NUMERICAL SIMULATION OF FREE SURFACE THERMALLY-INFLUENCED FLOWS FOR NONHOMOGENEOUS FLUIDS

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Abstract. In this paper a finite difference technique is presented to simulate the behavior of natural water bodies under the influence of pollutants and temperature differences.

The mathematical model which has been discretized is the closed system obtained by combining the Navier-Stokes equations, the heat transfer equation, the diffusion equations, and an equation relating fluid density to both the chemical concentration and the temperature.

The numerical method is based on the Marker-and-Cell method which has been extended to consider the volume expansion due to heat transfer and the density variations.
1. Introduction

Several numerical methods for simulation of density varying induced flows have been developed in the last few years. Spraggs and Street [1975] developed a numerical model capable of representing complex physical behavior such as stratification and thermally unstable flows. Roberts and Street [1975] studied a simplified two-dimensional numerical model for the same complex situation. A finite difference model for flow simulation in estuaries has been widely discussed by Caponi [1976]. Findikakis, Franzini and Street [1978] used the finite element method for simulation of stratified turbulent flows in closed water bodies. All these models have used the Boussinesq approximation for the density. Such an approximation simplifies the model in the case of small density variations. However, this is not always the case physically. The purpose of this paper is to introduce a finite difference model for thermally-influenced flows in nonhomogeneous fluids which does not require the Boussinesq approximation in the mathematical model and is, therefore, of more general applicability.

2. Governing Equations

The governing equations for thermally-influenced flows in nonhomogeneous fluids are derived from the principle of conservation of momentum, mass, chemical constituents and heat. Such equations (see Yih [1965]) are the following.
The Navier-Stokes equations of motion:

\[
\rho \frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} + \rho X_1 + \mu \frac{1}{3} \frac{\partial}{\partial x_i} \left( \frac{\partial u_i}{\partial x_j} \right) + \mu \nabla^2 u_i
\]

where \( \rho \) is the density of the fluid, \( u_i \) is a velocity component, \( p \) is the pressure, \( X_1 \) is a body force component, and \( \mu \) is the viscosity assumed to be constant. In (1), repeated indices in one term indicate summation.

The equation of heat transfer is

\[
\frac{dT}{Dt} + T \frac{\partial u_i}{\partial x_i} = \tau \nabla^2 T
\]

where \( T \) is the temperature and \( \tau \) is the thermal diffusivity.

The diffusion equation for each chemical constituent is given by

\[
\frac{Dc^k}{Dt} + c^k \frac{\partial u_i}{\partial x_i} = \tau_k \nabla^2 c^k
\]

where \( c^k \) is the concentration of the \( k \)th constituent, and \( \tau_k \) is the mass diffusivity.

The continuity equation for this model is given by

\[
\frac{Dc}{Dt} + \rho \frac{\partial u_i}{\partial x_i} = \sum_k \tau_k \nabla^2 c^k
\]

The equation relating fluid density to both the temperature and the chemical concentration is

\[
\rho = \rho_0 \left[ 1 - \alpha(T-T_0) \right] + \sum_k (c^k - c_0^k)
\]
where $\alpha$ is the coefficient of expansion, and $\rho_0$ is the density at temperature $T_0$ and concentration $c_0^k$.

From (3) and (4) it follows that

$$\frac{D}{Dt} \left( \rho - \sum_k c_k \right) + \left( \rho - \sum_k c_k \right) \frac{\partial u}{\partial x} = 0.$$  

(6)

Now, substituting (5) in (6) we have

$$\rho_0^k \left[ \frac{\partial T}{\partial t} + T \frac{\partial u}{\partial x} \right] = \rho_0^k \left[ 1 + \alpha T_0 - \frac{1}{\rho_0^k} \sum_k c_0^k \right] \frac{\partial u}{\partial x}$$

Using (2), equation (7) becomes

$$\frac{\partial u}{\partial x} = \gamma v^2 T$$  

(8)

where

$$\gamma = \frac{\alpha \tau}{1 + \alpha T_0 - \frac{1}{\rho_0^k} \sum_k c_0^k}$$

Equation (8) now will take the place of continuity equation (4), so the mathematical model (1), (2), (3), (5) and (8), written out in full in two dimensions, is

$$\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = -\nabla P - \rho \mathbf{g} + \frac{\eta}{\rho} \frac{\partial \mathbf{u}}{\partial t} \nabla^2 \mathbf{u} + \nabla \cdot \tau$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{v} + v \frac{\partial \mathbf{v}}{\partial y} \right] = \frac{\partial P}{\partial y} - \rho \mathbf{g} + \frac{\eta}{\rho} \frac{\partial \mathbf{v}}{\partial t} \nabla^2 \mathbf{v} + \nabla \cdot \tau$$

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = -\gamma c \nabla^2 T + \nabla \cdot \mathbf{c}$$

$$\frac{\partial \mathbf{u}}{\partial x} + \frac{\partial \mathbf{v}}{\partial y} = \gamma v^2 T$$

$$\rho = \rho_0 \left[ 1 - \alpha(T - T_0) \right] + \sum_k \left( c_k - c_0^k \right)$$

$$\sum_k \left( c_k - c_0^k \right)$$
When the free surface can be represented as a single valued function
\[ y = h(x, t) \] (see Chan and Street [1970]), the change in the surface elevation is determined by the kinematic condition

\[ \frac{\partial h}{\partial t} = v_s - u_s \frac{\partial h}{\partial x} \]

where \( u_s \) and \( v_s \) are the components of the velocity at the fluid surface.

3. The Equations of Motion.

The finite difference scheme which discretizes model (9) is based on the Marker-and-Cell (MAC) method (see Harlow and Welch [1965]).

The finite difference mesh consists of rectangular cells of width \( \Delta x \) and height \( \Delta y \). The field variables \( u, v, P, T \) and \( c^k \) are defined at the locations shown in fig. 1: \( u \)-velocity at center of each vertical side of a cell, \( v \)-velocity at center of each horizontal side, while pressure \( P \), temperature \( T \), and concentrations \( c^k \) are defined at each cell center.

\[
\begin{array}{c|c|c|c}
\text{\( u_{i} - \frac{1}{2} j \)} & \text{\( v_{ij} + \frac{1}{2} \)} & \text{\( P_{ij}, T_{ij}, c_{ij}^{k} \)} & \text{\( u_{i} + \frac{1}{2} j \)} \\
\hline
\text{\( v_{ij} - \frac{1}{2} \)} & \text{\( \ldots \)} & \text{\( \ldots \)} & \text{\( \ldots \)}
\end{array}
\]

Fig. 1: Position of field variables

The finite difference equations corresponding to the first two equations of system (9), that is to the equations of motion, are

\[ \begin{align*}
u_t + u \nu_x + v \nu_y = & \frac{1}{\rho} \left[ -\frac{\partial P}{\partial x} + \frac{\mu}{3} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \right] + \mu (\nu_x + \nu_y) \\
v_t + u \nu_x + v \nu_y = & \frac{1}{\rho} \left[ -\frac{\partial P}{\partial y} + \frac{\mu}{3} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \right] + \mu (\nu_x + \nu_y)
\end{align*} \]
where

\[ \dot{u}_t = \frac{u_{n+1}^{i+1/2j} - u_n^{i+1/2j}}{\Delta t} \]

\[ u \dot{u}_x = u^n_{i+1/2j} \frac{u^n_{i+1/2j} - u^n_{i-1/2j}}{\Delta x} \quad \text{if} \quad u^n_{i+1/2j} > 0 \]

\[ u \dot{u}_x = u^n_{i+1/2j} \frac{u^n_{i+1/2j} - u^n_{i+1/2j-1}}{\Delta x} \quad \text{if} \quad u^n_{i+1/2j} < 0 \]

\[ v \dot{u}_y = v^n_{i+1/2j} \frac{u^n_{i+1/2j} - u^n_{i+1/2j-1}}{\Delta y} \quad \text{if} \quad v^n_{i+1/2j} > 0 \]

\[ v \dot{u}_y = v^n_{i+1/2j} \frac{u^n_{i+1/2j+1} - u^n_{i+1/2j}}{\Delta y} \quad \text{if} \quad v^n_{i+1/2j} < 0 \]

\[ \dot{p}_x = \frac{\rho^{n+1}_{i+1/2j} - \rho^n_{i+1/2j}}{\Delta x} \]

\[ \hat{u}_{xx} + \hat{u}_{yy} = \frac{u^n_{i+3/2j} - 2u^n_{i+1/2j} + u^n_{i-1/2j}}{(\Delta x)^2} + \frac{u^n_{i+1/2j+1} - 2u^n_{i+1/2j} + u^n_{i+1/2j-1}}{(\Delta y)^2} \]

\[ \hat{p}_{xxx} = \frac{T^n_{i+2j} - 3T^n_{i+1j} + 3T^n_{i+1j-1} - T^n_{i+1j-1}}{(\Delta x)^3} \]

\[ \hat{T}_{yy} = \frac{T^n_{i+1j+1} + 2T^n_{i+1j} + T^n_{i+1j-1} - T^n_{i+1j-1}}{(\Delta y)^2} - \frac{T^n_{i+1j-1}}{\Delta x} \]

Similarly

\[ \dot{v}_t = \frac{v_{n+1}^{ij+1/2} - v^n_{ij+1/2}}{\Delta t} \]

\[ v \dot{v}_x = v^n_{ij+1/2} \frac{v^n_{ij+1/2} - v^n_{i-1j+1/2}}{\Delta x} \quad \text{if} \quad v^n_{ij+1/2} > 0 \]

\[ v \dot{v}_x = v^n_{ij+1/2} \frac{v^n_{ij+1/2} - v^n_{i+1j+1/2}}{\Delta x} \quad \text{if} \quad v^n_{ij+1/2} < 0 \]
\[ v_{ij+\frac{1}{2}} = \frac{v_{ij+1}^n - v_{ij}^n}{\Delta y} \] if \( v_{ij+\frac{1}{2}}^n \geq 0 \)

\[ v_{ij+\frac{1}{2}} = \frac{v_{ij}^n - v_{ij+1}^n}{\Delta y} \] if \( v_{ij+\frac{1}{2}}^n < 0 \)

\[ \begin{align*}
\hat{v}_x & = \frac{p_{ij+1}^{n+1} - p_{ij}^{n+1}}{\Delta y} \\
\hat{v}_y & = \frac{p_{ij+1}^{n+1} - p_{ij}^{n+1}}{\Delta y}
\end{align*} \]

\[ \hat{v}_{xx} + \hat{v}_{yy} = \frac{v_{i+1,j+1}^n - 2v_{i,j+1}^n + v_{i-1,j+1}^n}{(\Delta x)^2} + \frac{v_{i+1,j}^n - 2v_{i,j+1}^n + v_{i-1,j}^n}{(\Delta y)^2} \]

\[ \frac{\hat{T}_{i+1,j+1} - 2\hat{T}_{i,j} + \hat{T}_{i-1,j+1}}{(\Delta x)^2} + \frac{\hat{T}_{i+1,j+1} - 2\hat{T}_{i,j} + \hat{T}_{i-1,j+1}}{(\Delta y)^2} \]

\[ \hat{T}_{i,j+1}^n - 3\hat{T}_{i,j}^n + 3\hat{T}_{i,j-1}^n - \hat{T}_{i,j}^n \]

In the previous notation the discrete variables \( u_{i,ij+\frac{1}{2}}, v_{i,ij+\frac{1}{2}}, \rho_{i,ij+\frac{1}{2}} \) and \( \rho_{i,ij+\frac{1}{2}} \) are not defined (see fig. 1). Therefore, a simple average from the closest scalar grid points is to be used.


The finite difference equation for the heat transfer is simply given by

\[ \hat{T}_t + u_{ij} \hat{T}_x + v_{ij} \hat{T}_y = (\tau - \gamma T) \left( \hat{T}_{xx} + \hat{T}_{yy} \right) \]

where

\[ \hat{T}_t = \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} \]

\[ u_{ij} \hat{T}_x = u_{ij} \frac{T_{i+1,j}^n - T_{i-1,j}^n}{\Delta x} \] if \( u_{ij} > 0 \)
Again, the discrete variables $u_{ij}^n$ and $v_{ij}^n$ are not defined, and then a simple average from the closest scalar grid points is used.

Similarly, the finite difference equations for the diffusion equations are given by

\begin{equation}
\hat{c}_t^k + u \hat{c}_x^k + v \hat{c}_y^k = -\gamma \ c_k (\hat{T}_{xx} + \hat{T}_{yy}) + \tau_k (\hat{c}_{xx}^k + \hat{c}_{yy}^k)
\end{equation}

where

\begin{align*}
\hat{c}_t^k &= \frac{c_{ij}^{k+1} - c_{ij}^k}{\Delta t} \\
\hat{c}_x^k &= u_{ij} \frac{c_{i+1j}^k - c_{ij}^k}{\Delta x} \\
\hat{c}_y^k &= v_{ij} \frac{c_{ij+1}^k - c_{ij}^k}{\Delta y} \\
\hat{T}_{xx} &= \frac{T_{ij+1}^n - 2T_{ij}^n + T_{ij-1}^n}{(\Delta x)^2} + \frac{T_{ij+1}^n - 2T_{ij}^n + T_{ij-1}^n}{(\Delta y)^2}
\end{align*}
The terms \( \hat{T}_{xx} \) and \( \hat{T}_{yy} \) and the discrete variables \( u_{ij}^n \) and \( v_{ij}^n \) are defined as in the heat transfer equation.

5. Pressure Evaluation.

The finite difference equation corresponding to the fifth equation of system (9), that is, to the continuity equation, in each cell is given by

\[
\frac{u_{ij+1}^{n+1} - u_{ij-1}^{n+1}}{\Delta x} + \frac{v_{ij+1}^{n+1} - v_{ij-1}^{n+1}}{\Delta y} = \frac{\gamma (T_{xx}^{n+1} + T_{yy}^{n+1})}{\Delta t}
\]

As it is done in the MAC method, the pressure field \( p_{ij}^{n+1} \) at center of each cell must be computed in such a way that the discrete continuity equation (14) will be satisfied throughout.

Equation (14) in the MAC method, as well as in all the models using the Boussinesq approximation, has the right-hand side equal to zero.

To find a finite difference equation for the pressure, we assume that the velocities computed with (11) satisfy equation (14).

First define

\[
P_{ij+\frac{1}{2}}^1 = u_{ij+\frac{1}{2}}^n - \frac{\Delta t}{\rho_{ij+\frac{1}{2}}} (u_{ij+\frac{1}{2}} + v_{ij+\frac{1}{2}}) - \frac{\gamma (T_{xx} + T_{yy})}{\rho} (u_{ij+\frac{1}{2}} + v_{ij+\frac{1}{2}}) + g
\]

so that the finite difference equations (11) can be written in the following way

\[
\begin{align*}
\frac{u_{ij+\frac{1}{2}}^{n+1} - u_{ij-\frac{1}{2}}^{n+1}}{\Delta x} &= \frac{\Delta t}{\rho_{ij+\frac{1}{2}}} p_{ij+\frac{1}{2}}^{n+1} - p_{ij-\frac{1}{2}}^{n+1} \\
\frac{v_{ij+\frac{1}{2}}^{n+1} - v_{ij-\frac{1}{2}}^{n+1}}{\Delta y} &= \frac{\gamma (T_{xx} + T_{yy})}{\Delta t} p_{ij+\frac{1}{2}}^{n+1} - p_{ij-\frac{1}{2}}^{n+1}
\end{align*}
\]
Now, by substituting (15) in (14), we obtain the following finite
difference equation for pressure

\[
\frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{(\Delta x)^2 \rho_{i+1,j}} - \frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{(\Delta x)^2 \rho_{i,j}} + \frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{(\Delta y)^2 \rho_{i,j+1}} - \frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{(\Delta y)^2 \rho_{i,j+1}} =
\]

\[
\frac{F_{i+1,j}^{n+1} - F_{i,j}^{n+1}}{\Delta t \Delta x} + \frac{F_{i,j+1}^{n+1} - F_{i,j}^{n+1}}{\Delta t \Delta y} - \frac{\gamma}{\Delta t} \left( T_{xx}^{n+1} + T_{yy}^{n+1} \right)
\]

(16)

Equation (16), for constants \( c^k \) and \( T \), reduces to the finite
differences Poisson equation used in the MAC method to evaluate the pressure.

Equation (16), at each time step, is solved by an iterative algorithm
(see e.g. Nichols and Hirt [1973]) that adjusts the velocities through
changes in the pressure field. So if \( \delta p_{ij} \) denotes the pressure change in
cell \((i,j)\), according to equation (15), each velocity component specified
on the sides of cell \((i,j)\) is adjusted in the following way:

\[
u_{i+\frac{1}{2},j}^{n+1} = u_{i+\frac{1}{2},j}^{n+1} + \frac{\Delta t}{\rho_{i+\frac{1}{2},j}} \frac{\delta p_{ij}}{\Delta x}
\]

\[
v_{i-\frac{1}{2},j}^{n+1} = v_{i-\frac{1}{2},j}^{n+1} - \frac{\Delta t}{\rho_{i-\frac{1}{2},j}} \frac{\delta p_{ij}}{\Delta y}
\]

(17)

\[
u_{i,j+\frac{1}{2}}^{n+1} = v_{i,j+\frac{1}{2}}^{n+1} + \frac{\Delta t}{\rho_{i,j+\frac{1}{2}}} \frac{\delta p_{ij}}{\Delta y}
\]

\[
u_{i,j-\frac{1}{2}}^{n+1} = v_{i,j-\frac{1}{2}}^{n+1} - \frac{\Delta t}{\rho_{i,j-\frac{1}{2}}} \frac{\delta p_{ij}}{\Delta y}
\]
The expression for $\delta P_{ij}$ is derived by substituting the right-hand sides of equations (17) into the discrete continuity equation (14), and solving for $\delta P_{ij}$:

$$
\delta P_{ij} = -\frac{u_{i+1/2,j}^{n+1} - u_{i-1/2,j}^{n+1} + v_{i,j+1/2}^{n+1} - v_{i,j-1/2}^{n+1}}{\Delta x} \frac{\Delta x}{\rho_{i-1/2,j}^{n} + \Delta y} + \frac{\Delta y}{\rho_{i,j+1/2}^{n}} - \gamma(T_{x}^{n}T_{y}^{n+1}) \frac{1}{(\Delta x)^{2}} \frac{1}{\rho_{i-1/2,j}^{n}} + \frac{1}{(\Delta y)^{2}} \frac{1}{\rho_{i,j+1/2}^{n}}
$$

As a starting point for the iterative procedure, the intermediate velocities are taken by an explicit calculation from equations (15) that uses the previous-time velocities and pressure:

$$
\begin{align*}
\hat{u}_{i+1/2,j}^{n+1} &= \frac{1}{\rho_{i+1/2,j}^{n}} - \frac{\Delta t}{\rho_{i+1/2,j}^{n}} p_{i+1,j}^{n} - p_{i,j}^{n} \\
\hat{v}_{i,j+1/2}^{n+1} &= \frac{1}{\rho_{i,j+1/2}^{n}} - \frac{\Delta t}{\rho_{i,j+1/2}^{n}} p_{i,j+1}^{n} - p_{i,j}^{n}
\end{align*}
$$

Often, convergence of iteration can be accelerated by multiplying $\delta P_{ij}$ by an over-relaxation factor, which should not be larger than 2.


A finite difference scheme that discretizes the free surface equation (10), allowing for the proper boundary conditions (see Bulgarelli, Casulli and Greenspan [1980]), is the Courant-Isaacson and Rees method, which is implemented as follows. The surface height $h_{i+1/2}^{n}$ is defined on the sides of each vertical grid line, and the equation (10) is discretized in the following way:

$$
\hat{h}_{t} = v_{s} - u_{s} \hat{h}_{x}
$$
where

\[ h_{t}^{n} = \frac{h_{i+\frac{1}{2}}^{n+1} - h_{i+\frac{1}{2}}^{n}}{\Delta t} \]

\[ u_{s}^{n} \hat{h}_{x} = u_{s}^{n} \frac{h_{i+\frac{3}{2}}^{n} - h_{i+\frac{1}{2}}^{n}}{\Delta x} \text{ if } u_{s}^{n} > 0 \]

\[ u_{s}^{n} \hat{h}_{x} = u_{s}^{n} \frac{h_{i+\frac{1}{2}}^{n} - h_{i-\frac{1}{2}}^{n}}{\Delta x} \text{ if } u_{s}^{n} < 0 \]

The coefficients \( u_{s}^{n} \) and \( v_{s}^{n} \) are obtained as a weighted average of the four nearest cell velocities.

7. Boundary Conditions.

The solution to model (9)-(10) for any particular problem requires the specification of an appropriate set of initial and boundary conditions. Here the rigid bottom and the lateral boundaries will be considered fixed in time and impenetrable. Another simplifying assumption made here is that the lateral boundaries fall on sides of computational cells, while the rigid curved bottom and the free surface have a slope small enough that the direction of the y-axis is a good approximation for the direction of any normal vector to these boundaries (see fig. 2).

Under these assumptions, the boundary conditions for the motion equations on the rigid boundaries are given by assigning a value zero to the velocity orthogonal to the boundaries, and the tangential velocity is defined by giving a free slip boundary condition, that is:
\[
\frac{\partial v}{\partial x} = 0 \quad \text{on the lateral boundaries}
\]

(21)

\[
\frac{\partial u}{\partial y} = 0 \quad \text{on the bottom}.
\]

On the free surface, we take

\[
P = P_a + 2\mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \gamma v^2 T
\]

(22)

\[
\mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) = 0
\]

where \( P_a \) is the applied pressure on the free surface.

Forced flow through the rigid boundaries can be simulated by assigning to the velocity field values other than zero on the boundaries.

Fig. 2: The mesh region.

Boundary conditions (21) and (22) are easily discretized on the boundaries.
Care must be taken for the pressure boundary condition on the rigid curved bottom. Equation (14) can be written also as

\[
(23) \quad u_{i+1/2j}^{n+1} \Delta y - u_{i-1/2j}^{n+1} \Delta y + v_{ij+1/2}^{n+1} \Delta x - v_{ij-1/2}^{n+1} \Delta x = y(T_{xx}^{n+1} + T_{yy}^{n+1}) \Delta x \Delta y
\]

which has the following meaning: the rate of volume accumulation in a cell must balance the rate of volume expansion due to temperature differences.

Now, let us apply the same principle to a cell crossed by the curved bottom. With reference to fig. 3, the analogue of the discrete continuity equation (23) in such cells is given by

\[
(24) \quad u_{i+1/2j}^{n+1} \zeta_{i+1/2} - u_{i-1/2j}^{n+1} \zeta_{i-1/2} + v_{ij+1/2}^{n+1} \Delta x = y(T_{xx}^{n+1} + T_{yy}^{n+1}) \Delta x \frac{\zeta_{i+1/2} - \zeta_{i-1/2}}{2}
\]

Equation (24) states, also, that no fluid flux is permitted through the curved bottom.

Fig. 3: Bottom configuration.
The finite difference equation for pressure in a bottom cell is obtained by substituting (15) in (24):

\[
\begin{align*}
\frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{\Delta x \rho_{i+1/2,j}} - \frac{p_{i-1,j}^{n+1} - p_{i,j}^{n+1}}{\Delta x \rho_{i-1/2,j}} &\approx \frac{\Delta x}{\Delta y} \left( \frac{\partial^2 p}{\partial y^2} \right)_{i,j} \\
\frac{p_{i,j}^{n+1} - p_{i,j}^{n+1}}{\Delta y} &\approx \frac{\Delta x}{\Delta y} \left( \frac{\partial^2 p}{\partial x^2} \right)_{i,j} \\
\frac{p_{i,j}^{n+1} - p_{i,j}^{n+1}}{\Delta x} &\approx \frac{\Delta x}{\Delta y} \left( \frac{\partial^2 p}{\partial x \partial y} \right)_{i,j}
\end{align*}
\]

(25)

\[
\frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{\Delta x \rho_{i+1/2,j}} - \frac{p_{i,j}^{n+1} - p_{i-1,j}^{n+1}}{\Delta x \rho_{i-1/2,j}} = \frac{\gamma}{\Delta t} \left( \frac{T_{x}^{n+1} + T_{y}^{n+1}}{2} \right) \Delta x \left( \frac{\partial^2 p}{\partial x^2} \right)_{i,j} + \frac{\partial^2 p}{\partial y^2} \left( \frac{\partial^2 p}{\partial x \partial y} \right)_{i,j}
\]

The iterative algorithm for pressure evaluation on bottom cells must compute the pressure change for \( \delta P_{i,j} \) by substituting equations (17) in (24), and then must adjust each velocity component specified on the sides of such cells.

The boundary conditions for the heat transfer equation and for the diffusion equations are simply given by assigning the temperature and the chemical concentration as functions of time on those boundaries through which a flux of temperature and chemicals is allowed. On those boundaries through which no flux of temperature and chemicals is permitted, the corresponding normal derivative must vanish.

8. Stability Considerations. A rigorous stability analysis for this numerical model is an open problem. From an heuristic point of view, analyzing the convective and the diffusive terms only, we get the following restrictions for the time step \( \Delta t \) (see Roache [1972]):

\[
\Delta t \leq \min_{u,v} \left[ \frac{|u|}{\Delta x} + \frac{|v|}{\Delta y} + 2 \frac{u}{\rho} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)^{-1} \right]^{-1}
\]

(26)
where $\lambda$ is the maximum wave speed. The last condition is the so-called surface wave condition due to the presence of the free surface of the fluid.

The use of the forward and backward finite differences to discretize the convective terms in equations (9) and (10) permits the method to remain stable even in absence of diffusive terms.


The fluid flow is advanced by a series of time steps which begin from the initial data

$$u(x,y,t_0) = u_1(x,y)$$
$$v(x,y,t_0) = v_1(x,y)$$
$$T(x,y,t_0) = T_1(x,y)$$
$$c^k(x,y,t_0) = c^k_1(x,y)$$
$$h(x,t_0) = h_1(x).$$

Each time step consists of the following stages:

**Stage i** Determination of the intermediate values of the velocities
Fig. 4: Initial fluid configuration.
The time step is $\Delta t = 0.01$.

In the first example a chemical constituent at concentration $c = 0.5$ is present at all times on the lateral boundary near the bottom of the shallower side of the basin, and no heat sources are present in any part of the boundary.

Figures 5, 6, 7 and 8 show the development of the flow at times $t = 5$, $t = 10$, $t = 15$ and $t = 20$, respectively.

As expected, the flow, from the chemical source, follows the sloped bottom to bring the heavy chemical constituent down to the lowest part of the basin. A large eddy forms quickly, and is succeeded in time by two eddies, one on top of the other, developing a stratification phenomenon which should occur in this case.

A second run was made with all parameters the same except that the temperature $T = 1.0$ is assumed at the free surface. Figures 9, 10, 11 and 12 show the development of the flow for this example at times $t = 5$, $t = 10$, $t = 15$, and $t = 20$, respectively. An additional phenomenon occurs in this case: the fluid near the free surface becomes lighter and tends to remain on top generating a third eddy as shown in figure 12.

It is also important to note a slow increasing of the surface height due to the volume expansion caused by the heat source in this last example.

For the convenience of the interested reader, the precise computer results (velocities, temperature, concentrations and free surface height) obtained from this last run, are given in appendix B of the technical report by Casulli [1980].

The computations were performed on the IBM 370-155 of the University of Texas at Arlington.
Fig. 7: $t = 15$. 
ACKNOWLEDGMENT

I wish to express my gratitude to Donald Greenspan for his encouragement and useful suggestions for the development of this model.
APPENDIX A-FORTRAN PROGRAM

```
DIMENSION U(22,22), V(22,22), UN(22,22), VN(22,22), P(22,22), 
1J1(22), JB(22), HB(22), H(22), HN(22), R(22,22), VT(22,22)

INT(22,22), TN(22,22), C(22,22), CN(22,22)

INTEGER CYCLE
REAL NU

C INPUT AND OUTPUT DATAS
C
READ 2, IMAX, JMAX, DELX, DELY, DELT, NU, EPSI, OMG
READ 3, UZERO, VZERO, TZERO, RZERO, CZERO, ALPH, TAU, TAU1
PRINT 919, IMAX, JMAX, DELX, DELY, DELT, NU, EPSI, OMG
PRINT 929, UZERO, VZERO, TZERO, RZERO, CZERO, ALPH, TAU, TAU1
CWPRT=500.
TWFIN=20.

C COMPUTE CONSTANT TERMS AND INITIALIZE NECESSARY VARIABLES
C
GX=0.
GY=-9.81
CALL INT(IMAX, JMAX, DELX, DELY, PDX, RDX, RDY, S, IM1, UZERO, VZERO
1, RZERO, TZERO, CZERO, ALPH, U, V, P, R, T, C, VT)

C DETERMINE SLOPE BOUNDARY LOCATION
C
C COMPUTE INITIAL TOP CONFIGURATION
C
CALL SLOP(IMAX, DELX, DELY, RDX, RDY, H, HB, JT, JB)
TIME=0.0
ITER=0
CYCLE=0
CWPRT=CWPRT*DELT
GO TO 4280

C START CYCLE
C
1000 CONTINUE
C
C COMPUTE INTERMEDIATE U AND V
C
CALL COMUV(JT, JB, DELX, DELY, DELT, RDX, RDY, PDX, RDY, S, GX, GY, R, VT, U, V, UN, VN,
1, IM1)
CALL UVBND(IMAX, JMAX, IM1, S, DELY, RDX, RDY, VT, U, V, JT, JB)

C COMPUTE TEMPERATURE AND CONCENTRATION
C
C CALL COMIC(JT, JB, DELX, DELY, DELT, RDX, RDY, TAU1, S, UN, VN, C, CN, T, TN, VT,
1, IM1)
C CALL TCBND(IMAX, JMAX, JT, JB, IM1, T, C)
C CALL VTcal(1M1, DELX, DELY, TAU, JT, JB, T, VT)

C COMPUTE UPDATED CELL PRESSURE AND VELOCITIES
C
ITER=1
2000 CONTINUE
FLG=0.0
CALL PRESS(IM1, DELX, DELY, S, OMG, EPSI, FLG, NU, DELT, VT, R, U, V, P
1, HN, JT, JB, VN, HB, RLX, RDY)
CALL UVBND(IMAX, JMAX, IM1, S, DELY, RDX, VT, U, V, JT, JB)

C HAS CONVERGENCE BEEN REACHED
```
IF (FLG.EQ.0.) GO TO 4000
ITER=ITER+1
IF (ITER.LT.1000) GO TO 2000
TIME=1.E+10
4000 CONTINUE

CALL SURF(IM1,IMAX,DELX,DELY,DELT,RDX,RDY,HN,H,UN,VN,JT)

4280 CONTINUE
CALL TCBND(IMAX,JMAX,JB,IM1,T,C)
CALL VTCAL(IMAX,JMAX,IM1,S,DELY,RTX,VT,U,V,VT,VT)
CALL UVBND(IMAX,JMAX,IM1,S,DELY,RTX,VT,UT,VT,VT,VT)

IF (TIME.EQ.1) GO TO 5800
IF (TIME.EQ.1.E-3.LT.TWPRT) GO TO 6000
TWPRT=TWPRT+DELT
5800 CONTINUE

CALL LIST (ITER,TIME,CYCLE,IMAX,JB,UN,V,T,CH)
6000 CONTINUE
IF (TIME.GE.TWP1N) STOP

CALL SET(IMAX,JMAX,H,HN,UN,V,VT,TN,C,CN,R,ALPH,ZERO,TZERO,1,CZERO)

ADVANCE TIME T=TIME+DELT
CYCLE=CYCLE+1
GO TO 1000

2 FORMAT(2I10,6F10.5)
3 FORMAT(3F10.5)
919 FORMAT(1H1,' DATI: ',2I10,6F10.5)
929 FORMAT(' ',F10.5)

END
SUBROUTINE INIT (IMAX, JMAX, DELX, DELY, RDX, RDY, S, IM1, UZERO, VZERO)
DIMENSION U (22, 22), V (22, 22), P (22, 22), R (22, 22), T (22, 22)
I, C (22, 22), VT (22, 22)
IM1 = IMAX - 1
RDX = 1.0 / DELX
RDY = 1.0 / DELY
S = ALPH / (1. * ALPH + TZERO - CZERO / RZERO)
DO 1 I = 1, IMAX
DO 1 J = 1, JMAX
U (I, J) = UZERO
V (I, J) = VZERO
P (I, J) = 0.
R (I, J) = RZERO
T (I, J) = TZERO
C (I, J) = CZERO
VT (I, J) = 0.
1 CONTINUE
RETURN
END

SUBROUTINE SLOP (IMAX, DELX, DELY, RDX, RDY, H, HB, JT, JB)
DIMENSION H (1), HB (1), JT (1), JB (1)
HBHT = 0.0
HB (1) = HBHT + 4.0 * DELY
DO 240 I = 2, IMAX
HB (I) = HBHT + 4.0 * DELY - 0.5 * DELX * (I - 1)
IF (I.GE.9) HB (I) = HBHT
JT (I) = MAX 1.0 * RDX + 1.0 * E-5, HB (I - 1) * RDX + 1.0 * E-5) + 2
240 CONTINUE
JB (1) = JB (2)
FLHT = 2.0
DO 260 I = 2, IMAX
H (I) = FLHT
260 CONTINUE
JT (I) = INT (0.5 * (H (I) + H (I - 1)) * RDX + 1.0 * E-8) + 2
RETURN
END
SUBROUTINE COMUV (JT, JB, DELX, DELY, DELT, RX, RY, NU, S, GX, GY, R, VT, U, V, UN, VN, P, IM1)
DIMENSION R (22, 22), VT (22, 22), U (22, 22), V (22, 22), UN (22, 22), VN (22, 22)
1, P (22, 22), JT (1), JB (1)
REAL NU
DO 1100 I=2, IM1
JT1 = JT (I)
JB1 = JB (I)
DO 1100 J = JB1, JT1
IF (UN (I, J) * GE. 0.) FXU = UN (I, J) * RDX * (UN (I, J) - UN (I - 1, J))
IF (UN (I, J) .LT. 0.) FXU = UN (I, J) * RDX * (UN (I + 1, J) - UN (I, J))
VV = (VN (I, J) + VN (I + 1, J) + VN (I, J - 1) + VN (I, J - 1)) / 4.
IF (VV .GE. 0.) FUY = VV * RDY * (UN (I, J) - UN (I, J - 1))
IF (VV .LT. 0.) FUY = VV * RDY * (VN (I, J + 1) - VN (I, J))
UU = (UN (I, J) + UN (I, J + 1) + UN (I - 1, J) + UN (I - 1, J + 1)) / 4.
IF (UU .GE. 0.) FXV = UU * RDX * (VN (I, J) - VN (I - 1, J))
IF (UU .LT. 0.) FXV = UU * REX * (VN (I + 1, J) - VN (I, J))
IF (VN (I, J) * GE. 0.) FVY = VN (I, J) * RDX * (VN (I, J) - VN (I, J - 1))
IF (VN (I, J) .LT. 0.) FVY = VN (I, J) * RDX * (VN (I, J) - VN (I, J + 1))
VVX = NU * ((UN (I + 1, J) - 2. * UN (I, J) + UN (I - 1, J)) / DELX**2 + 1.
(VN (I + 1, J) - 2. * VN (I, J) + VN (I - 1, J)) / DELX**2)
VVY = NU * ((VN (I + 1, J) - 2. * VN (I, J) + VN (I - 1, J)) / DELX**2 + 1.
VFX = VNX * FYX = FYX * (P (I, J) - P (I + 1, J)) * RDX / RX
VFY = VFY * (P (I, J) - P (I, J + 1)) * RDX / RX
1100 CONTINUE
RETURN
END

SUBROUTINE COMTC (JT, JB, DELX, DELY, DELT, RX, RY, NU, S, UN, VN, C, CN, T, TN, VT, IM1)
DIMENSION UN (22, 22), VN (22, 22), C (22, 22), CN (22, 22), T (22, 22),
TN (22, 22), VT (22, 22), JT (1), JB (1)
DO 1100 I = 2, IM1
JT1 = JT (I)
JB1 = JB (I)
DO 1100 J = JB1, JT1
UC = 0.5 * (UN (I, J) + UN (I - 1, J))
VC = 0.5 * (VN (I, J) + VN (I, J - 1))
IF (UC * GE. 0.) FTX = UC * RDX * (TN (I, J) - TN (I - 1, J))
IF (UC .LT. 0.) FTX = UC * RDX * (TN (I + 1, J) - TN (I, J))
IF (VC * GE. 0.) FTY = VC * RDY * (TN (I, J) - TN (I, J - 1))
IF (VC .LT. 0.) FTY = VC * RDY * (TN (I, J + 1) - TN (I, J))
T (I, J) = TN (I, J) - DELT * (FTX + FTY + (TN (I, J)) * S - 1.) + VT (I, J))
IF (UC * GE. 0.) FCX = UC * RDX * (CN (I, J) - CN (I - 1, J))
IF (UC .LT. 0.) FCX = UC * RDX * (CN (I + 1, J) - CN (I, J))
IF (VC .GE. 0.) FCY = VC * RDY * (CN (I, J) - CN (I, J - 1))
IF (VC .LT. 0.) FCY = VC * RDY * (CN (I, J + 1) - CN (I, J))
VC = TAU1 * (CN (I, J) + 2. * CN (I, J) + CN (I, J - 1)) / DELY**2
1 + (CN (I, J + 1) - 2. * CN (I, J) + CN (I, J - 1)) / DELY**2
C (I, J) = CN (I, J) - DELT * (FCX + FCY - VC + CN (I, J) * S * VT (I, J))
1100 CONTINUE
RETURN
END
SUBROUTINE PRESS (IM1, DELX, DELY, S, EPSI, FLG, NU, DELT, VT, R, U, V, P
1, HN, JT, JB, VN, HR, RDY, FDY)
DIMENSION JT(1), JB(1), VT (22, 22), R (22, 22), U (22, 22), V (22, 22),
1P (22, 22), HN (1), HB (1), VN (22, 22)
REAL NU
DO 3500 I=2, IM1
JT1=JT (I)
JB1=JB (I)
DO 3500 J=JB1, JT1
IF (J .EQ. JT1) GO TO 3100
IF (J .EQ. JB1) GO TO 3060
GO TO 3200
3060 CONTINUE
F1=DELY* (JB1-1) - HN (I-1)
F2=DELY* (JB1-1) - HN (I)
D=U (I, J) * F2 - U (I-1, J) * F1 + V (I, J) * DELX
Z = (F2/(R (I, J) * R (I+1, J))) * F1/(R (I-1, J)*R (I, J))/DELX
1 + DELX*RDY/(R (I, J) + R (I, J+1))
DELP = (S*VT (I, J) * DELX * 0.5 * (F1 + F2) - 0)/(2. * DELT * Z)
IF (ABS (S*VT (I, J) * 0.5 * (F1 + F2) / DELY - D*RDY*RDY) .GT. EPSI) FLG = 1.
GO TO 3300
3100 CONTINUE
PETA=DELY/ (0.5 * (HN (I) + HN (I-1)) - (FLOAT (JT1) - 2.5) * DELY)
DELP = (1.0 - PETA)* P (I, J-1) - P (I, J) * PETA * 2. * NU * (VN (I, J) - VN (I, J-1))
1*RDY-S*VT (I, J)/3.
GO TO 3300
3200 CONTINUE
D=RDY* (U (I, J) - U (I-1, J)) + RDY* (V (I, J) - V (I, J-1))
IF (ABS (D-S*VT (I, J)) .GT. EPSI) FLG = 1.
Z = (1. / (R (I, J) + R (I+1, J))) + 1. / (R (I-1, J) + R (I, J))] / DELX**2
R (I, J) = 1. /((R (I, J) + R (I, J+1)) + 1. / (R (I, J-1) + R (I, J)))/DELX**2
DELP-OMG* (S*VT (I, J) - E)/ (2. * DELT * Z)
3300 CONTINUE
P (I, J) = P (I, J) + DELP
U (I, J) = U (I, J) + DELT * RDY * DELP / (0.5 * (R (I, J) + R (I+1, J)))
U (I-1, J) = U (I-1, J) - DELT * RDY * DELP / (0.5 * (R (I-1, J) * R (I, J)))
V (I, J) = V (I, J) + DELT * RDY * DELP / (0.5 * (R (I, J) + R (I, J+1)))
V (I, J-1) = V (I, J-1) - DELT * RDY * DELP / (0.5 * (R (I, J-1) + R (I, J)))
3500 CONTINUE
RETURN
END
SUBROUTINE SURF(IM1, IMAX, DELX, DELY, DELT, RDX, RDY, HN, H, UN, VN, JT)
DIMENSION H(1), HN(1), JT(1), UN(22,22), VN(22,22)

DO 4100 I = 1, IM1
JT1=INT(HN(I) *RDY+1.E-8) + 2
HV=RDY*(HN(I)-FLOAT(JT1-2)*DELY)/2.
UN=UN(I, JT1)

JS1=JT (I+1)
VV=HV* (VN(I, JS1) + VN(I+1, JS1) ) + ( 0.5-HV) * (VN(I, JT1-1) + VN(I+1, JT1-1) )
IF (I.EQ.1) HX=0.
IF (I.EQ.1) GO To 4050
IF (UU.EQ.0.) HX=0.
IF (UU.GT.0.) HX=(HN(I)-HN(I-1)) *RDX
IF (UU.LT.0.) HX=(HN(I+1)-HN(I)) *RDX

4050 H(I) = HN(I) + DELT* (VV-UU*HX)

4100 CONTINUE
H(IMAX)=H(IM1)

C CALCULATE CELL IN WHICH SURFACE IS LOCATED AND UPDATE ARRAY

DO 4250 I=2, IM1
JT (I)=INT (0.5*(H (I) + H( I-1)))*RDY+1.E-8) + 2
4250 CONTINUE

JT (1)= JT (2)
JT (IMAX)= JT (IM1)
RETURN

END

SUBROUTINE LIST(ITER,TIME,CYCLE,IMAX, JT, JB, U, V, T, C, H)
DIMENSION JT(1), JB(1), H(1), U(22, 22), V(22, 22), T(22, 22), C(22, 22)
INTEGER CYCLE
PRINT 49, ITER, TIME, CYCLE
PRINT 47
DO 5900 I = 1, IMAX
JT=JT(I)
JB1=JB(I)
JT2=JT(I)+1
JB2=JB(I)-1
DO 5900 J=JB2, JT2
PRINT 48, I, J, U(I, J), V(I, J), T(I, J), C(I, J), H(I), JT1, JB1
5900 CONTINUE

47 FORMAT(//' , 3X,' I',' I', 2X,' J', 12X,' U', 17X,' V', 18X,' T', 18X,' C', 18X,' H'
      ,11X, 'S', ' B')

48 FORMAT(1X, I3, I3, 5(6X, 1PE12.5), 6X, 2I4)

49 FORMAT(1H1, 6X, ' ITER=', 15, 10X, ' TIME=', 1PE12.5, 10X, ' CYCLE=', 1X, I4)
RETURN
END
SUBROUTINE SET (IMAX, JMAX, H, HN, U, UN, V, VN, T, TN, C, CN, R, ALPH, RZERO)

DIMENSION H (1), HN (1), U (22, 22), UN (22, 22), V (22, 22), VN (22, 22)
1, T (22, 22), TN (22, 22), C (22, 22), CN (22, 22), R (22, 22)

DO 6100 I=1, IMAX

HN (I) = H (I)
DO 6100 J=1, JMAX
UN (I, J) = U (I, J)
VN (I, J) = V (I, J)
CN (I, J) = C (I, J)

TN (I, J) = T (I, J)
R (I, J) = RZERO*(1.0 - ALPH*(T (I, J) - TZERO)) + C (I, J) - CZERO

6100 CONTINUE
RETURN
END

SUBROUTINE UBVNC (IMAX, JMAX, IM1, S, DELY, RDX, VT, U, V, JT, JB)

DIMENSION JT (1), JB (1), U (22, 22), V (22, 22), VT (22, 22)

C
C SET VELOCITY BOUNDARY CONDITIONS
C

DO 2200 J=1, JMAX
U (1, J) = 0.0
V (1, J) = V (2, J)
U (IM1, J) = 0.0
V (IMAX, J) = V (IM1, J)

2200 CONTINUE

DO 2620 I=2, IM1
JT1 = JT (I)
JB1 = JB (I)
IF (JT (I+1), LT, JT (I)) U (I, JT1) = U (I, JT1-1)
V (I, JT1) = V (I, JT1-1) - DELY*RDY*(U (I, JT1) - U (I-1, JT1)) + DELY*S
1

IF (JB (I+1), LT, JB (I)) U (I, JB1) = U (I, JB1+1)
V (I, JB1-1) = V (I, JB1) + DELY*RDY*(U (I, JB1) - U (I-1, JB1)) - DELY*S
1

2620 CONTINUE

IM2 = IM1 -1

DO 2630 I=2, IM2
JT1 = JT (I)
IF (JT (I+1), LT, JT (I)) U (I, JT1) = U (I, JT1-1) - DELY*RDY*
1*(V (I+1, JT1-1) - V (I, JT1-1))

IF (JB (I+1), LT, JB (I)) V (I+1, JT1) = V (I+1, JT1-1)
U (I, JT1+1) = U (I, JT1) - DELY*RDY*(V (I+1, JT1) - V (I, JT1))

2630 CONTINUE

JT1 = JT (1)
JT2 = JT (IMAX)
V (1, JT1) = V (2, JT1)
V (IMAX, JT2) = V (IM1, JT2)
RETURN
END
SUBROUTINE TCEND(IMAX, JMAX, JT, JB, IM1, T, C)
DIMENSION JT(1), JB(1), T(22, 22), C(22, 22)

C C TEMPERATURE AND CONCENTRATION BOUNDARY CONDITIONS
C
DO 1200 J=1, JMAX
C (1, J) = C (2, J)
T (1, J) = T (2, J)
D (IMAX, J) = D (IM1, J)
1 (IMAX, J) = T (IM1, J)
1200 CONTINUE
DO 1300 I=1, IMAX
JT1 = JT (I)
JB1 = JB (I)
C (I, JT1+1) = C (I, JT1)
T (I, JT1+1) = T (I, JT1)
C (I, JB1-1) = C (I, JB1)
T (I, JB1-1) = T (I, JB1)
1300 CONTINUE
C C CONCENTRATION AND TEMPERATURE SPECIAL BOUNDARY CONDITIONS
C
JB1 = JB (1)
JB2 = JB1 + 1
C (1, JB1) = 0.5
C (1, JB2) = 0.5
DO 1350 I=1, IMAX
JT1 = JT (I) + 1
T (I, JT1) = 1.
1350 CONTINUE
RETURN
END

SUBROUTINE VTCLC(IM1, DELX, DELY, TAU, JT, JB, T, VT)
DIMENSION JT(1), JB(1), T(22, 22), VT(22, 22)

C C V1 CALCULATION
C
DO 1400 I=2, IM1
JT1 = JT (I)
JB1 = JB (I)
DO 1400 J=JB1, JT1
VT (I, J) = TAU * ((T (I+1, J) - 2. * T (I, J) + T (I-1, J)) / DELX**2
1 + (T (I, J+1) - 2. * T (I, J) + T (I, J-1)) / DELY**2)
1400 CONTINUE
RETURN
END
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<th>N</th>
<th>V</th>
<th>T</th>
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