynolds numbers describing the turbulence. When the result for the root mean square of the velocity fluctuations and the characteristic length scale is set into equation (8) we obtain:

$$Re = \frac{(\overline{u^2})^{\frac{1}{2}} \cdot l}{\nu} = \frac{\sqrt{2}\, a^2\omega}{\nu} \qquad (12)$$

In the experiments this Reynolds number was varied from $1 \cdot 10^4$ to $1.6 \cdot 10^4$, which indicates that a well developed turbulence was obtained.

It is possible to obtain a dimensionless parameter that describes the process, simply by forming the ratio between the stability frequency (the Brunt-Väisälä frequency N) and the agitating cyclic frequency ω.

$$\theta = \frac{N}{\omega} \qquad (13)$$

All data for diffusion coefficients obtained in 3 different tests with the horizontal grid and with 3 different agitating frequencies were then correlated with this dimensionless number and presented in a dimensionless form, so that the ratio between diffusion coefficient and the kinematic viscosity is given. The result is shown in Fig. 9.

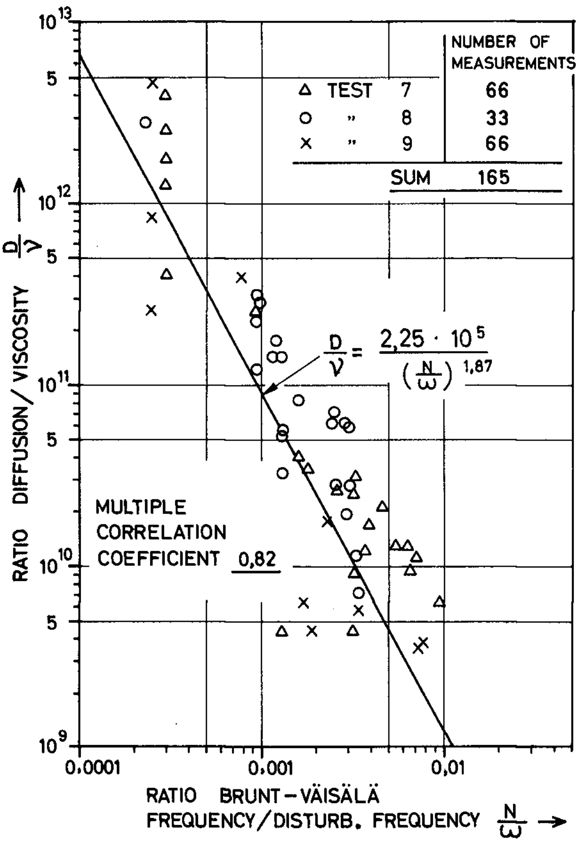

Fig. 9. Diffusion coefficients as a function of the ratio between stabilizing and agitating frequencies.

All data in the 3 different tests, 165 altogether, correlated with a multiple correlation frequency 0.82 and the equation obtained was:

$$\frac{D}{\nu} = \frac{2.25 \cdot 10^5}{\theta^{1.87}} = \frac{\text{CONSTANT}}{(N/\omega)^{1.87}} \qquad (14)$$

The ratio between the diffusion coefficient and the kinematic viscosity can thus be expressed as a constant divided by the frequency ratio to the power 1.87.

A typical order of magnitude for the diffusion coefficients involved here is $10\ cm^2/sec$.

EXTENSION TO CASE INCLUDING ADVECTION

The general equation for three-dimensional diffusion with varying diffusion coefficients is:

$$\frac{\partial s}{\partial t} + U_x \frac{\partial s}{\partial x} + U_y \frac{\partial s}{\partial y} + U_z \frac{\partial s}{\partial z} = \frac{\partial}{\partial x}\left(D_x \cdot \frac{\partial s}{\partial x}\right) +$$

$$\frac{\partial}{\partial y}\left(D_y \cdot \frac{\partial s}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \cdot \frac{\partial s}{\partial z}\right) \quad (15)$$

Here x is the vertical coordinate while y and z are horizontal coordinates. If advection in one direction dominates, as in the case in many estuaries with wind driven circulation, we obtain:

$$\frac{\partial s}{\partial t} + U_y \frac{\partial s}{\partial y} = \frac{\partial}{\partial x}\left(D_x \frac{\partial s}{\partial x}\right) \quad (16)$$

Horizontal diffusion terms might be included here on the left side as a constant or as a function of space coordinates. For the vertical diffusion coefficient we can then obtain:

$$D_x = \frac{\int_o^x \frac{\partial s}{\partial t}\, dx + \int_o^x U_y \frac{\partial s}{\partial y} \cdot dx}{\frac{\partial s}{\partial x}} \quad (17)$$

If the current velocity is recorded the algorithm can then be extended and operated for a case with advection.

Field data in the form of density profiles, current profiles and wind, tide and wave recordings have already been collected from a typical Norwegian fjord which has been found suitable for further studies. This is the Romsdalsfjord earlier mentioned and shown in Fig. 1.

Use of the algorithm on the field data obtained here is in progress.

CONCLUSION

The purpose of this project was to develop a mathematical method that is able to treat the case of vertical diffusion with a diffusion coefficient varying with time and dept.

This was done and a computer programme was developed for the one-dimensional case without advection.

Model experiments were performed to test the algorithm. The results from these showed that the ratio between the stabilizing Brunt-Väisälä frequency and the agitating cyclic frequency was a governing parameter for the system and dimensionless diffusion coefficients could be expressed as a funtion of this parameter.

The algorithm can easily be extended to include advection, and is therefore usefull also for the treatment of field data in more complex situations.

This extension can be made step by step, and might include more and more terms in the general equation for diffusion in space and time with variable diffusion coefficients.

Further knowledge concerning development and decay of turbulence in the presence of a density profile is urgently needed.

ACKNOWLEDGEMENT

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REFERENCE

[1] H. Rye 1973: " Wind currents in the Langfjord Norway". Division of Port and Ocean Engineering. The Norwegian Institute of Technology, Trondheim.