

行政院國家科學委員會特約研究專題結案（完整）報告

非線性三維河口污染物擴散模式之研究-速度／渦度法（3/3）

Nonlinear 3D Mathematical Modeling of Pollutant Transport In
Estuaries by the Method of Velocity-Vorticity Formulation (3/3)

計畫類別：☐個別型計畫

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計畫編號：NSC89-2611-E-002-048

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一. 中文摘要 (關鍵字：河口水理污
染物傳輸與擴散、速度 - 渦度法、
邊界元素法、有限元素法)

本研究目的，在於以數值模式模擬非線性三維河口污染物擴散之物理現象。由於物理包涵的層面廣泛，因此在盡量以數值模式呈現實際的現象，又必須顧及數值計算上的限制，所以在模式上盡量減低處理非線性方程式，因而我們在水理模式採用以速度 - 渦度觀念，使得處理速度分佈，祇分離之線性 Poisson 方程式，而在渦度場方面，則為傳統之傳輸 - 擴散 - 反應方程式。因此本研究重點，即著重於線性 Poisson 方程式之邊界元素及有限元素模式的建立與應用及速度 - 渦度觀念之可行性。

本文利用速度 (Velocity) - 渦度 (Vorticity) 法搭配有限元素法 (Finite element method)，邊界元素法 (Boundary element method) 及二階朗吉庫達法 (Runge-Kutta method) 求解三維慣性座標和非慣性座標不可壓縮黏性流場，文中以簡單之三維箱型穴室流 (Cavity flow) 作為驗證程式的依

據。在驗證過程中，對奈維爾 - 司徒克斯

(Navier - Stokes) 方程式在中低雷諾茲數流場作分析，以瞭解流場變化和渦度變化的關係。由驗證的結果中發現邊界的黏滯力將導致渦度的改變，而渦度會擴散至整個流場中，帶動整個流場變化，造成速度改變，而流場速度變化又相繼改變渦度，如此相互反制影響。

英文摘要 ((Keywords : Estuary hydrodynamics, Pollutant advection-diffusion, Velocity-vorticity method, Boundary element method, Finite element method)

The main purpose of present study aims at the establishment of a mathematical model for predicting the pollutant transport in a nonlinear 3D estuary. To reduce the handling of nonlinear partial differential equations, the concept of velocity-vorticity formulation is adopted to model the estuary hydrodynamics. Thus the governing

equations for the velocity field are deduced to the linear Poisson equations, To further lower the dimension, the BEM or FEM is again applied to solve the velocity Poisson equations. The distribution of pollutant, temperature, as well salinity are all solved by the FEM or BEM algorithms as well as the feasibility of the concept of velocity-vorticity formulation.

In this study, we use the velocity-vorticity method, in combination with finite element method, boundary element method and Runge-Kutta method to solve the three-dimensional inertial and non-inertial unsteady incompressible viscous flows. The correctness of the model is verified by a simple driven cavity flow by comparing with existing literature.

As for as flow verification is concerned, we analyze the flows satisfying the Navier-Stokes equations with low Reynolds numbers. In computation, one can understand the relation between the change of flow velocity and vorticity. By the process of verification, we know the fact that the viscous force on the boundary induces the generation of the vorticity, and interacts with velocity. The vorticity would diffuse into the whole flows, and cause the variation of the flows. However the variation of the flow also will change the vorticity. Finally, they are influenced and coupled each other.

二、計畫的原由與目的

台灣地區地狹人稠四面環海，土地利用的限制及環境保護意識的抬

頭，促使發展的觸角伸向河流及海洋。因此，河口及沿海之開發日益頻繁，人口快速的成長及高科技工業之發展，對水域之水質與環境造成負面之影響，水質規劃與管理之工作成為重要之課題，然而，河口及沿海水域之污染物傳輸與擴散機制深受河川流量及水質、海洋潮汐、洋流運動、風力、地球自轉之科氏力、海水密度層變及河口與海岸地形等因素所影響。欲瞭解河口及沿海水域複雜污染物對流、擴散與反應現象，水理與水質數值模擬應是最佳之分析方法。

研究方向將分為三個階段進行，第一階段進行沒有密度層變與有密度層變之非線性水理與污染物邊界積分及有限元素法數值模式之建立與比較，以瞭解慣性力與水平擴散相對於水理之影響。第二階段則著重有密度層變之非線性三維河口污染物之擴散模式之研究，並了解各項參數值對於模擬結果之影響，以利找出最佳組合，符合實際水理條件，最後階段則著重能以現場資料，尤其是淡水河口為例，探討模式應用於實際例子之可行性。

三、研究方法

3-1 水理模式

本研究為研究非線性極強之廣義 Navier-Stokes 方程式及連續方程式，為避開處理壓力及降低非線性與希望達成分割(decoupling)而有利於平行計算(parallel computing)，今以速度渦度法(velocity-vorticity method)來求解均值(即沒有密度層變)之河口水理。其基

本方程式為

$$\nabla^2 \bar{u} = -\bar{\nabla} \times \bar{\omega} \quad (1)$$

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \bar{\nabla} \bar{\omega} = \nu \bar{\nabla}^2 \bar{\omega} + (\bar{\omega} + f \bar{k}) \cdot \bar{\nabla} \bar{u} \quad (2)$$

式中 $f = 2\Omega \sin \theta$, $\bar{\omega} = \bar{\nabla} \times \bar{u}$

3-2 污染物傳輸模式

描述污染物傳輸模式，一般以所謂之傳輸(advection)、擴散(diffusion)及反應(reaction)方程式為之，即

$$\frac{\partial \bar{C}}{\partial t} + \bar{u} \cdot \nabla^2 \bar{C} = k_c \nabla^2 \bar{C} + \bar{S}_c(\bar{C}, \bar{x}, t) \quad (3)$$

我們以所發展之有限元素法(FEM)來處理渦度、溫度、鹽度及污染物之傳輸擴散，及反應方程式。因為在第二階段有密度層變(density stratification)之計畫中，吾人只要在第(2)式中增加密度而增加之渦度即可。

$$\begin{aligned} \frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nu \bar{\nabla} \bar{\omega} = \nu \bar{\nabla}^2 \bar{\omega} + (\bar{\omega} + f \bar{k}) \cdot \bar{\nabla} \bar{u} \\ + \bar{\nabla} \times \left(-g \frac{\rho - \rho_0}{\rho} \bar{k} \right) \end{aligned} \quad (4)$$

及狀態方程式

$$\rho = \rho(T, S, \bar{C}) \quad (5)$$

及溫度方程式

$$\frac{\partial T}{\partial t} + \bar{u} \cdot \bar{\nabla} T = k_T \nabla^2 T + S_T(T, \bar{x}, t) \quad (6)$$

及鹽度方程式

$$\frac{\partial S}{\partial t} + \bar{u} \cdot \bar{\nabla} S = k_S \nabla^2 S + S_S(S, \bar{x}, t) \quad (7)$$

3-3 數值模擬結果

本文在三年研究期間，總共發表 13 篇期刊論文；14 篇會議論文；6 篇研究技術報告及完成 4 篇碩士論文及正在指導中之 2 篇博士及 2 篇碩士論文，詳細之數值模擬結果，分別附在本總結研究之報告中。

四、結論與建議

1. 本研究利用邊界元素法及有限元素法求解速度場之 Poisson 方程式，利用邊界元素法及有限元素法及二階郎吉庫特性法求解渦度、溫度、污染物濃度場之傳輸-擴散-反應方程式，發現是一個解決非線性三維河口污染物擴散研究之可行方法。
2. 為探討更有效率之數值方法，建議繼續研究改進並引進目前正在研究發展無須網格之其他數值方法。

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THE USE OF DUAL RECIPROCITY BOUNDARY ELEMENTS FOR SIMULATION OF GROUNDWATER FLOW AND POLLUTANT TRANSPORT

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ABSTRACT

The dual reciprocity boundary element method (DRBEM) has been established as an effective numerical tool in the modeling of various engineering problems. Here the application of the DRBEM in groundwater flow and pollutant transport is described. Several cases analyzed prove that DRBEM is an effective numerical tool in simulating these problems.

I. INTRODUCTION

Groundwater, in recent years, has been an important consideration in the water plans of many countries due to over exploitation and non-availability of surface water. In the development and management of groundwater resources, two major problems of interest are the quantity of available water and the quality of extracted water. For the efficient management of groundwater basins subjected to pumping and recharge, it is necessary to analyze and predict the hydraulic response of the system using effective tools. Similarly for the assessment of groundwater quality, it is necessary to identify the source of pollution and predict the movement of pollutants using effective techniques.

Generally, the hydrodynamic response of groundwater basins and pollutant movement in

porous media are predicted using analytical, physical, field and numerical models. For the simulation of groundwater flow and pollution transport, very few exact analytical solutions are available and the physical and field models are cumbersome and difficult in practice. Hence, numerical models are in common use for the prediction of groundwater flow and pollution transport.

Commonly used numerical models are based on the finite difference method (FDM), the finite element method (FEM) and the boundary element method (BEM). FDM and FEM are in common use for the solution of groundwater flow and pollution dispersion problems for which domain discretization is required. For large-scale groundwater flow and pollutant transport problems, the discretization of the domain using FDM or FEM takes huge effort and the solution becomes cumbersome. Using BEM, if there

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are no convective or time dependent terms in the governing equations, only the boundary of the domain is to be discretized for solution, hence, it is easier in field applications. But if there are convective terms or time dependent terms in the governing equations, (which is the usual case with groundwater flow or pollutant transport problems), a solution using the general BEM (Brebbia, 1978) requires domain integration which reduces the attraction of the method.

The dual reciprocity boundary element method (DRBEM), converts all time dependent terms and convective terms into boundary integrals using a special technique and hence is totally boundary oriented. The internal points are defined wherever a solution is required. Hence, in DRBEM, a three dimensional problem is solved, computationally, in two dimensions and a two dimensional problem is solved, computationally, in one dimension. Here, the application of dual reciprocity boundary elements in the modeling of groundwater flow and pollution transport is briefly described, with some case studies.

The dual reciprocity boundary element method (DRBEM) was introduced by Nardini and Brebbia (1982) and was later generalized to a wide range of engineering problems (Partridge *et al.*, 1992). Various authors presented formulations for diffusion equations and diffusion-convection equations based on dual reciprocity boundary elements (De-Figueriredo and Wrobel, 1990; Partridge and Brebbia, 1992; Zhou and Zhang, 1994). Eldho (1995) used DRBEM for the solution of transient groundwater flow problems and pollution dispersion problems. Eldho and Rao (1997) presented the applications of DRBEM for two dimensional contaminant transport problems in porous media. In this paper, the general applications of DRBEM in groundwater flow and pollution dispersion modeling are described with the help of two case studies.

II. GROUNDWATER FLOW MODELING

1. Governing Equation and Formulation

The general governing equation for transient groundwater basin flow (both confined and unconfined aquifers) in homogeneous isotropic porous media can be expressed as Bear (1979):

$$\nabla^2 \phi = \frac{1}{D} \frac{\partial \phi}{\partial t} - \frac{W}{T} \quad (1)$$

where ϕ - the potential or hydraulic head, T - the transmissivity of the aquifer, D - the diffusivity of the aquifer ($D=T/S$), S - storativity of the aquifer, t - the

time and W - recharge or pumping rate (positive for recharge and negative for pumping). The following dimensionless form of variables are used in the solution:

$$X=x/L; Y=y/L; \Phi=\phi/\bar{\phi}; t=\tau D_0/L^2; \\ \bar{W}=WL^2/T_0 \bar{\phi}; D'=D/D_0 \quad (2)$$

where L is a reference length, $\bar{\phi}$ is a reference hydraulic head, D_0 is a reference diffusivity, T_0 is the transmissivity corresponding to the reference diffusivity and τ is the time step.

For transient groundwater flow, the initial and boundary conditions should be prescribed. The initial condition, usually prescribed head, is described throughout the domain at some initial time. Two common types of boundary conditions may be defined in a typical aquifer problem. One is a Dirichlet condition (boundary of prescribed head) and another one is a Neumann condition (boundary of prescribed flux).

Considering the transient flow in aquifers without any pumping or recharge, Eq. (1) becomes,

$$\nabla^2 \phi = \frac{1}{D} \frac{\partial \phi}{\partial t} \quad (3)$$

Here, in the solution of Eq. (3) using DRBEM, the time dependent term is approximated using the dual reciprocity method and then Green's theorem is applied to get a boundary solution. The fundamental solution of the Laplace equation is used for approximation. This procedure gives a boundary only solution with less complexity in the solution process of the governing equation.

In the dual reciprocity method, the term $\partial \phi / \partial t$ is approximated and Eq. (3) is represented as:

$$\nabla^2 \phi = \frac{1}{D} \sum_{j=1}^{N+L} f_j(x, y) \alpha_j(t) = \frac{1}{D} \sum_{j=1}^{N+L} (\nabla^2 \hat{\phi}_j) \alpha_j(t) \quad (4)$$

where f_j - a set of approximating functions, α_j - a set of initially unknown coefficients, N - number of boundary nodes, L - number of internal nodes and $\hat{\phi}_j$ is a series of particular solutions. Here the right hand side of Eq. (3) has been represented by a set of basis functions $f_j(x, y)$ multiplied by a set of unknown functions of time $\alpha_j(t)$ which in turn is replaced by a summation of products of coefficients α_j and the Laplacian operating on the particular solution $\hat{\phi}_j$. The number of $\hat{\phi}_j$ is equal to the number of nodes $N+L$.

Now, using the reciprocity principle on both sides of Eq. (4), discretizing the boundary into N linear elements and using L internal nodes, the

boundary integral equation can be written in discretized form for a source node i as follows:

$$g_i \phi_i + \sum_{k=1}^N \int_{\Gamma_k} \frac{\partial \phi^*}{\partial n} \phi d\Gamma - \sum_{k=1}^N \int_{\Gamma_k} \phi^* \frac{\partial \phi}{\partial n} d\Gamma$$

$$= \frac{1}{D} \sum_{j=1}^{N+L} \alpha_j (g_i \tilde{\phi}_{ij} + \sum_{k=1}^N \int_{\Gamma_k} \frac{\partial \phi^*}{\partial n} \tilde{\phi}_j d\Gamma - \sum_{k=1}^N \int_{\Gamma_k} \phi^* \frac{\partial \tilde{\phi}_j}{\partial n} d\Gamma) \quad (5)$$

where ϕ^* is the fundamental solution of the Laplace equation, n is the unit outward normal and g_i is Green's constant; $g_i=1$ for a point inside the domain, $g_i=0$ for a point outside the domain and $g_i=\theta/2\pi$ for a point on the boundary, in which θ is the internal angle at point i in radians.

After introducing the interpolation function and integrating over each boundary element, applying to all boundary nodes using a collocation technique and using the initial and boundary conditions, a system of linear equations can be formed. The solution of this linear system of equations gives the unknown function values first on the boundary of the domain and then the internal values can be found from Eq. (5). The detailed formulation of DRBEM for groundwater flow can be found elsewhere (Eldho, 1995, 1996).

The approximating function ' f ' used here is ' $1+r$ ' where r is the distance from the point i of application of the concentrated source or sink to any other point under consideration. Here the pumping and recharge effects (Eq. 1) are considered as concentrated sinks and sources (Brebbia, 1978).

The presented model has been compared with one analytical solution given in Liggett and Liu (1983) and one FEM model given in Pinder and Gray (1977) for confined aquifer conditions (Eldho, 1995). Here the comparison with the analytical solution is presented. The aquifer considered is a square region of unit dimension without any pumping or recharge and unit diffusivity. On the left hand side of the domain boundary, unit potential ($\phi(0, y, t)=1.0$) and right hand side of the domain boundary zero potential ($\phi(1, y, t)=0.0$) are assumed. On other boundaries, no flow boundary condition ($\partial\phi/\partial n=0$) are assumed. Initially, throughout the domain zero potential ($\phi(x, y, 0)=0.0$) are assumed. Here, dimensionless variables as given in Eq. (2) are used. For the problem described, the exact analytical solution is described in Liggett and Liu (1983).

In the DRBEM model, the boundary of the domain is discretized into 20 linear elements and 12 internal nodes are considered and a

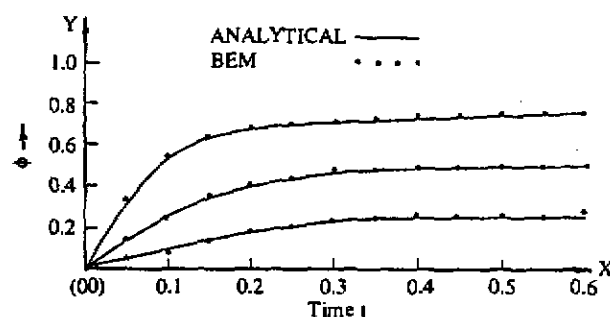


Fig. 1. Comparison of ϕ variation for DRBEM model and analytical solution

dimensionless time step of 0.05 is used. Figure 1 shows the potential variation with respect to time at various points in comparison with the analytical solution. Good agreement is observed between the DRBEM solution and the analytical solution. In the transient groundwater flow analysis using DRBEM, the accuracy and stability of the results depend on the use of optimal dual reciprocity boundary element model parameters like time steps, number of boundary elements, number of internal nodes, weighting factors and approximating functions used in the investigation. A detailed sensitivity study of these parameters can be found in Eldho (1996).

2. Case Study

To show the effectiveness of DRBEM in groundwater flow analysis, a case study of regional aquifer modeling is presented here. An unconfined aquifer in Pochampad Ayacut, Andhra Pradesh, India is considered to determine the effects of continued pumping on the regional groundwater basin (Eldho, 1995). The aquifer considered has a specific area of 67 sq.km. It is wedge shaped bounded by two streams, Peddavagu and Kortavagu, on two sides and the Pochampad main canal on the third side as in Fig. 2. Groundwater mainly occurs in this basin under unconfined conditions. From the pumping tests, the average transmissivity and storativity are observed to be 79.5 m²/day and 4.55×10⁻³ respectively. For the study purpose, the aquifer is considered to be homogeneous and isotropic. The two boundary streams are considered as recharging boundaries. The other boundary, the Pochampad main canal is a lined canal, having been excavated beyond the average depth of weathering in the region, and is assumed to be impermeable. The groundwater levels available in 1971 without any pumping effect varying from 270 to 304 m, are taken as the initial groundwater levels for the purpose of analysis. All these data are taken from the publication of Baig and Prabhakar (1980).

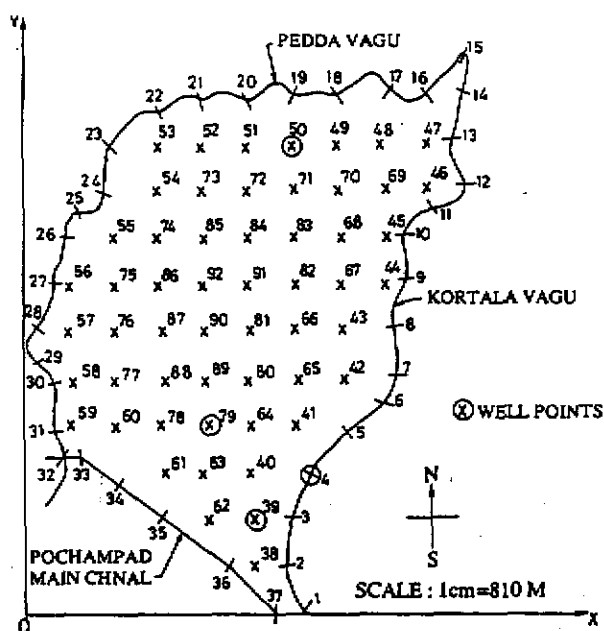


Fig. 2. Aquifer plan and DRBEM discretization

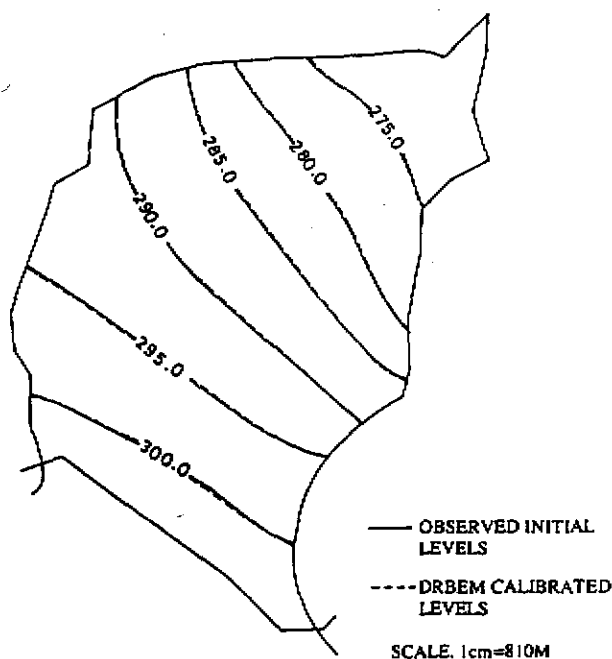


Fig. 3. Model Calibration - case study

3. Calibration of The Model

For the simulation of a real aquifer, it is essential that the model used is calibrated with the initial data available so that the model reflects back the response of the original situation within reasonable limits. In the present case study, the data available is a record of initial water levels observed in 1971, when there was no pumping. No data is available about the recharging stream boundaries. Hence, in the absence of any other data, the initial water levels of 1971 have been considered as the unknown steady state solution of potential head distribution over the entire basin. A steady state analysis is carried out for calibration. The boundary of the domain is discretized into 37 linear elements and 55 internal points are considered as in Fig. 2. From the given conditions and initial boundary heads, the fluxes (discharges and recharges) at the boundary nodes and the heads at internal points are predicted. These boundary recharges and discharges are assumed to exist over future times as the boundary conditions of the basin in addition to the future prescribed pumping activities.

To ascertain the accuracy of the calibrated model, the boundary discharges and recharges are redistributed to see whether given boundary heads and internal nodes are obtained, if so, the model is calibrated. The calibrated groundwater levels and the initially observed water levels of 1971 are plotted in the form of contours in Fig. 3. Both the contours agree closely and establishes the validity of the calibration.

4. Prediction of Future Transient Water Levels with Pumping

For the prediction of future transient water levels with pumping effects, a case study is considered with pumping wells located at nodal points 4, 39, 50 and 79 (see Fig. 2) pumping at a rate of 169, 169, 338 and 338 m^3/day respectively. The pumping wells are treated as concentrated sinks in the model (Brebbia, 1978). The boundary of the domain is discretized into 37 linear elements and 55 internal points are considered to find the potential distribution. The recharge and discharge rates obtained from steady state analysis are used as boundary conditions. The given initial potential is described as the initial condition on the nodes and a time step of 1 day is used in the analysis. The groundwater levels are predicted at the end of 1 year, 5 years and 10 years, due to continuous pumping and the corresponding contours are shown in Fig. 4. The potential variation at some selected nodes (42, 53, 63, 70, 77 and 92) with respect to time is shown in Fig. 5.

This case study shows the effectiveness of DRBEM in groundwater flow modeling. The transient groundwater flow problem with pumping and recharge is solved entirely based on boundary discretization. Internal points are defined wherever a solution is needed. Using DRBEM, the two dimensional problem is solved computationally in one dimension. The irregular shape of the boundaries of the problem is considered such that computation is not possible with other numerical methods, only with

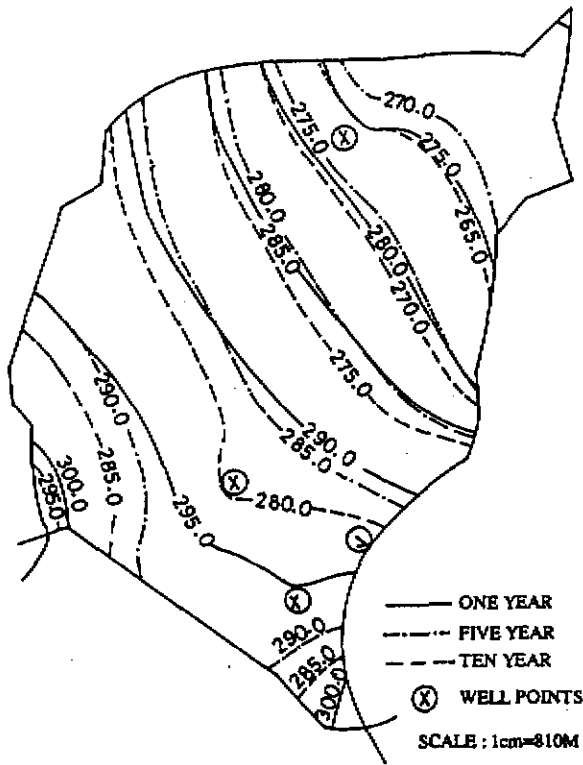


Fig. 4. Contours of predicted potential - case study

DRBEM. The pumping and recharge are considered as concentrated sinks and sources. As is clear from the case study, the data required and prepared are much less than needed by other numerical methods.

III. GROUNDWATER POLLUTANT TRANSPORT MODELING

1. Governing equation and formulation

The two-dimensional governing equation for groundwater contaminant transport in saturated, homogeneous and isotropic porous media (Van Genuchten *et al.*, 1977) can be expressed as:

$$D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} = R \frac{\partial C}{\partial t} + \frac{1}{n_e} (U_x \frac{\partial C}{\partial x} + U_y \frac{\partial C}{\partial y}) + \lambda RC \quad (6)$$

where C is the pollutant solution concentration, D_{xx} and D_{yy} are the dispersion coefficients in x and y directions, t is the time, U_x and U_y are the Darcy velocity components in x and y directions, n_e is the effective porosity, R is the retardation factor of the porous media and λ is a first-order decay constant for solutes that undergo decay. A dimensionless form of Eq. (6) can be achieved by substituting,

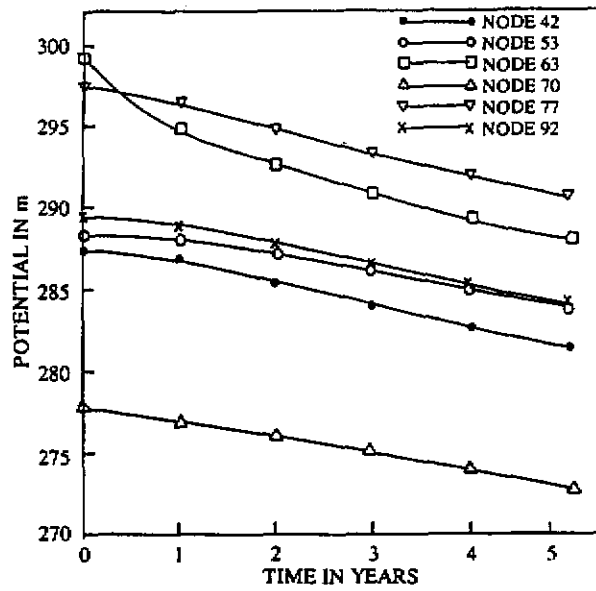


Fig. 5. Potential variation with time - case study

$$c = \frac{C n_e}{C_0}; X = \frac{x}{L'}; Y = \frac{\beta y}{L'}; u_x = \frac{U_x L'}{D_{xx}};$$

$$u_y = \frac{\beta U_y L'}{D_{yy}}; t' = \frac{D_{xx} t}{L'^2} \quad (7)$$

in which C_0 and L' are some reference concentration and length and $\beta = (D_{xx}/D_{yy})^{1/2}$.

To solve a particular problem, the governing equation has to be supplemented by appropriate initial and boundary conditions. The initial condition, usually prescribed concentration, is described throughout the domain at some initial time. Two boundary conditions are commonly used in the solution of pollution dispersion problems. One is a Dirichlet condition (boundary of prescribed concentration) and another one is a Neumann condition (boundary of normal gradient of the concentration).

Here in the solution of the dispersion equation using DRBEM, the time dependent term and convective terms are approximated using the dual reciprocity method and then Green's theorem is applied to get a boundary solution. The fundamental solution of the Laplace equation is used for approximation. This procedure gives a boundary only solution with less complexity in the solution process and allows any of the coefficients to have variable values without adopting special techniques. Assuming D_T as the longitudinal dispersion coefficient, $V_x = U_x/n_e$, $V_y = U_y/n_e$ and using Eq. (7) (while keeping the symbols same as in Eq. (6)), then

$$\nabla^2 C = \frac{1}{D_T} (V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} + \lambda RC + R \frac{\partial C}{\partial t}) = \frac{b}{D_T} \quad (8)$$

In the DRBEM, the right hand side of Eq.(8) can be represented as:

$$\nabla^2 C = \frac{1}{D_T} \sum_{j=1}^{N+L} \alpha_j (\nabla^2 \hat{C}_j) = \frac{1}{D_T} \sum_{j=1}^{N+L} f_j(x, y) \alpha_j(t) \quad (9)$$

where $\hat{C}_j$ is a series of particular solutions, N is the number of boundary nodes, L is the number of internal nodes, α_j is a set of initially unknown coefficients and f_j are approximating functions. Here, the right hand side of Eq. (9) has been represented by a set of coordinate functions $f_j(x, y)$ multiplied by an unknown function of time $\alpha_j(t)$, which in turn is replaced by a summation product of coefficients α_j and the Laplacian operating on the particular solution $\hat{C}_j$. The number of $\hat{C}_j$ is equal to the total number of nodes $N+L$.

Now using reciprocity principle on both sides of Eq. (9), discretizing the boundary into N linear elements and using L internal nodes, the boundary integral equation can be written in discretized form for a source node i as follows:

$$\begin{aligned} g_i C_i + \sum_{k=1}^N \int_{\Gamma_k} \frac{\partial C^*}{\partial n} C d\Gamma - \sum_{k=1}^N \int_{\Gamma_k} C^* \frac{\partial C}{\partial n} d\Gamma \\ = \frac{1}{D_T} \sum_{j=1}^{N+L} \alpha_j [g_i \hat{C}_{ij} + \sum_{k=1}^N \int_{\Gamma_k} \frac{\partial C^*}{\partial n} \hat{C}_j d\Gamma \\ - \sum_{k=1}^N \int_{\Gamma_k} C^* \frac{\partial \hat{C}_j}{\partial n} d\Gamma] \end{aligned} \quad (10)$$

where C^* is the fundamental solution of the Laplace equation, n is the unit outward normal and g_i is Green's constant, as defined earlier.

After introducing the interpolation function and integrating over each boundary element, applying to all boundary nodes using a collocation technique and using the initial and boundary conditions, a system of linear equations can be formed. The solution of this linear system of equation gives the unknown function values first on the boundary of the domain and then the internal concentration values can be found from Eq. (10). The detailed formulation of DRBEM for pollution dispersion in porous media can be found elsewhere (Eldho and Rao, 1997).

The approximating function 'f' used here is '1+r' where r is the distance from the point i of application of the concentrated source or sink to any other point under consideration.

The DRBEM model has been compared with some one-dimensional and two-dimensional analytical solutions (Eldho and Rao, 1997). Here, the comparison with one analytical solution is presented. The porous media considered is a rectangular region

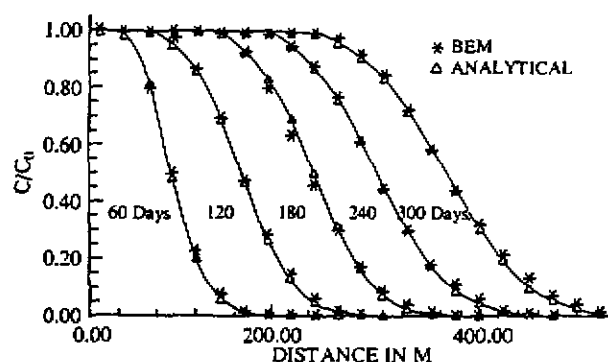


Fig. 6. Comparison of pollutant distribution for DRBEM and analytical solution

of 600m×100m size and is homogeneous, isotropic and fully saturated. The longitudinal dispersion coefficient of the media (D_T) is assumed to be 7.616 m²/day, the retardation factor $R=1.0$, radioactive decay coefficient is assumed to be zero, seepage velocity = 1.219 m/day and source fluid discharge is assumed to be zero. On the left hand side of the domain boundary, unit relative concentration ($C(0, y, t)=1.0$) and on the right hand side of the domain boundary zero relative concentration ($C(600, y, t)=0.0$) is assumed. On other boundaries, no flow condition and derivative of concentration ($\partial C/\partial n=0$) is assumed as zero. Initially, throughout the domain zero concentration ($C(x, y, 0)=0.0$) is assumed. Here, dimensionless variables, as given in Eq. (7), are used. For the problem described, the exact analytical solution is described in Marino (1974).

In the DRBEM model, the boundary of the domain is discretized into 52 linear elements and 11 internal nodes are considered and a time step of 1 day is used. The dispersion analysis is carried out for 300 time steps and concentration distribution is found. Figure 6 shows the relative concentration distributions along the domain at various times in comparison with the analytical solution. Good agreement is observed between the DRBEM solution and the analytical solution.

As in the case of groundwater flow modeling, the accuracy, stability, convergence and computational efficiency of the DRBEM model for pollutant dispersion analysis also depends on the use of optimal dual reciprocity boundary element model parameters like time steps, boundary discretizations, internal nodal distributions, weighting factors and approximating functions used in the investigation. A detailed sensitivity study of these parameters can be found in Eldho and Rao (1997).

IV. CASE STUDY

To show the effectiveness of DRBEM in

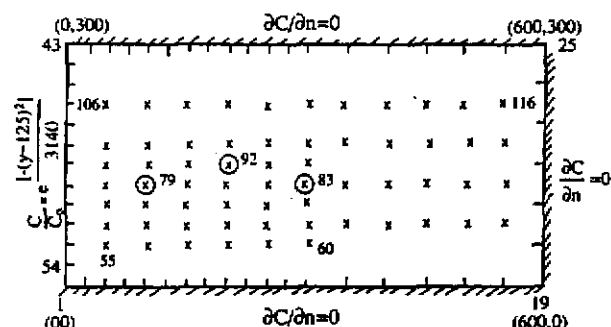


Fig. 7. Solution region for pollution dispersion case study with discretization

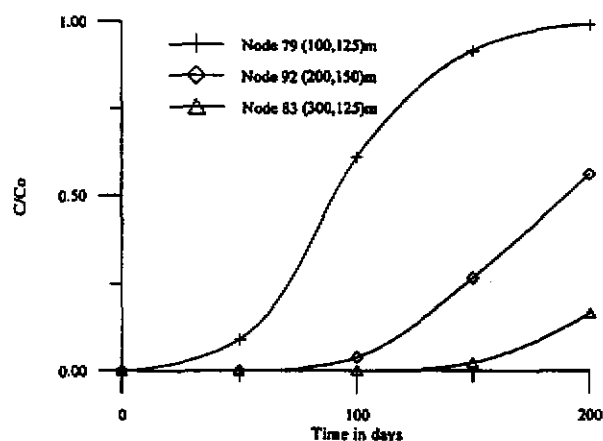


Fig. 8. Solute concentration distribution with time

groundwater pollution analysis, a case study of pollution dispersion in an aquifer is presented here. An unconfined aquifer of domain size 600m×300m is considered to determine the effects of pollution dispersion in porous media (Eldho, 1995). The boundary of the domain is discretized with 54 linear elements and 62 internal nodes are used. Fig. 7 shows the discretization with the input concentration that varies along the y-axis. The dispersion coefficient in the x-direction (D_{xx}) is 7.622 m²/day and in the y-direction (D_{yy}) is 0.4795 m²/day. The unidirectional seepage velocity through the aquifer media is 1.22 m/day.

A time step of 2 days is used in the analysis. The pollutant dispersion analysis is carried out for 200 days. Figure 8 shows the concentration development with time at three nodes, 79 (100, 125), 92 (200, 150) and 83 (300, 125). Figs. 9a and 9b show the contours of the relative pollutant concentration distribution after 100 days and 200 days from the beginning of the pollution. To analyze the pollution movement after stopping the contamination source, numerical analysis is continued for 200 more days after the removal of the contamination source.

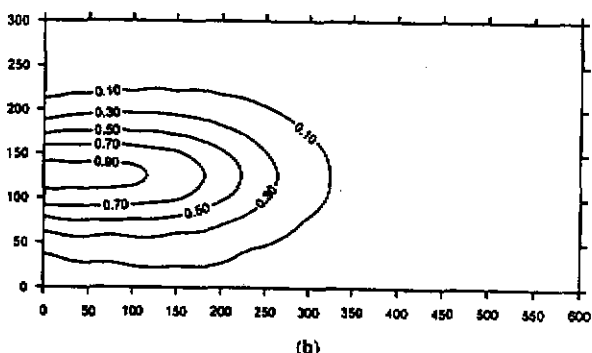
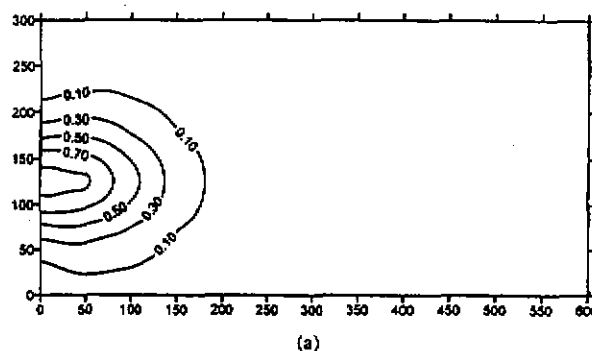


Fig. 9. (a) Contours of the relative pollutant distribution after 100 days. (b) Contours of the relative pollutant distribution after 200 days

Figs. 10a and 10b show the relative contours of the pollutant concentration distribution 100 days and 200 days after stopping the contamination source (300 days and 400 days after the beginning of the pollution).

This case study shows the effectiveness of DRBEM in groundwater pollutant transport modeling. The time dependent and convective terms in the governing equation are approximated in such a way that the problem is solved entirely based on boundary discretization. Internal points are defined wherever a solution is needed. Using DRBEM, the two dimensional, problem is solved computationally, in one dimension. In the present model, the effect of numerical dispersion is found to be negligible compared to other numerical methods (Eldho and Rao, 1997). As is clear from the case study, the data required and prepared are much less than compared to other numerical methods.

V. CONCLUDING REMARKS

Here the applications of the dual reciprocity boundary element method in the analysis of groundwater flow and pollution modeling are described. The time-dependent term and convective terms in the diffusion equation and dispersion equation are approximated using the dual reciprocity method to achieve a boundary only solution. Various case

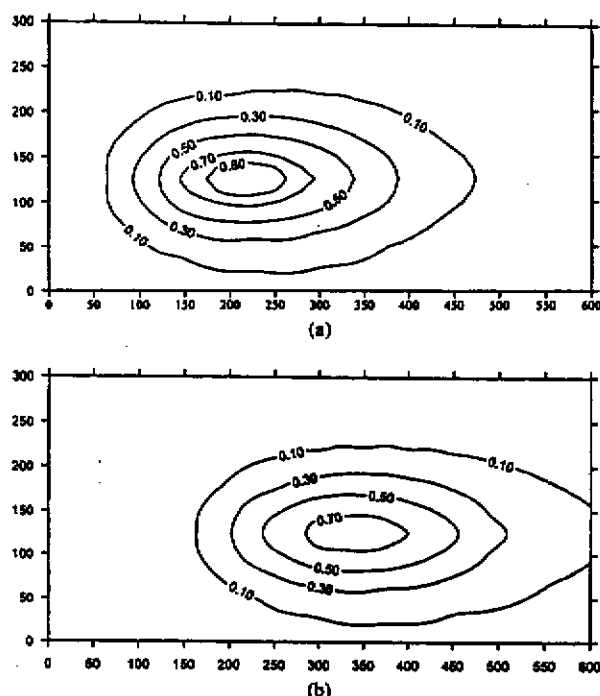


Fig. 10. (a) Contours of pollutant distribution after the source removal (100days). (b) Contours of pollutant distribution after the source removal (200days)

studies analyzed show the effectiveness of the DRBEM in groundwater flow and pollution dispersion analysis. In DRBEM, all the basic advantages of the BEM, like reduction in computational dimension, ease of data handling and less numerical dispersion are achieved. DRBEM is particularly advantageous in the analysis of large groundwater basins with irregular boundaries as only the boundary of the domain is discretized and internal nodes are considered at the desired points.

NOMENCLATURE

C	pollutant solution concentration
C^*	fundamental solution of Laplace equation
D	diffusivity of the aquifer
D_{xx}, D_{yy}	Dispersion coefficient in x, y directions
f_j	approximating functions
g_i	Green's constant
L	number of internal nodes
N	number of boundary nodes
n	unit outward normal
n_e	effective porosity
R	retardation factor
S	storativity of the aquifer
t	time
T	transmissivity of the aquifer
U	Darcy velocity
W	recharge or pumping rate

Greek symbol

ϕ	potential
λ	first order decay constant
τ	time step
α	a set of initially unknown coefficients
ϕ^*	fundamental solution of Laplace equation

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以雙倒易邊界元素法模擬地下水流及污染物傳輸

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摘 要

雙倒易邊界元素法已廣泛有效地被利用於模擬各種工程上的問題，本文利用雙倒易邊界元素法應用於地下水流及污染物傳輸之研究，許多例子證明雙倒易邊界元素法對於處理這種問題是一十分有效率的數值工具。

關鍵詞：地下水，污染物擴散，雙倒易邊界元素法。

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THREE-DIMENSIONAL STOKES FLOW SOLUTION USING COMBINED BOUNDARY ELEMENT AND FINITE ELEMENT METHODS

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ABSTRACT

This paper describes a model using boundary element and finite element methods for the solution of three-dimensional incompressible viscous flows in slow motion, using velocity-vorticity variables. The method involves the solution of diffusion-advection type vorticity equations for vorticity whose solenoidal vorticity components are obtained by solving a Poisson equation involving the velocity and vorticity components. The Poisson equations are solved using boundary elements and the vorticity diffusion type equations are solved using finite elements and both are combined. Here the results of Stokes flow with very low Reynolds number, in a typical cavity flow are presented and compared with other model results. The combined BEM-FEM model has been found to be efficient and satisfactory.

Keywords : Velocity-vorticity method, Stokes flow, Boundary elements, Finite elements.

1. INTRODUCTION

The incompressible viscous flow problems governed by very small velocities (consequently very low Reynolds number), known as Stokes flow problems, are very important in fluid dynamics. Stokes flow problems can be considered as a subset of Navier-Stokes flow problems, in which the effects of nonlinear convective terms are very small or can be neglected. Three formulations are well known for the solution of the incompressible Navier-Stokes equations, in terms of: primitive variables of pressure and velocity, velocity-stream function and velocity-vorticity. The first two formulations have been thoroughly investigated by various researchers for two-dimensional and three-dimensional problems using various numerical methods like finite difference (FDM), finite elements (FEM) and boundary element methods (BEM), e.g., [1-3]. The third formulation in terms of velocity and vorticity also has been explained in the last decade, mainly in two dimensions using various numerical schemes.

For the solution of Navier-Stokes flow problems using the velocity-vorticity formulation, the governing equations have been written as a system of diffusion-advection type and Poisson type equations for the components of the vorticity and velocity fields, respectively. The main advantage of this formulation includes the numerical separation of the kinematic and kinetic aspects of the fluid flow from the pressure computation, which is determined afterwards from the

known velocity and vorticity fields.

The theoretical potentials of FEM [4] and BEM [3] have been adequately exposed for the solution of Stokes flow and Navier-Stokes equations by various researchers. In this paper, an effort has been made to combine the well-known BEM and FEM techniques for solving the velocity-vorticity form of the Stokes flow equations and for very low Reynolds number Navier-Stokes equations in three-dimensions. In the present model, the vorticity transport equations in the velocity-vorticity formulation of Stokes flow and Navier-Stokes equations are approximated using a standard Galerkin finite element technique [5] and combined with velocity-vorticity Poisson type equations, which are solved using a standard boundary-domain integral method [6]. The vorticity boundary conditions are exactly obtained by the BEM solution of the Poisson equation. An iterative scheme is used in the solution of the system of equations after the numerical discretization using BEM and FEM.

The accuracy and feasibility of the combined BEM-FEM model has been demonstrated using the well-known model problem of flow in a driven cubic cavity. The cavity flow problem is of continuing interest because it offers a relatively simple model on which numerical techniques may be examined and verified with other numerical schemes. Using the combined BEM-FEM model, even for a coarse mesh, accurate results comparable with other models using fine meshes, in literature are obtained.

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After presenting the governing equations, the numerical formulation using BEM and FEM are briefly described. Then the solution procedure and numerical results for three-dimensional driven cavity flow problem is provided, followed by a few concluding remarks.

2. GOVERNING EQUATIONS

The governing equations for mass and linear momentum transport in a domain Ω with boundary Γ occupied by incompressible Newtonian fluid, can be written as [7]:

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \bar{u} \quad (1)$$

$$\nabla \cdot \bar{u} = 0 \quad (2)$$

where $\bar{u}$ is the velocity vector, p is the pressure, Re is the Reynolds number and t is the time. Equations (1) and (2) represent the Navier-Stokes equations in the pressure-velocity formulation.

The vorticity vector $\bar{\omega}$ can be expressed as:

$$\bar{\omega} = \nabla \times \bar{u} \quad (3)$$

By taking the curl of both sides of Eq. (1) and using Eqs. (2) and (3), we can obtain the vorticity transport equation as:

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{\text{Re}} \nabla^2 \bar{\omega} \quad (4)$$

By taking the curl of Eq. (3) and using Eq. (2) we get,

$$\nabla^2 \bar{u} = -\nabla \times \bar{\omega} \quad (5)$$

which is a vector form of the Poisson equation for $\bar{u}$.

Equations (4) and (5) with $\bar{u}$ (u, v, w) as velocity and $\bar{\omega}$ (ξ, η, ζ) as vorticity vectors are known as velocity-vorticity formulation of Navier-Stokes equations and can replace Eqs. (1) and (2) in which $\bar{u}$ and p are variables.

The Stokes flow problems are characterized by very small velocities (consequently very low Reynolds number), such that the nonlinear convective terms in the Navier-Stokes equations can be neglected. If in addition the flow is steady, the whole inertia force is everywhere small in magnitude compared with either pressure or viscous forces. The flow can then be approximated by the motion of a fluid with zero density (or infinite viscosity) with $\text{Re} = 0$, generating the linear creeping flow equations [8]:

$$-\nabla p + \nabla^2 \bar{u} = 0 \quad (6)$$

$$\nabla \cdot \bar{u} = 0 \quad (7)$$

The basic equations of Stokes flow in the velocity-vorticity formulation can be derived from the Navier-Stokes Eqs. (4) and (5) as:

$$\nabla^2 \bar{\omega} = \frac{\partial \bar{\omega}}{\partial t} \quad (8)$$

$$\nabla^2 \bar{u} = -\nabla \times \bar{\omega} \quad (9)$$

If (u, v, w) are the velocity vectors and (ξ, η, ζ) are the vorticity vectors, then from Eq. (8), the three vorticity transport equations can be written as:

$$\nabla^2 \xi = \frac{\partial \xi}{\partial t} \quad (10)$$

$$\nabla^2 \eta = \frac{\partial \eta}{\partial t} \quad (11)$$

$$\nabla^2 \zeta = \frac{\partial \zeta}{\partial t} \quad (12)$$

In steady state conditions, Eqs. (10) ~ (12) can be written as:

$$\nabla^2 \xi = 0 \quad (13)$$

$$\nabla^2 \eta = 0 \quad (14)$$

$$\nabla^2 \zeta = 0 \quad (15)$$

For Stokes flow, Eq. (9) can be written as:

$$\nabla^2 u = -\frac{\partial \zeta}{\partial y} + \frac{\partial \eta}{\partial z} \quad (16)$$

$$\nabla^2 v = \frac{\partial \zeta}{\partial x} - \frac{\partial \xi}{\partial z} \quad (17)$$

$$\nabla^2 w = -\frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \quad (18)$$

For Navier-Stokes equations, the solution of vorticity transport equations in ξ, η, ζ (Eq. (4)), in combination with the Poisson equations, (16) ~ (18), gives the velocity and vorticity distribution all over the domain at the concerned time step. For unsteady Stokes flow, the solution of vorticity transport equations, (10) ~ (12), in combination with the Poisson equations, (16) ~ (18), gives the velocity and vorticity distributions all over the domain at the concerned time step. Similarly in steady state conditions, solution of Eqs. (13) ~ (15), in combination with the Poisson equations, (16) ~ (18), gives the velocity and vorticity distributions all over the domain.

We seek a solution in the domain Ω which satisfies the initial conditions,

$$\bar{u} = \bar{u}_0 ; \quad \bar{\omega} = \nabla \times \bar{u}_0 \quad \text{at } t = 0 \quad (19)$$

and the boundary conditions,

$$\bar{u} = \bar{u}_\Gamma ; \quad \bar{\omega} = (\nabla \times \bar{u})|_\Gamma \quad \text{at } t = 0 \quad (20)$$

on the boundary Γ of Ω .

3. NUMERICAL FORMULATION

As mentioned in Sect. 1, in the solution of velocity-vorticity formulation of Navier-Stokes equations and Stokes flow equations using the combined BEM-FEM formulation, the vorticity transport equations are solved using Galerkin FEM and the Poisson type velocity equations are solved using direct BEM. In this section, the numerical formulation for both BEM and FEM are briefly described.

3.1 Boundary Element Formulation

Consider the Poisson type velocity equation in u and assuming the vorticity vectors ($\bar{\omega}$) and its derivatives are known, Eq. (16) can be written as follows:

$$\nabla^2 u = -\frac{\partial \bar{\omega}}{\partial y} + \frac{\partial \eta}{\partial z} = b \quad (21)$$

with velocity boundary conditions as,

$$u = \bar{u} \text{ on } \Gamma_1; \quad \bar{q} = \frac{\partial u}{\partial n} \text{ on } \Gamma_2 \quad (22)$$

where n is the unit outward normal vector. In the present model, an iterative algorithm is used such that the right hand side of Eq. (21) is known in the current iteration and time step from the previous step by solving the vorticity transport Eq. (8).

A weighting function u^* can now be introduced such that it has continuous first derivatives within Ω . The following weighted residual statement can now be written:

$$\int_{\Omega} (\nabla^2 u - b) u^* d\Omega = \int_{\Gamma_2} (q - \bar{q}) u^* d\Gamma - \int_{\Gamma_1} (u - \bar{u}) q^* d\Gamma \quad (23)$$

where $q = \partial u / \partial n$ and $q^* = \partial u^* / \partial n$.

Let u^* be the fundamental solution of the Laplace equation in three dimensions, represented as $u^* = 1/(4\pi r)$, where r is the distance from the collocation point (k) to other field points (i) given as:

$$r = \sqrt{(x_k - x_i)^2 + (y_k - y_i)^2 + (z_k - z_i)^2} \quad (24)$$

Now applying Green's second identity theorem to Eq. (23) and using the standard boundary element procedure [6], we can get the boundary integral equation as:

$$C_i u_i + \int_{\Gamma} u q^* d\Gamma + \int_{\Omega} b u^* d\Omega = \int_{\Gamma} q u^* d\Gamma \quad (25)$$

where C_i is the Green's constant which can be calculated by surrounding the boundary point i by a small sphere of radius ϵ and taking each term in Eq. (25) in the limit as $\epsilon \rightarrow 0$. Generally C_i can be represented as $\theta/4\pi$ where θ is the internal solid angle at point i in radians.

In Eq. (25), we have boundary integrals and volumetric-domain integrals. In the present model, the

domain integration is carried out by subdividing the domain into a series of internal cells, on each of which a numerical integration is performed. Here two-dimensional isoparametric quadrilateral linear elements are used for the boundary discretization and three-dimensional isoparametric quadrilateral cells are used for the internal discretization. The details of the element properties, shape functions, coordinate transformation and numerical integration used here are described in Brebbia, *et al.*, [6] which is not repeated here.

If the domain is discretized into M internal cells, then the domain integral can be written as,

$$D_i = \int_{\Omega} b u^* d\Omega = \sum_{e=1}^M \left[\sum_{k=1}^{NI} w_k (b u^*)_k \right] \Omega_e \quad (26)$$

where the integral has been approximated by a summation over different cells (e varies from 1 to M), w_k are the Gauss integration weights, the function $(b u^*)_k$ needs to be evaluated at integration points k on each cell (k varies from 1 to NI , where NI is the total number of integration points on each cell) and Ω_e is the volume of cell e . The term D_i is the result of the numerical integration and is different for each position i of the boundary nodes.

Assuming that the boundary of the domain is discretized into NE isoparametric quadrilateral linear elements with N nodes, Eq. (25) can be discretized and written in matrix form as,

$$C_i u_i + \sum_{j=1}^N \bar{H}_{ij} u_j + D_i = \sum_{j=1}^N G_{ij} q_j \quad (27)$$

Combining the effect of the constant term C with the $\bar{H}$ matrix, we can write the system of matrix as,

$$H u + D = G q \quad (28)$$

In Eq. (28), the boundary conditions are introduced and the known values are taken to the right hand side to form a system of linear equations of the form,

$$A b = F \quad (29)$$

where b is a vector of unknown boundary values of u and q , and F is a known vector. Equation (29) is solved using Gauss elimination scheme and all the boundary values will be then known. Once this is done, it is possible to calculate internal values of u or its derivatives. The values of u are calculated at any internal point using the Eq. (25) that can be written in condensed form as:

$$u_i = \int_{\Gamma} q u^* d\Gamma - \int_{\Gamma} u q^* d\Gamma - \int_{\Omega} b u^* d\Omega \quad (30)$$

The same discretization is used for the boundary integrals, that is,

$$u_i = \sum_{j=1}^N G_{ij} q_j - \sum_{j=1}^N \bar{H}_{ij} u_j - D_i \quad (31)$$

where i is an internal point.

The values of the internal fluxes in the Cartesian directions are calculated by carrying out derivatives on (30), i.e.,

$$\begin{aligned}(q_x)_i &= \left(\frac{\partial u}{\partial x} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial x} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial x} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial x} d\Omega \\(q_y)_i &= \left(\frac{\partial u}{\partial y} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial y} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial y} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial y} d\Omega \\(q_z)_i &= \left(\frac{\partial u}{\partial z} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial z} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial z} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial z} d\Omega\end{aligned}\quad (32)$$

Notice that the derivatives are carried out only on the fundamental solution u^* and q^* as we are computing the variations of flux around the point i .

The main advantage of using BEM in the solution of the velocity Poisson equation is the exact determination of the vorticity boundary conditions. The vorticity boundary conditions, which are essential to solve the vorticity transport equations are directly obtained as the velocity normal derivative from the solution of Eq. (25).

3.2 Finite Element Formulation

Consider one of the vorticity transport equations in ξ as,

$$\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} - \xi \frac{\partial u}{\partial x} - \eta \frac{\partial u}{\partial y} - \zeta \frac{\partial u}{\partial z} - \frac{1}{\text{Re}} \nabla^2 \xi = 0 \quad (33)$$

Using the method of weighted residuals and Galerkin criterion [5], Eq. (33) can be written as,

$$\begin{aligned}0 &= \iiint_V N_i \left(\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} - \xi \frac{\partial u}{\partial x} - \eta \frac{\partial u}{\partial y} - \zeta \frac{\partial u}{\partial z} \right. \\&\quad \left. - \frac{1}{\text{Re}} \left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2} \right) \right) dV\end{aligned}\quad (34)$$

where $N_i = N_i(x, y, z)$ is the shape function. Approximating ξ using the shape function as,

$$\xi = \xi(x, y, z, t) = \sum N_i(x, y, z) \bar{\xi}_i(t) \quad (35)$$

and using a time integration for the time derivative of ξ , Eq. (34) can be written as,

$$\begin{aligned}0 &= \sum \iiint_V N_i N_j \bar{\xi}_j' dV \\&+ \sum \iiint_V \left(u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z} \right) \bar{\xi}_j dV \\&- \sum \iiint_V N_i \left(\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} \right) dV - \sum \iint_{\Gamma} q_n N_i dA \\&+ \frac{1}{\text{Re}} \sum \iiint_V \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) \bar{\xi}_j dV\end{aligned}\quad (36)$$

$$\text{where, } q_n = \frac{\partial \xi}{\partial x} n_x + \frac{\partial \xi}{\partial y} n_y + \frac{\partial \xi}{\partial z} n_z.$$

Equation (36) can be written in the form,

$$\sum [M^*] \{\bar{\xi}\} + [L^*] \{\bar{\xi}\} - [R^*] - [Q^*] + \frac{1}{\text{Re}} [K^*] \{\bar{\xi}\} = 0 \quad (37)$$

where,

$$\begin{aligned}M_{ij}^* &= \iiint_V N_i N_j dV; \\L_{ij}^* &= \iiint_V \left(u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z} \right) dV; \\R_i^* &= \iiint_V N_i \left(\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} \right) dV; \\Q_i^* &= \iint_{\Gamma} q_n N_i dA; \\K_{ij}^* &= \iiint_V \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) dV\end{aligned}\quad (38)$$

Here, isoparametric quadrilateral linear elements are used for the three-dimensional discretization. The details of the interpolation functions, integration and formation of the conductance matrix are described in Reddy [5]. For the solution of the vorticity transport equations, an iterative algorithm is used in which it is assumed that at the current time step, the values of $u, v,$

$w, \eta, \zeta, \frac{\partial u}{\partial x}, \frac{\partial v}{\partial y}, \frac{\partial w}{\partial z}$ are known from the previous

step. Using a difference scheme to approximate the time derivative of ξ between time steps $(n+1)$ and n as

$$\{\bar{\xi}\}' = \frac{\{\bar{\xi}_{n+1}\} - \{\bar{\xi}_n\}}{\Delta t} \text{ and putting } \{\bar{\xi}\} = \{\bar{\xi}_n\}, \text{ we can}$$

write the final system of equations for the low Reynolds number flows in matrix form as,

$$\begin{aligned}[M^*] \{\bar{\xi}_{n+1}\} &= [M^*] \{\bar{\xi}_n\} - \Delta t [L^*] \{\bar{\xi}_n\} + \Delta t [R^*] + \Delta t [Q^*] \\&- \frac{\Delta t}{\text{Re}} [K^*] \{\bar{\xi}_n\} = 0\end{aligned}\quad (39)$$

For unsteady Stokes flow problems, Eq. (39) can be modified and written as,

$$[M^*] \{\bar{\xi}_{n+1}\} = [M^*] \{\bar{\xi}_n\} + \Delta t [Q^*] - \Delta t [K^*] \{\bar{\xi}_n\} \quad (40)$$

Here the vorticity boundary conditions obtained from the solution of velocity Poisson equations by BEM is used and the system of equations are solved to find the unknown values of ξ . The derivatives of ξ in Cartesian coordinates are also found which is used in the Poisson equation for the successive iterations and time steps. Here a second order Runge-Kutta (R.K.) method is used to relax the vorticity values in each iteration, if necessary. Let $\{\bar{\xi}_p\} = \{\bar{\xi}_{n+1}\}$ in Eq. (40). We then obtain the predictor step as,

$$[M^*]\{\bar{\xi}_p\} = [M^*]\{\bar{\xi}_n\} + \Delta t [Q^*] - \Delta t [K^*]\{\bar{\xi}_n\} \quad (41)$$

Putting $\{\bar{\xi}_n\} = \frac{1}{2}(\{\bar{\xi}_p\} + \{\bar{\xi}_n\})$ in Eq. (40), we finally get the second-order Runge-Kutta method as,

$$[M^*]\{\bar{\xi}_{n+1}\} = [M^*] \frac{\{\bar{\xi}_p\} + \{\bar{\xi}_n\}}{2} + \Delta t [Q^*] - \Delta t [K^*] \frac{\{\bar{\xi}_p\} + \{\bar{\xi}_n\}}{2} \quad (42)$$

Similar modification is performed for the low Reynolds number problems, in Eq. (39) using Runge-Kutta method. In a similar way, other two vorticity transport equations can be solved in the three-dimensional domain.

4. SOLUTION PROCEDURE

Here an iterative scheme is used in the solution of the velocity-vorticity formulation of Navier-Stokes equations and Stokes flow equations. In most of the incompressible viscous flow problems, the most natural boundary conditions arise when the velocity is prescribed all over the boundaries of the problem. The vorticity boundary conditions are seldom prescribed and hence should be determined from computation. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary condition which are used in the solution of the vorticity transport equations. The solution procedure adopted here includes the following iterative steps:

For the time step $n = 1$,

1. Assume some initial values for vorticity distribution and derivatives.
2. Solve the velocity Poisson equations using BEM
 - Get the unknown boundary velocity or velocity flux values
 - Calculate the velocity distribution and velocity derivatives at all nodal points
 - Determine the new vorticity boundary values
3. Solve the vorticity transport equations using FEM
 - Get the unknown vorticity values throughout the domain
 - Calculate the derivatives of the vorticity vectors to be used in the velocity Poisson equation
 - Relax the vorticity values using second order Runge-Kutta method, if necessary
4. Check for the convergence of the velocity and vorticity components in the present iteration, for example,

$$\frac{|w_{n+1}^k - w_n^k|}{|w_n^k|} \leq 0.001$$

If convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to step 2.

5. In the successive time step, use the velocity and

vorticity components from the previous time step as initial conditions and use the iterative procedure, steps 2 to 4. The procedure is repeated until the prescribed time step is reached.

5. NUMERICAL EXAMPLE

The described BEM-FEM model has been applied on a bench-mark problem to verify the numerical procedure. The test problem is the classical 'driven flow in a cubic cavity' for which many numerical model results are available in literature (see Fig. 1). The model problem consists of a cubic cavity of size $1 \times 1 \times 1$ (dimensionless) with a moving top lid with constant velocity of unity (dimensionless) in the x -direction, totally filled with an incompressible viscous fluid. Figure 1 shows the geometry and boundary conditions of the problem. Reynolds number is so low that the induced motion can be classified as a Stokes flow. It is to be noticed that the boundary conditions of the present problem are all velocities wherein non-zero values are horizontal u -component velocities along the top lid of the cavity. Due to the computational limitations (we used an IBM AIX workstation with 128MB RAM), the present analysis is limited to two sets of computational mesh points of $11 \times 11 \times 11$ and $13 \times 13 \times 13$ (on the boundary as well as internal domain).

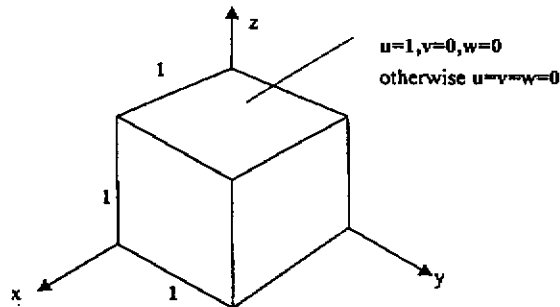


Fig. 1 Model problem with boundary conditions

Two cases have been presented here, for steady state Stokes flow conditions ($Re = 0$) and very low Reynolds number ($Re = 1$) Navier-Stokes equations problems. Figure 2 shows the x -component velocity profile (u) on the vertical centerline and Fig. 3 shows the z -component velocity profile (w) on the horizontal centerline of the cavity for steady state Stokes flow ($Re = 0$) conditions. The results are compared with a series solution [9], FEM solution [10] and BEM solution [11] in two dimensions and are in good agreement, bearing in mind that the mesh density is coarse. As it is obvious, for the two-dimensional comparison, the results vary slightly due to the three dimensional boundary effects.

As a convergence test for the grid, analysis has been done at $Re = 1$ for both the meshes ($11 \times 11 \times 11$ and $13 \times 13 \times 13$). Figure 4 shows the x -component velocity profiles (u) on the vertical centerline and Fig. 5 shows

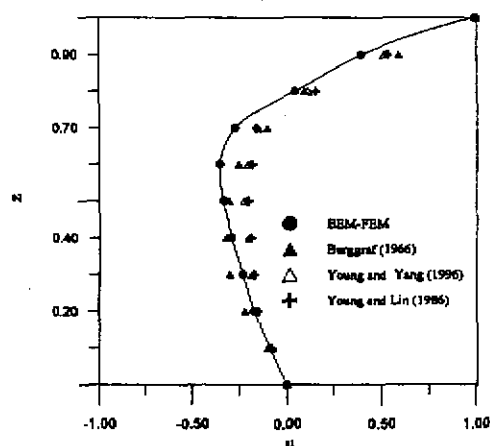


Fig. 2 Velocity profile (u) on vertical centerline of a cubic cavity for $Re = 0$

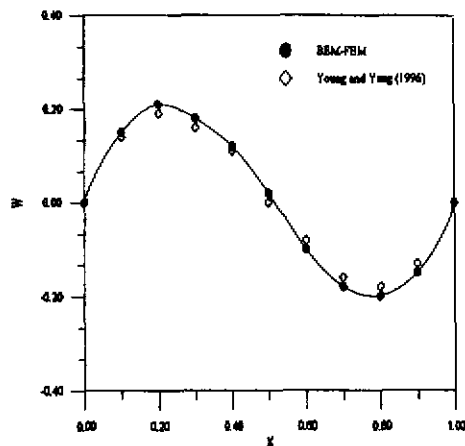


Fig. 3 Velocity profile (w) on horizontal centerline of a cubic cavity for $Re = 0$

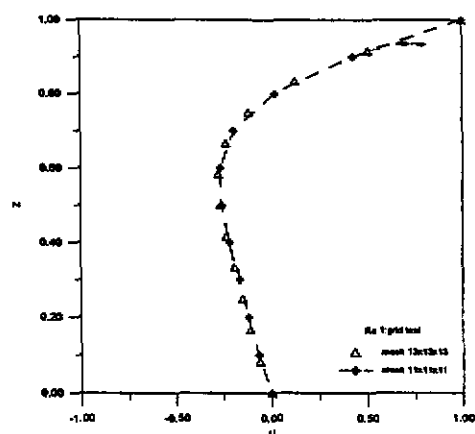


Fig. 4 Velocity profile (u) on vertical centerline of a cubic cavity for $Re = 1$

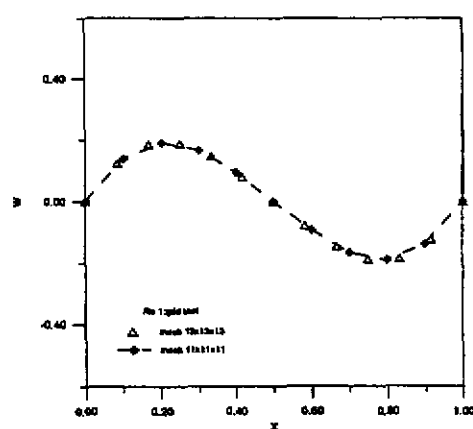


Fig. 5 Velocity profile (w) on horizontal centerline of a cubic cavity for $Re = 1$

the z -component velocity profile (w) on the horizontal centerline of the cavity for $Re = 1$, for both the meshes. The results seem to be almost the same for both the meshes and hence $11 \times 11 \times 11$ mesh has been used in further analysis. The velocity vectors, u vs. w at $y = 1/2$ plane, u vs. v at $z = 1/2$ plane and v vs. w at $x = 1/2$ plane for $Re = 1$, are shown in Figs. 6(a), 6(b) and 6(c), respectively. The distribution of vorticity components ξ at $x = 1/2$ plane, η at $y = 1/2$ and ζ at $z = 1/2$ plane, are also shown in Figs. 7(a), 7(b) and 7(c), respectively.

A comparison of the x -component velocity profiles (u) on the vertical centerline for $Re = 0$ (steady state Stokes flow) and $Re = 1$ (very low Reynolds number Stokes flow problem solved with Navier-Stokes equations) is shown in Fig. 8. As obvious from the Fig. 8, there is an observable difference in the velocity profile for both Stokes flow regimes for $Re = 0$ and $Re = 1$. A comparison of vorticity profile of η component in the $y = 1/2$ plane for $Re = 0$ and $Re = 1$ also shows that large vorticity is obtained for the $Re = 1$ case, although the pattern is almost the same. The nonlinear convective effects have a tendency to increase the vorticity and

velocity intensities. Hence, when low Reynolds number Stokes flow are to be solved, Navier-Stokes equations should be considered for accurate solutions.

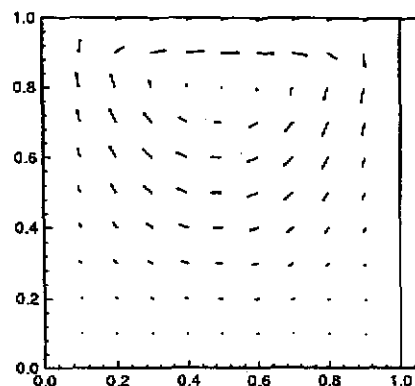


Fig. 6(a) Profile of the flow vector (u vs. w) in the $y = 1/2$ plane for $Re = 1$

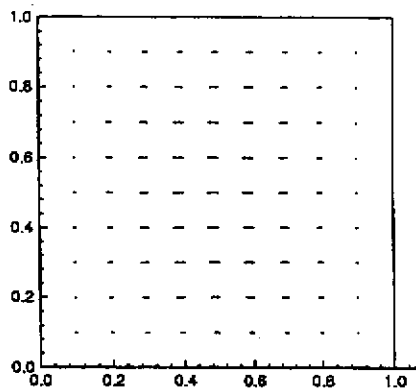


Fig. 6(b) Profile of the flow vector (u vs. v) in the $z = 1/2$ plane for $Re = 1$

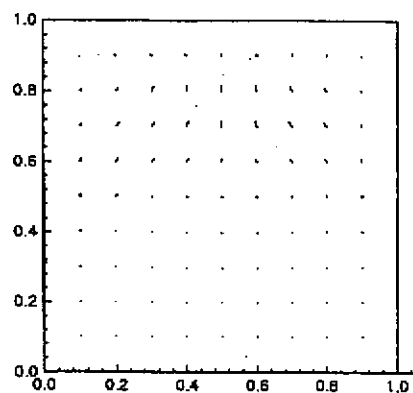


Fig. 6(c) Profile of the flow vector (v vs. w) in the $x = 1/2$ plane for $Re = 1$

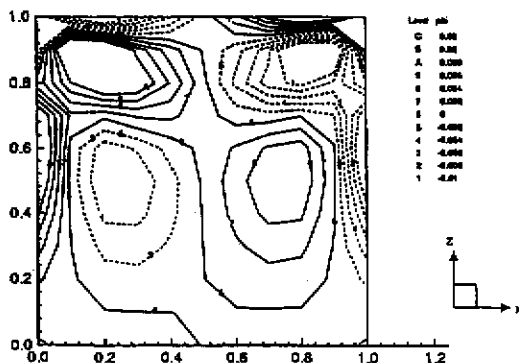


Fig. 7(a) Vorticity profile (ξ) in the $x = 1/2$ plane for $Re = 1$

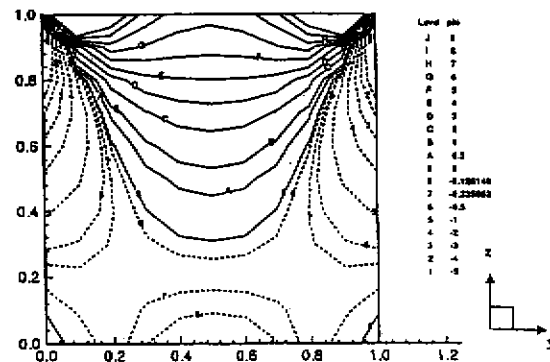


Fig. 7(b) Vorticity profile (η) in the $y = 1/2$ plane for $Re = 1$

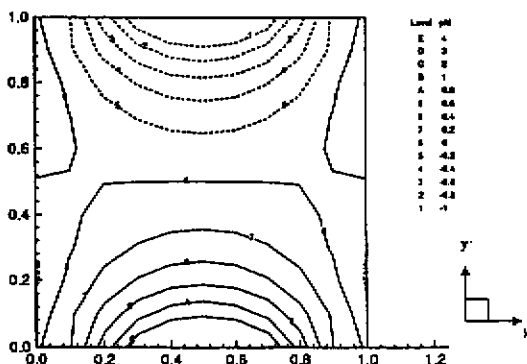


Fig. 7(c) Vorticity profile (ζ) in the $z = 1/2$ plane for $Re = 1$

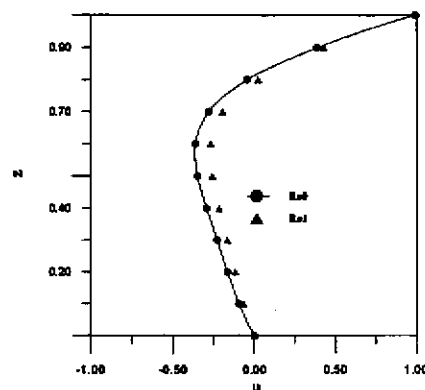


Fig. 8 Comparison of velocity profile (u) on vertical centerline of a cubic cavity for $Re = 0$ and $Re = 1$

The merit of the present model is that, it provides the best way to treat the velocity-vorticity formulation for three-dimensional flow by combining BEM and FEM together. In general, the boundary conditions of vorticity are not known *a priori*, so that the solution of vorticity transport equation is rather difficult. However the BEM solution of the velocity Poisson equation will automatically render the necessary vorticity boundary condition. This study demonstrates that even with a very coarse mesh, the solutions are very stable and accurate as shown in Figs. 4, 5, 6 and 7.

6. CONCLUDING REMARKS

A combined BEM-FEM model has been developed for solving the velocity-vorticity Navier-Stokes and Stokes flow equations in three dimensions. The vorticity boundary conditions for the solution of vorticity transport equations are exactly obtained directly from the BEM solution of velocity Poisson equations. Here the results of low Reynolds number Stokes flow problems, in a typical cubic cavity flow are

presented and compared with other numerical models. Computational results show that the combined BEM-FEM presented here provides an efficient tool for numerical investigation of three-dimensional incompressible viscous fluid in slow motion.

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以速度－渦度列式法求解三維不可壓縮流場

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摘要

本文利用速度－渦度列式法採用有限差分法來求解不可壓縮、粘性流體之運動，以三維穴流及三維後向階梯流場為例，分別進行數值計算工作。數值模式以顯示Adams-Bashforth法來求解Helmholtz vorticity transport equation；對速度之Poisson方程式則利用快速傅利葉轉換(FFT)法直接解出。配合MAC交錯網格系統，在求解過程不需要渦度的邊界條件，且速度與渦度在求解過程中可以不必疊代程序，數值解的精確度不論在時間或空間上都具二階精確度。初步研究結果經與前人研究之實驗及數模比較，顯示本文數值模式相當成功。

關鍵字：速度－渦度列式法，三維流，穴流，後向階梯流。

Velocity -Vorticity Formulation for 3D Incompressible Flow

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Abstract

The motion of incompressible and viscous fluid in a three-dimensional square cavity and three-dimensional backward-facing step are solved by the finite difference method using the velocity-vorticity formulation.

For the calculation of vorticity transport equation, explicit Adams-Bashforth scheme is proposed. The Fast Fourier Transform (FFT) is suggested to directly solve the velocity Poisson's equation. In conjunction with staggered grid system, the boundary condition of vorticity is satisfied automatically and without any consideration.

Iteration process is not necessary in the solving process between velocity and vorticity of proposed numerical method. By the way, the numerical solution reaches second-order accuracy in both time and space. The preliminary results of this study show that the numerical method is quite successful.

Keywords: velocity-vorticity formulation, three-dimensional flows, cavity flow, backward-facing step flow.

一、前言

流體中分離流的行為在流體力學上一直是受關注的研究課題，為瞭解其特有之物理意義亦吸引眾多學者投入研究，往往從較簡單之幾何形狀著手，從事相關實驗或數值計算之研究工作。分離流可定義為：鄰近固體邊界迴流區流場，其迴流區位置以“渦流泡”之離開和再接觸而定，通常以鄰近邊界之零渦度來區分。例如：1.凸擴管流場 2.孔口流場 3.渠流越流過一階梯或薄欄 4.穴流流場 5.後向階梯流場。

每一結構流場皆有其不同的邊界條件，亦隨趨動流體和質量傳遞與動量交換亦會使流場問題更顯示不同狀況。這些流動問題為典型的初始~邊界值問題，配合流場適當的初始及邊界條件，即能求得任何時刻之流場解答。本文研究以穴流及後向階梯流場為主軸，以數值模式測試流場穴流之流場特徵，三維穴流為上部流體受拉動，順沿邊壁於中央形成一大尺度之主漩渦生成過程中，由於邊壁剪力阻減邊界層流內動量及邊壁折角駐壓的阻滯效應，遂在角落產生分流，生成小尺度的二次漩渦(secondary eddies)。它常見於許多工程上之應用，如土木水利工程中河川渠道、水壩、輸水管路之閘門導槽及衛生下水道之底槽等之相關應用。至於後向階梯流特徵，為入流場流向一突擴區域，會有向下角落產生分離流及在更下游處分別于上下邊界有再接觸長度之分離迴流泡產生，其間流場會隨Re數之增加而有不同變化。至於後向階梯流場猶如流經一突然擴大流場，隨入流之長寬不同流場亦會有不同變化，本文於此流場之比較採用 Armaly *et. al.* [1]之實驗資料作用數值模擬驗證。

由頂蓋拖動之穴流流場實驗首先由 Pan and Acrivos [2]從事研究，數值模擬由頂蓋拖動之穴流流場問題之先鋒者為 Burggraf [3]，很多此型之相關研究皆為二維模式 Ghia *et. al.* [4]，但實際穴流流況則為三維流場。近年來PC硬體之快速發展促使三維流場之數值研究較為可行，如 Babu and Korpela [5]及 Chiang, Hwang and Sheu [6]等。對於數值方法，速度-渦度法是利用渦度傳輸擴散方程式，及速度的Poisson方程式來求解流場，其主要困難在於渦度的邊界條件之處理及速度與渦度間互相關聯，必需疊代求解。利用本方法來求解流場如 Fusegi and Farouk [7], Giannattasio and Napolitano [8]，劉與楊[9]等。

本文延伸廖等人[10]所發展的二維模式推廣至三維流場，利用有限差分交錯網格(staggered grid system)，不需要渦度的邊界條件，且速度與渦在求解過程不須疊代程序，數值計算結果顯示本研究之數值模式相當成功。

二、理論模式

2.1 控制方程式

1.不可壓縮Navier-Stokes方程式

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \frac{1}{Re} \nabla^2 \vec{u} \quad (2)$$

式中 $\vec{u} = u\vec{i} + v\vec{j} + w\vec{k}$ 為流體速度， p 為流體壓力， ρ 為流體密度， Re 為 Reynolds number， $Re = VL/\nu$ ， V 為特性速度， L 為特性長度， ν 為流體運動粘滯性係數。

2.定義渦度 $\vec{\omega}$

$$\vec{\omega} = \nabla \times \vec{u} \quad (3)$$

$$\omega_1 = \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} \quad (4)$$

$$\omega_2 = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \quad (5)$$

$$\omega_3 = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (6)$$

$$\vec{\omega} = \omega_1 \vec{i} + \omega_2 \vec{j} + \omega_3 \vec{k}$$

3.渦度傳輸方程式

對(2)式取旋度(curl)，可得

$$\frac{\partial \vec{\omega}}{\partial t} - \nabla \times (\vec{u} \times \vec{\omega}) = \frac{1}{Re} \nabla^2 \vec{\omega} \quad (7)$$

(7)式可進一步寫成

$$\frac{\partial \vec{\omega}}{\partial t} + \vec{u} \cdot \nabla \vec{\omega} = \vec{\omega} \cdot \nabla \vec{u} + \frac{1}{Re} \nabla^2 \vec{\omega} \quad (8)$$

我們可利用(7)式或(8)式來求解渦度。(8)式一般稱為 Helmholtz vorticity transport equation。

4.速度的Poisson方程式

由(4)-(6)式及(1)式，吾人可導出速度必須滿足下列的 Poisson 方程式

$$\nabla^2 u = \frac{\partial \omega_2}{\partial z} - \frac{\partial \omega_3}{\partial y} \quad (9)$$

$$\nabla^2 v = \frac{\partial \omega_3}{\partial x} - \frac{\partial \omega_1}{\partial z} \quad (10)$$

$$\nabla^2 w = \frac{\partial \omega_1}{\partial y} - \frac{\partial \omega_2}{\partial x} \quad (11)$$

所謂速度-渦度法就是利用(7)或(8)式配合(9)-(11)式來求解流場，而不由原來的 Navier-Stokes 方程式，即(1)和(2)式來求解。由於速度及渦度都是向量，在三維流場中共有6個變數待解，較原來問題4個變數要多解二條方程式，故一般很少使用這種方法來求解三維流動問題，但本文嘗試此方法來求解，在數值模式中為一大挑戰。

2.2 邊界條件

1. 固體邊界條件

不可滑動條件，即速度在固體邊界上為零。

$$\vec{u} = 0 \text{ on solid boundary} \quad (12)$$

2. 出流邊界條件

對於出流邊界之處理，本文採用線性對流條件，即在出流附近流體的渦度係以平均速度向下游傳遞。

$$\frac{\partial \omega}{\partial x} + V \frac{\partial \omega}{\partial x} = 0 \text{ on outflow } x = L \quad (13)$$

V為入流之平均速度。

三、數值計算方法

3.1 渦度方程式的計算方法

利用顯式二階Adams-Bashforth法來離散(7)式，可得

$$\frac{\omega_1^{n+1} - \omega_1^n}{\Delta t} + 1.5A^n - 0.5A^{n-1} = 0 \quad (14)$$

$$\frac{\omega_2^{n+1} - \omega_2^n}{\Delta t} + 1.5B^n - 0.5B^{n-1} = 0 \quad (15)$$

$$\frac{\omega_3^{n+1} - \omega_3^n}{\Delta t} + 1.5C^n - 0.5C^{n-1} = 0 \quad (16)$$

式中

$$A = \frac{\delta_y}{\Delta y}(\nu \omega_1) + \frac{\delta_z}{\Delta z}(w \omega_1) - \frac{\delta_y}{\Delta y}(\omega_2 u) - \frac{\delta_z}{\Delta z}(\omega_3 u) - \frac{1}{\text{Re}} \left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2} + \frac{\delta_z^2}{\Delta z^2} \right) \omega_1$$

$$B = \frac{\delta_x}{\Delta x}(u \omega_2) + \frac{\delta_z}{\Delta z}(w \omega_2) - \frac{\delta_x}{\Delta x}(\omega_1 u) - \frac{\delta_z}{\Delta z}(\omega_3 u) - \frac{1}{\text{Re}} \left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2} + \frac{\delta_z^2}{\Delta z^2} \right) \omega_2$$

$$C = \frac{\delta_x}{\Delta x}(u \omega_3) + \frac{\delta_y}{\Delta y}(\nu \omega_3) - \frac{\delta_x}{\Delta x}(\omega_1 w) - \frac{\delta_y}{\Delta y}(\omega_2 w) - \frac{1}{\text{Re}} \left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2} + \frac{\delta_z^2}{\Delta z^2} \right) \omega_3$$

其中 $\Delta x, \Delta y, \Delta z$ 為網格在 x, y, z 方向的間距， $\delta_x, \delta_y, \delta_z$ 為一次中央差分運算子， $\delta_x^2, \delta_y^2, \delta_z^2$ 為二次中央差分運算子。

以上的數值方法，不論在時間或空間上都可獲得二階精確度的數值解答，而數值穩定條件仍受CFL條件及擴散項條件控制，即

$$\left| \frac{u \Delta t}{\Delta x} \right| \leq 1, \left| \frac{v \Delta t}{\Delta y} \right| \leq 1, \left| \frac{w \Delta t}{\Delta z} \right| \leq 1 \quad (17)$$

$$\text{及 } \frac{\Delta t}{\text{Re}} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) \leq \frac{1}{2} \quad (18)$$

對高雷諾數流場數值模式之數值穩定條件主要仍受(17)式控制， Δt 與網格間距同級序(order)，對於時變問題的求解較為可行。

3.2 速度Poisson方程式之計算方法

(a) 速度 u^{n+1}

$$\left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2} + \frac{\delta_z^2}{\Delta z^2} \right) u^{n+1} = \frac{\delta_x}{\Delta x} \omega_2^{n+1} - \frac{\delta_y}{\Delta y} \omega_3^{n+1} \quad (19)$$

$$\text{with } u^{n+1} = 0 \text{ on } x=0, M \text{ 邊界} \quad (20)$$

$$\frac{\delta_y}{\Delta y} u^{n+1} = -\omega_3^{n+1} + \frac{\delta_x}{\Delta x} v^{n+1} \text{ on } y=0, N \text{ 邊界} \quad (21)$$

$$\frac{\delta_z}{\Delta z} u^{n+1} = \omega_2^{n+1} + \frac{\delta_x}{\Delta x} w^{n+1} \text{ on } z=0, L \text{ 邊界} \quad (22)$$

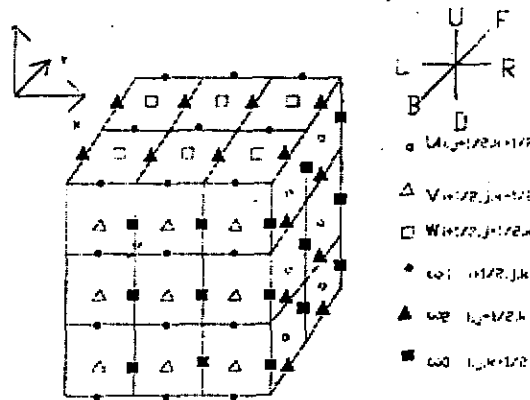


圖1 三維流場之網格配置圖

在MAC交錯網格系統下(如圖1所示)，以上系統可整理為

$$\nabla^2 u^{n+1} = F^* \quad (19)$$

$$\text{with } u^{n+1} = 0 \text{ on } x=0, M \text{ 邊界} \quad (20)$$

$$\frac{\delta_y}{\Delta y} u^{n+1} = 0 \text{ on } y=0, N \text{ 邊界} \quad (21)$$

$$\frac{\delta_x u^{n+1}}{\Delta x} = 0 \quad \text{on } z=0, L \text{ 邊界} \quad (22)$$

(M·N·L依序為X·Y·Z方向之網格數)

對於上述系統，我們利用快速傅利葉法(FFT)直接解出，詳細的計算方法如下：

令

$$u_{i,j+1/2,k+1/2}^{n+1} = \sum_{\ell} \sum_m \sum_n a_{\ell mn} \sin(\ell \pi x_i) \cos(m \pi y_{j+1/2}) \cos(n \pi z_{k+1/2}) \quad (23)$$

則 u^{n+1} 自動滿足(20')、(21')、(22')之邊界條件。又令

$$F^* = \sum_{\ell} \sum_m \sum_n b_{\ell mn} \sin(\ell \pi x_i) \cos(m \pi y_{j+1/2}) \cos(n \pi z_{k+1/2}) \quad (24)$$

將(23)·(24)式代入(19')式中整理可得

$$a_{\ell mn} = \frac{-b_{\ell mn}}{4 \left(\frac{\sin^2 \frac{\ell \pi \Delta x}{2}}{\Delta x^2} + \frac{\sin^2 \frac{m \pi \Delta y}{2}}{\Delta y^2} + \frac{\sin^2 \frac{n \pi \Delta z}{2}}{\Delta z^2} \right)} \quad (25)$$

其求解程序如下：

(1)由(24)式利用快速傅利葉轉換求出 $b_{\ell mn}$

(2)利用(25)式計算出 $a_{\ell mn}$

(3)由(23)式利用快速傅利葉反轉換求出 u^{n+1}

對於速度的邊界條件在(21)、(22)式中，我們採用Neumann邊界條件，而不直接使用速度的Dirichlet邊界條件，這種處理方式可以不必先知道渦度之邊界值，即能解出速度場。也就是這種數值處理方法，才使得速度與渦度在求解程序中可以不需疊代，大大的提昇數值計算的效率。

(b)速度 v^{n+1}

$$\left(\frac{\delta_x^2}{\Delta x^2} + \frac{\delta_y^2}{\Delta y^2} + \frac{\delta_z^2}{\Delta z^2} \right) v^{n+1} = \frac{\delta_x}{\Delta x} \omega_3^{n+1} - \frac{\delta_z}{\Delta z} \omega_1^{n+1} \quad (26)$$

$$\text{with } \frac{\delta_x v^{n+1}}{\Delta x} = \omega_3^{n+1} + \frac{\delta_y}{\Delta y} u^{n+1} \quad \text{on } x=0, M \text{ 邊界} \quad (27)$$

$$v^{n+1} = 0 \quad \text{on } y=0, N \text{ 邊界} \quad (28)$$

$$\frac{\delta_x v^{n+1}}{\Delta x} = -\omega_1^{n+1} + \frac{\delta_y}{\Delta y} w^{n+1} \quad \text{on } z=0, L \text{ 邊界} \quad (29)$$

整個系統與 u^{n+1} 相似，故數值計算方法與解 u^{n+1} 相同，不再贅述。

(c)速度 w^{n+1} 之計算方法

w^{n+1} 可由 w 的 Poisson 方程式中直接解出，但也可由連續方程式(1)式中計算出來，本文由(1)式中解出，其計算方法如下：

由(1)式

$$\frac{\delta_x}{\Delta x} w^{n+1} = - \left(\frac{\delta_x}{\Delta x} u^{n+1} + \frac{\delta_y}{\Delta y} v^{n+1} \right) \quad (30)$$

對 z 方向微分一次可得

$$\frac{\delta_x^2}{\Delta x^2} w^{n+1} = - \frac{\delta_x}{\Delta x} \left(\frac{\delta_x}{\Delta x} u^{n+1} + \frac{\delta_y}{\Delta y} v^{n+1} \right) \quad (31)$$

$$\text{with } w^{n+1} = 0 \quad \text{on } z=0, L \quad (32)$$

利用(31)·(32)式直接計算出 w^{n+1} ，由於僅為三對角線代數系統故很容易求解。

3.3 數值計算程序

1. 給定流場初始及邊界條件
2. 由(14)·(15)·(16)式中計算所有內點的 $\omega_1^{n+1}, \omega_2^{n+1}, \omega_3^{n+1}$
3. 由(19)·(20)·(21)·(22)式中利用FFT解出 u^{n+1}
4. 由(26)·(27)·(28)·(29)式中利用FFT解出 v^{n+1}
5. 由(31)·(32)式中解出 w^{n+1}
6. 設定 $u^{n+1}, v^{n+1}, w^{n+1}$ 及 $\omega_1^{n+1}, \omega_2^{n+1}, \omega_3^{n+1}$ 之邊界值。
7. 重複2-6直到所求時間之流場解。

四、計算結果與討論

4.1 數值模式之驗證

利用速度-渦度法來求解三維流動問題，模式建立成功後，我們以三維穴流問題進行驗證前人的工作。在一長寬高為1:3:1的長方形渠槽中，上板以 $u=1$ 的速度拖動，流場示意圖如圖2所示。數值計算以 $Re=1500$ 為模擬對象，採用 $48 \times 144 \times 48$ 的網格系統， $\Delta t=0.01$ 。數值計算所採用的網格為 u, v, w 及 $\omega_1, \omega_2, \omega_3$ 交錯配置的網格系統，如圖1所示。這種變數交互配置的網格系統，在邊界條件上的處理有很大的優點，即速度與渦度在求解過程不需要疊代程序。圖3為數值計算結果之流場解答，經與蔣(1996)之結果比較，如圖4，證實數值模式確實無誤。

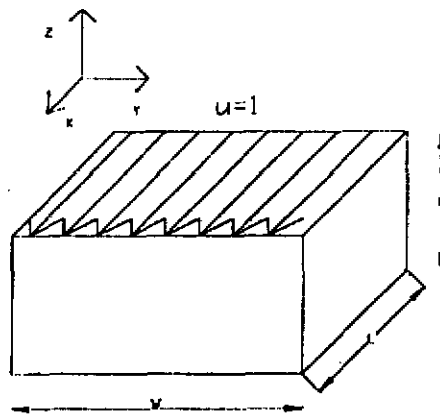
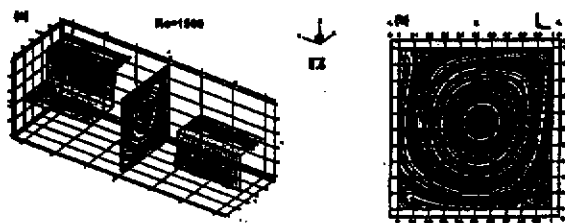
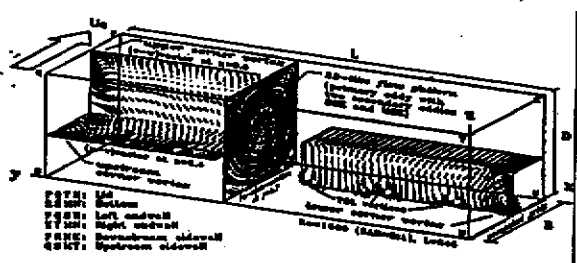
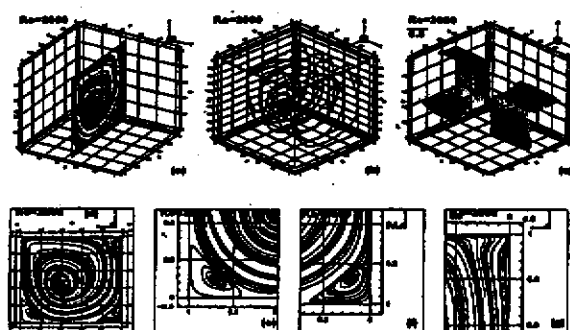


圖2 三維穴流流場示意圖

圖3 三維穴流 $Re=1500$ 之數值模擬圖圖4 三維穴流 $Re=1500$ 之流場 (蔣, 1996)圖6 三維穴流 $Re=2000$ 之數值模擬圖

2. $Re=2000$, $72 \times 72 \times 72$ 網格, 流場已為暫態(Transient), 不再具有穩態解。其流場解答繪於圖6中。可以看出較 $Re=1000$ 之流況更強烈, 其中右下角之迴流區變大, 流線改由上向下以順時鐘旋轉, 右下角及左下角迴流區間有一狹長之流線分離區。整個流況非常穩定, 數值計算結果相當可靠。

(二)三維後向梯流場

根據 Armaly *et al.* [1] 之實驗, 長150mm, 寬180mm, 高10.1mm之渠道中, 入流渠道高5.2mm, 階梯高4.9mm, 如圖7所示。由於具對稱關係, 數值計算取只一半寬, 渠長則取30倍階梯高, 來進行數值模擬, 入流條件係由充分發展之矩形断面流之解析解代入模式中。在層流範圍上述的入流條件與實驗相當一致, 故吾人採用上述的入流條件進行了 $Re=100, 200, 300, 397, 500, 600, 648, 800$ 等案例之計算, 一律採用 $128 \times 64 \times 32$ 的網格系統, 計算結果如圖8、9所示, 圖8為雷諾數100, 200, 300, 397, 圖9則為雷諾數500, 600, 648, 800等中央對稱面速度 u_z 之等值線圖, 左下角落有一迴流區。我們將渠道中央對稱面 ($y=0$ 處) 階梯後迴流泡之再接觸長度 X_r 與雷諾數 Re 之關係繪於圖10, 由圖中可以看出數值計算結果與實驗值相當一致, 且較 Ku *et al.* [11], Jiang *et al.* [12] 及 Williams *et al.* [13] 之三維數值計算亦顯優異。由圖十亦可看出於上邊界處有二次迴流泡 (Secondary vortex structure) 形成, 將其上邊界之再接觸長度 X_r 與 Re 數之關係繪於圖11, 由圖中可以看出數值計算結果大致與實驗值相當。

4.2 數值計算結果

本文以三維穴流及三維後向階梯流場進行數值計算工作, 數值計算結果分別討論如下:

(一)三維方型穴流

我們以1:1:1的三維方型穴流問題, 進行流場模擬, 計算結果如下:

1. $Re=1000$, $48 \times 48 \times 48$ 網格, 流場穩定解如圖5所示。

(a)圖為三維切面流線圖, 在靠近邊界及中心流線較密, 速度較快, 中間帶之流線較稀疏, 流速較慢; (b)圖為三維流線圖, 其水流繞中心以逆時鐘方向轉動, 流況非常穩定; (c)圖為向量圖, 可看出在頂部之水流作用力量相當大, 中央之水流作用較小; (d)圖為(a)圖為之二維流線, 左下角之迴流區比右下角之迴流區大, 兩迴流區內之轉動方向與主要迴流區轉動相反, 為順時鐘; (e)圖為(d)圖左下角迴流區放大圖, 在中心及邊界之迴流較強, 流線由下向上以順時鐘旋轉; (f)圖為(d)圖右下角迴流區放大圖, 水流流動方向為順時鐘, 流況正在發展中; (g)圖為(d)圖右上角迴流區放大圖, 流線上升至頂部時, 遇到強大的水流, 使流線作接近90度的轉彎, 在頂部速度異常大。

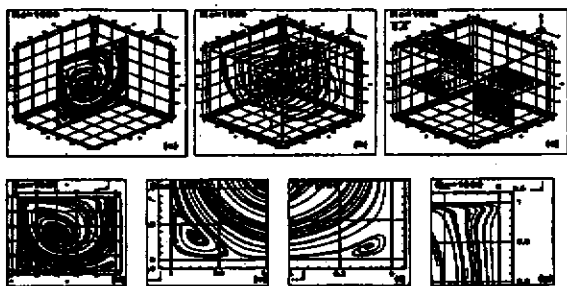
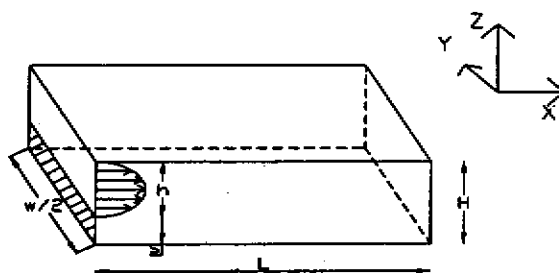
圖5 三維穴流 $Re=1000$ 之數值模擬圖

圖7 三維後向階梯流場示意圖

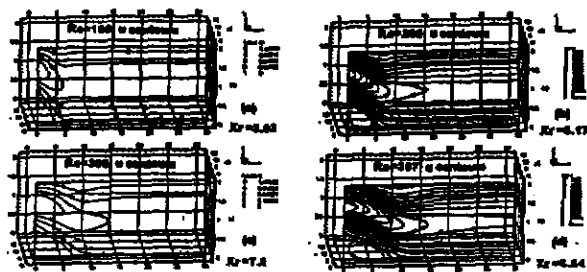


圖8 三維後向階梯流 $Re=100, 200, 300, 397$ 在對稱面速度 u 之等值線圖

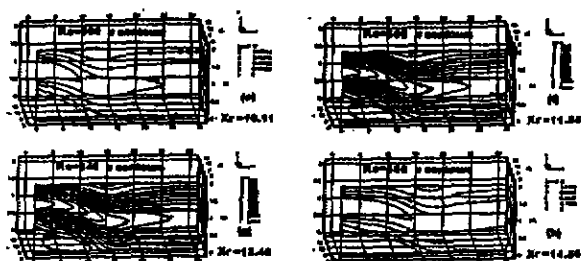


圖9 三維後向階梯流 $Re=500, 600, 648, 800$ 在對稱面速度 u 之等值線圖

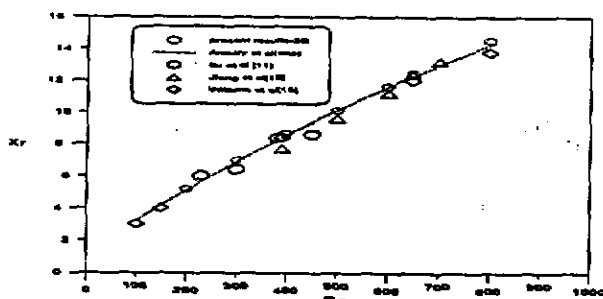


圖10 三維後向階梯流再接觸長度 X_r 與 Re 數之關係實驗與數值模式比較圖

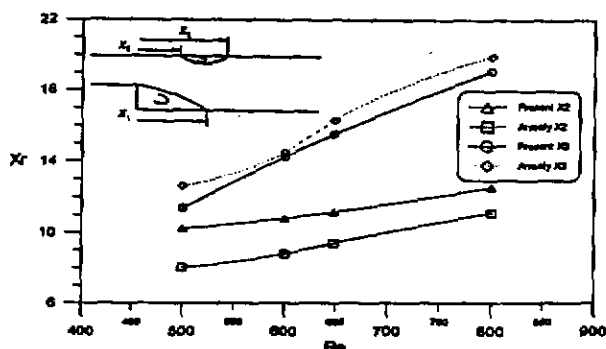


圖11 三維後向階梯流二次迴流泡再接觸長度 X_r 與 Re 數之關係實驗與數值模式比較圖

以上之計算工作皆在個人電腦上執行，PC機型為PENTIUM II-450，所需計算時間，以 $Re=648$ 流場為例： $\Delta t=0.01517$ ，採用 $128 \times 64 \times 32$ 網格，至定常狀態時， $T=156.12$ ，PC每跑一時步需時間為4.52秒，共需實時約12.92小時。

對於 $Re=800$ 的案例，我們再將其流場解答繪於圖12。由(a)圖中可看出，除了在階梯後方出現一個大迴流區外，在上邊界 $X=15$ 處，亦產生一迴流區，其流線相當密集，流況非常激烈；(b)圖為三維流線圖，受到階梯之影響，後方之迴流區相當大，流場解答非常不錯。經過初步的數值模擬結果顯示，本文所提出的速度-渦度法確實可以應用於三維不可壓縮流之求解上。

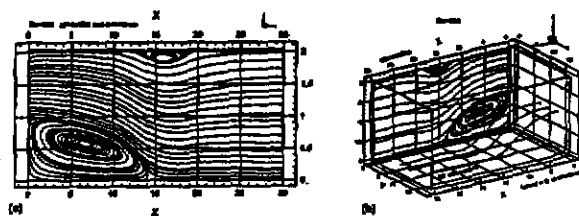


圖12 三維後向階梯流 $Re=800$ 之流線圖

五、結論

1. 本文以速度-渦度列式法來求解三維不可壓縮流動問題，經三維穴流及三維後向階梯流兩案例與前人研究之數值及實驗結果的比較後，證實數值模式相當成功。數值模式採用交錯網格配置，使得在二階精確度下，渦度與速度在求解過程不需要疊代程序，大大地提昇數值計算效率，較傳統速度與壓力間需要疊代略勝一籌。
2. 在後向階梯流的案例中，其出流條件採用線性對流條件，即在出口附近流體係以平均速度向下游傳遞，確實是一種相當不錯的處理方式。
3. 以速度-渦度列式法求解三維流場，需解六條方程式，較原來Navier-Stokes方程式多出二條，但連續方程式可自動滿足，因此仍值得採用。
4. 本文所有計算都在個人電腦上執行，而不必使用大型主機或工作站。將來可朝平行計算發展，改善數值計算速度。

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符號說明

$\bar{\omega}$	: 渦度
V	: 特性速度 (入流之平均速度)
L	: 特性長度
u	: x方向之速度分量
v	: y方向之速度分量
w	: z方向之速度分量
P	: 流體壓力
ρ	: 流體密度
μ	: 流體之動力黏滯係數(dynamic viscosity)
ν	: 流體之運動黏滯係數(kinematic viscosity)
Re	: $Re = \frac{VL}{\nu}$ 雷諾數
Δ	: 網格數及時間間距
Δt	: 時間間距
Δx	: x方向間距
Δy	: y方向間距
Δz	: z方向間距
δ	: 一次差分運算符號
M	: x方向之網格數
N	: y方向之網格數
L	: z方向之網格數

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Solution of the Navier–Stokes equations in velocity–vorticity form using a Eulerian–Lagrangian boundary element method

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SUMMARY

This paper describes the Eulerian–Lagrangian boundary element model for the solution of incompressible viscous flow problems using velocity–vorticity variables. A Eulerian–Lagrangian boundary element method (ELBEM) is proposed by the combination of the Eulerian–Lagrangian method and the boundary element method (BEM). ELBEM overcomes the limitation of the traditional BEM, which is incapable of dealing with the arbitrary velocity field in advection-dominated flow problems. The present ELBEM model involves the solution of the vorticity transport equation for vorticity whose solenoidal vorticity components are obtained iteratively by solving velocity Poisson equations involving the velocity and vorticity components. The velocity Poisson equations are solved using a boundary integral scheme and the vorticity transport equation is solved using the ELBEM. Here the results of two-dimensional Navier–Stokes problems with low–medium Reynolds numbers in a typical cavity flow are presented and compared with a series solution and other numerical models. The ELBEM model has been found to be feasible and satisfactory. Copyright © 2000 John Wiley & Sons, Ltd.

KEY WORDS: boundary element method; Eulerian–Lagrangian method; Navier–Stokes equations; velocity–vorticity formulation

1. INTRODUCTION

The velocity–vorticity form of the Navier–Stokes equations pioneered by Fasel [1] has been established as an effective formulation for the solution of incompressible viscous flow problems. In the recent times, many researchers used the velocity–vorticity formulation for the calculations of two- and three-dimensional steady and unsteady flows using various numerical methods, such as the finite difference method (FDM) [2], the finite element method (FEM) [3]

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and the boundary element method (BEM) [4]. In most investigations, the governing equations have been written as a system of parabolic- and Poisson-type equations for the components of the vorticity and velocity fields respectively. The main advantage of this formulation includes the numerical separation of the kinematic and kinetic aspects of the fluid flow from the pressure computation, which is determined afterwards from the known velocity and vorticity fields.

The theoretical potential of the BEM for the solution of Navier–Stokes equations has been adequately exposed by various researchers [5]. In the solution of the velocity–vorticity formulation of the Navier–Stokes equations, two different types of equations (Poisson-type and parabolic-type) are to be solved. While the Poisson-type equations can be accurately solved with the BEM [6], the method is not so stable in the solution of the parabolic-type transport equations [7].

While solving the parabolic-type transport equations, the numerical diffusion and dispersion are the two major problems to be concerned with. The popular methods like the upwind FDM [8] and upwind FEM [9] work well only for the problems in which the diffusion effect dominates. In general, the high-order upwind schemes produce numerical oscillations in the results, while the lower-order upwind schemes cannot avoid the numerical diffusion.

The Eulerian–Lagrangian method is a widely used scheme for the transport modeling. It is a combination of the Eulerian method, in which the equation is solved on a fixed grid in space, and the Lagrangian method, which utilizes either a deforming grid or a fixed grid in deforming co-ordinates. The Eulerian–Lagrangian method (ELM) combines aspects of both approaches so as to merge the simplicity of a fixed Eulerian grid with the computational power of the Lagrangian method [10]. In the transport modeling using the ELM, the advection part is solved by the Lagrangian method, which can be computed independently at each time step by the method of characteristics applied to a grid fixed domain. The remaining diffusion part can be solved by the FEM [10,11] or by the FDM [12], or by the BEM on a separate grid. The influence of the advection is projected from one grid to another by local interpolation.

In the present study, an accurate Eulerian–Lagrangian boundary element method (ELBEM) is proposed for the first time for the velocity–vorticity formulation of the Navier–Stokes equations. The Poisson-type equations are solved using the general boundary integral technique with domain integration for the source terms and from which the vorticity boundary conditions are exactly determined. The vorticity transport equation is solved using the ELBEM on a transformed characteristic domain. Based on the concept of the ELM, the formulation of the ELBEM and its associated fundamental solution is obtained for vorticity transport equations. By combining the ELM and BEM, the BEM is made easier to handle the variable velocity field. In this paper, the interpolation procedure for the ELM computation of the convection part is replaced with the process of the more accurate BEM interior point evaluation, and hence the interpolation error is avoided.

The application of the ELBEM model to incompressible viscous flow problems has been demonstrated using the well-known model problem of flow in a driven square cavity. The cavity flow problem is of continuing interest because it offers a relatively simple model on which numerical techniques may be examined and verified with other numerical schemes. Using the ELBEM model, satisfactory results comparable with other models in literature are presented for Reynolds number of up to 2000.

After presenting the governing equations, the numerical formulation using the ELBEM are briefly described. Then the solution procedure and numerical results for the two-dimensional driven cavity flow problem are described, followed by a few concluding remarks.

2. GOVERNING EQUATIONS

The governing equations for mass and linear momentum transport for an incompressible Newtonian fluid can be written as [13]

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{Re} \nabla^2 \bar{u} \quad (1)$$

$$\nabla \cdot \bar{u} = 0 \quad (2)$$

where $\bar{u}$ is the velocity vector, p is the pressure, Re is the Reynolds number and t is the time. Equations (1) and (2) represent the Navier–Stokes equations in the velocity–pressure formulation.

The vorticity vector $\bar{\omega}$ can be expressed as

$$\bar{\omega} = \nabla \times \bar{u} \quad (3)$$

By taking the curl of both sides of Equation (1) and using Equations (2) and (3), we can obtain the vorticity transport equation as follows:

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{Re} \nabla^2 \bar{\omega} \quad (4)$$

By taking the curl of Equation (3) and using Equation (2) we get

$$\nabla^2 \bar{u} = -\nabla \times \bar{\omega} \quad (5)$$

which is the vector form of Poisson's equation for $\bar{u}$.

Equations (4) and (5), with $\bar{u}$ and $\bar{\omega}$ as velocity and vorticity vectors, are known as the velocity–vorticity formulation of the Navier–Stokes equations, and can replace Equations (1) and (2) in which $\bar{u}$ and p are primitive variables.

We seek a solution in the domain Ω , which satisfies the initial conditions

$$\bar{u} = \bar{u}_0, \quad \bar{\omega} = \nabla \times \bar{u}_0 \quad \text{at } t = 0 \quad (6)$$

and the boundary conditions

$$\bar{u} = \bar{u}_\Gamma, \quad \bar{\omega} = (\nabla \times \bar{u})|_\Gamma \quad \text{at } t \geq 0 \quad (7)$$

on the boundary Γ of Ω .

For two-dimensional problems, if (u, v) are the velocity vectors $(\vec{u})$ and ω is the associated vorticity, then from Equation (4), the vorticity transport equation can be written as

$$\frac{\partial \omega}{\partial t} + \vec{u} \cdot \nabla \omega = \frac{1}{Re} \nabla^2 \omega \quad (8)$$

Equation (5) can be written as

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (9)$$

$$\nabla^2 v = \frac{\partial \omega}{\partial x} \quad (10)$$

The solution of the vorticity-transport equation (8), in combination with the velocity Poisson equations (9) and (10) with reference to initial and boundary conditions, gives the velocity and the vorticity distribution all over the domain at the concerned time step.

For the velocity-vorticity formulation, there are certain aspects to be noted [1,14]. Even though the continuity equation has been assumed to be satisfied for the derivation of velocity Poisson equations (9) and (10), it may not be necessarily guaranteed for the integral or difference equations based on the velocity-vorticity formulation. In two-dimensional problems, the continuity equation (2) can be described as

$$D = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (11)$$

Differentiating Equations (9) and (10) for x and y respectively and adding the resulting equations, we get

$$\frac{\partial^2}{\partial x^2} (D) + \frac{\partial^2}{\partial y^2} (D) = 0 \quad (12)$$

As explained by Fusegi and Farouk [14], from the 'maximum principle' it follows that $|D|$ is maximal on the boundary. It can be concluded that continuity ($D = 0$) is ensured in the entire integration domain if it is satisfied on the boundary of the problem. Hence, if care is taken to satisfy the continuity condition to a high degree of accuracy on the boundaries, mass conservation is ensured to an even higher accuracy in the interior of the integration domain of the problem. The vorticity definition can be considered in a similar way [1,14]. For the class of problem analyzed in the present investigations, and by the assumption of no-slip walls on the boundaries, the continuity condition is automatically satisfied.

3. NUMERICAL FORMULATION

As mentioned earlier, in the solution of the velocity-vorticity formulation of Navier-Stokes equations using the present model, the vorticity transport equation (8) is solved using the ELBEM and the Poisson-type velocity equations (9) and (10) are solved using the boundary integral equation scheme. In this section, the numerical formulation is briefly described.

3.1. BEM formulation of velocity Poisson equations

Consider the Poisson-type velocity equation in u and ω , say Equation (9)

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} = b \quad (13)$$

with velocity boundary conditions as

$$u = u_0 \quad \text{on } \Gamma_1, \quad q_0 = \frac{\partial u_0}{\partial n} \quad \text{on } \Gamma_2 \quad (14)$$

where n is the unit outward normal vector. In the present model, an iterative scheme is used such that the vorticity is known in the current iteration and time step from the previous step by solving the vorticity transport equation (8).

Considering $u^* = \ln(r)$ as the fundamental solution of the Laplace equation in two dimensions, from Green's theorem, the boundary integral equation for Equation (13) can be written as

$$C_i u_i = \int_{\Gamma} u q^* d\Gamma - \int_{\Gamma} q u^* d\Gamma + \int_{\Omega} b u^* d\Omega \quad (15)$$

where C_i is Green's constant, $q = \partial u / \partial n$, $q^* = \partial u^* / \partial n$ and r is the distance from the collocation point (k) to other field points (i), defined as

$$r = \sqrt{(x_k - x_i)^2 + (y_k - y_i)^2} \quad (16)$$

Considering Equation (13), $b = -(\partial \omega / \partial y)$. In Equation (15), let the domain integral be represented as

$$B = \int_{\Omega} -\frac{\partial \omega}{\partial y} u^* d\Omega \quad (17)$$

Now from Green's theorem, we can write Equation (17) as

$$B = + \int_{\Omega} \omega \frac{\partial u^*}{\partial y} d\Omega + \int_{\Gamma} \omega u^* dx \quad (18)$$

Now $\partial u^*/\partial y$ can be found as

$$\frac{\partial \ln(r)}{\partial y} = \frac{y_k - y_i}{(x_k - x_i)^2 + (y_k - y_i)^2} \quad (19)$$

Therefore, Equation (18) can be written as

$$B = + \int_{\Omega} \omega \frac{y_k - y_i}{(x_k - x_i)^2 + (y_k - y_i)^2} d\Omega + \int_{\Gamma} \omega u^* dx \quad (20)$$

Now we can write Equation (15) as

$$C_i u_i = \int_{\Gamma} u q^* d\Gamma - \int_{\Gamma} q u^* d\Gamma + \int_{\Omega} \omega \frac{y_k - y_i}{(x_k - x_i)^2 + (y_k - y_i)^2} d\Omega + \int_{\Gamma} \omega u^* dx \quad (21)$$

In a similar way, the boundary integral equation for Equation (10) can be derived using Green's theorem as

$$C_i v_i = \int_{\Gamma} v q^* d\Gamma - \int_{\Gamma} q' u^* d\Gamma - \int_{\Omega} \omega \frac{x_k - x_i}{(x_k - x_i)^2 + (y_k - y_i)^2} d\Omega + \int_{\Gamma} \omega u^* dy \quad (22)$$

where $q' = \partial v / \partial n$.

In Equations (21) and (22), we have boundary integrals and domain integrals. In the present model, the domain integration is carried out by sub-dividing the domain into a series of internal cells, on each of which a numerical integration is performed. Here linear elements are used for the boundary discretization and two-dimensional isoparametric quadrilateral cells are used for the internal discretization. The details of the element properties, shape functions, co-ordinate transformation and numerical integration used here are described in Brebbia *et al.* [6], which are not repeated here.

Here, considering Equation (21), if the domain is discretized into L internal cells, then the domain integral can be written as

$$D_i = \int_{\Omega} \omega \frac{y_k - y_i}{(x_k - x_i)^2 + (y_k - y_i)^2} d\Omega = \sum_{e=1}^L \left[\sum_{k=1}^{NI} w_k \left(\omega \frac{y_k - y_i}{(x_k - x_i)^2 + (y_k - y_i)^2} \right)_k \right] \Omega_e \quad (23)$$

where the integral has been approximated by a summation over different cells (e varies from 1 to L), w_k are the Gauss integration weights, the function needs to be evaluated at integration points k on each cell (k varies from 1 to NI , where NI is the total number of integration points on each cell) and Ω_e is the area of cell e . The term D_i is the result of the numerical integration and is different for each position i of the boundary nodes.

Assuming that the boundary of the domain is discretized into NE linear elements with N nodes, Equation (21) can be discretized and written in matrix form as

$$-C_i u_i + \sum_{j=1}^N \bar{H}_{ij} u_j + D_i = \sum_{j=1}^N (G_{ij} q_j - P_{ij} \omega_j) \quad (24)$$

Combining the effect of the constant term C with the $\bar{H}$ matrix, we can write the system of matrix as

$$Hu + D = Gq - P\omega \quad (25)$$

In Equation (25), the boundary conditions are introduced and the known values are taken to the right-hand side to form a system of linear equations of the form

$$AX = F \quad (26)$$

where X is a vector of unknown boundary values of u and q , and F is a known vector. Equation (26) is solved using a Gauss elimination scheme and all the boundary values will be then known. Once this is done, it is possible to calculate internal values of u or its derivatives. The values of u are calculated at any internal point using Equation (24). Similar procedures are used to calculate the values of v at any internal point using Equation (22).

The main advantage of using the BEM in the solution of the velocity Poisson equations is the exact determination of the vorticity boundary conditions from the velocity flux values that are obtained by the solution of Equation (25). The vorticity boundary condition that is essential to solve the vorticity transport equation is directly obtained as the velocity normal derivative from the solution of Equations (21) and (22), together with the no-slip boundary conditions. If other numerical methods like the FDM or the FEM are used in the solution of velocity Poisson equations, then the vorticity values are to be separately calculated from the velocity values. By doing so, computational error for vorticity may be introduced. Besides, the accuracy of the vorticity boundary conditions is very crucial for the convergence of the velocity-vorticity formulation.

3.2. ELBEM formulation of vorticity transport equation

The vorticity transport equation (8) is very similar to the form of unsteady convective diffusion equation for transport phenomena [Young DL, Wang YF, Eldho TI. Solution of the advection diffusion equation using the Eulerian-Lagrangian boundary element method. *Engineering Analysis with Boundary Elements* 2000 (in press)]. For the solution of Equation (8), the initial and boundary conditions should be prescribed. The initial condition, usually prescribed vorticity, is described throughout the domain at some initial time as

$$\omega = \omega_i(\bar{x}) \quad \text{in } \Omega, \quad t = 0 \quad (27)$$

Two common types of boundary conditions prescribed are

$$\omega = \omega_0(t) \quad \text{on } \Gamma, \quad 0 < t \quad (28)$$

$$q = -\frac{1}{Re} \frac{\partial \omega}{\partial n} + (\bar{u}\omega) \cdot \bar{n} = q_0(t) \quad \text{on } \Gamma_q, \quad 0 < t \quad (29)$$

where q is the normal flux, Ω is the domain and $\Gamma = (\Gamma_t \cup \Gamma_q)$ the boundary.

Owing to the Eulerian–Lagrangian concept, the computational domain is now chosen along the characteristic domain, as shown in Figure 1. The vorticity transport equation is rewritten by a hydrodynamic derivative within this new domain as

$$\frac{D\omega}{Dt} = \frac{1}{Re} \nabla^2 \omega \quad \text{in } \Omega_E \quad (30)$$

where the hydrodynamic derivative is defined as

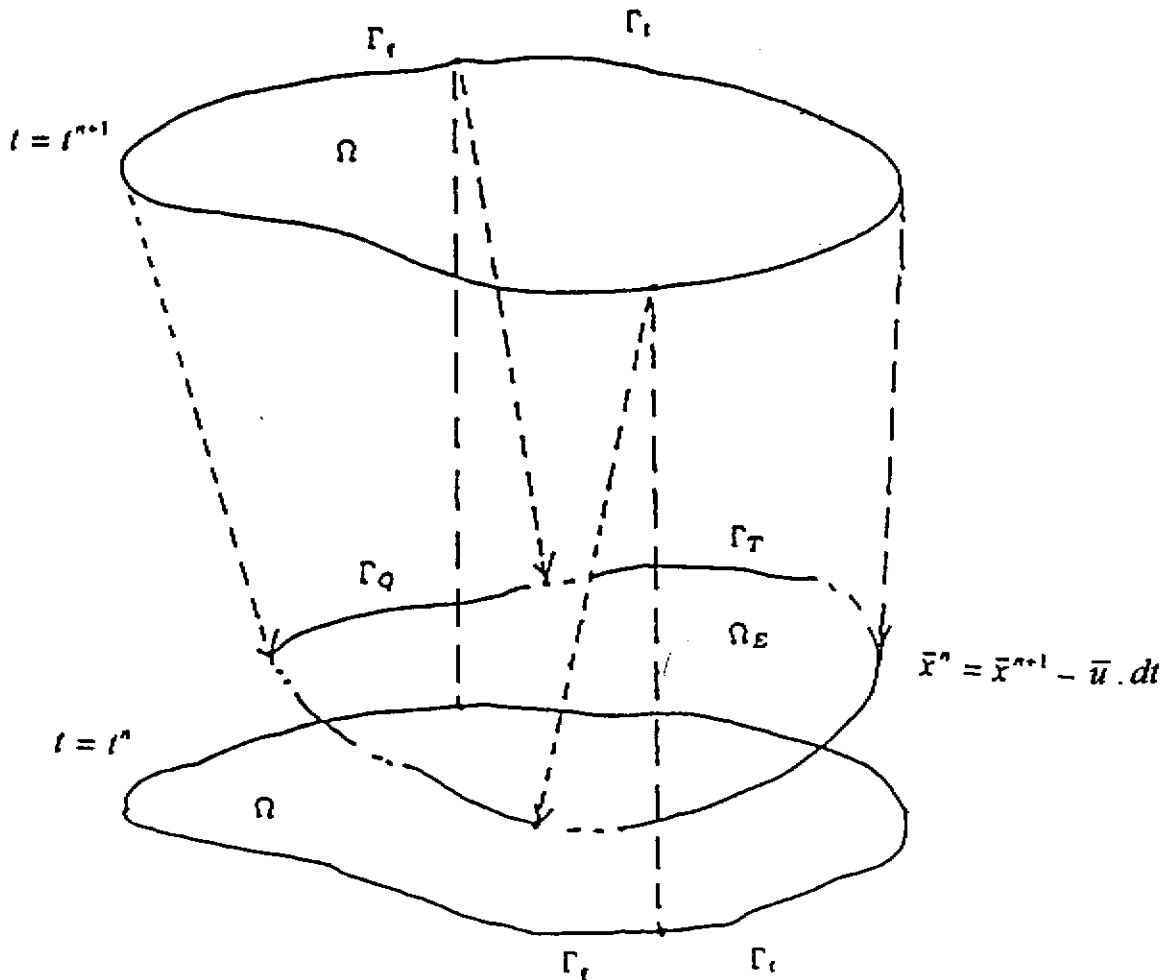


Figure 1. Characteristic domain and boundaries.

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla \quad (31)$$

The initial and boundary conditions are now defined as

$$\omega = \omega_i(\vec{x}) \quad \text{in } \Omega_E, \quad t = 0 \quad (32)$$

$$\omega = \omega_0(t) \quad \text{on } \Gamma_T, \quad 0 < t \quad (33)$$

$$q = -\frac{1}{Re} \frac{\partial \omega}{\partial n} = q_0(t) \quad \text{on } \Gamma_Q, \quad 0 < t \quad (34)$$

Now using Green's second identity, the boundary integral equation can be derived on the characteristic domain as

$$\begin{aligned} \alpha(\vec{x}_b, t^{n+1})\omega(\vec{x}_b, t^{n+1}) &= \int_{t^n}^{t^{n+1}} \int_{\Gamma} \hat{q}(\vec{x}_b, t^n; \vec{x}, t)\omega(\vec{x}, t) d\Gamma_E dt \\ &- \int_{t^n}^{t^{n+1}} \int_{\Gamma} \hat{\omega}(\vec{x}_b, t^n; \vec{x}, t)q(\vec{x}, t) d\Gamma_E dt + \int_{\Omega_E} \hat{\omega}(\vec{x}_b, t^{n+1}; \vec{x}, t^n)\omega(\vec{x}, t^n) d\Omega_E \end{aligned} \quad (35)$$

in which α is the Cauchy principle value, $\vec{x}_b$ is the position vector of base point, $\vec{x}$ is any field point, and q and $\hat{q}$ are the flux terms defined in the following equations:

$$q(\vec{x}, t) = -\frac{1}{Re} \frac{\partial \omega}{\partial n} \quad (36)$$

$$\hat{q}(\vec{x}, t) = -\frac{1}{Re} \frac{\partial \hat{\omega}}{\partial n} \quad (37)$$

The associated fundamental solution $\hat{\omega}$ satisfies the source varying formally adjoint operator of the governing equation (30). That is

$$\frac{D\hat{\omega}}{Dt} - \frac{1}{Re} \nabla^2 \hat{\omega} = \delta(\vec{x} - \vec{x}_i)\delta(t - t^n) \quad (38)$$

Now the fundamental solutions can be easily derived for the one-, two- and three-dimensional problems [15]

$$\hat{\omega}(\vec{x}, t; \vec{x}_b, t^n) = \frac{Re}{[4\pi(t - t^n)]^{k/2}} \exp\left[-\frac{Rer^2}{4(t - t^n)}\right] \quad (39)$$

where $r = |\vec{x} - \vec{x}_i|$ is the Cartesian distance between the base point and the any field point. For one-, two- and three-dimensional problems, k is equal to 1, 2 and 3 respectively.

The integral equation (35) implies that the boundary conditions and initial condition are treated as a continuous distribution of the impulse acting on the domain boundary. The third term on the right-hand side of the integral equation (35), which is in the form of a volume integral, represents the initial effect of the transport equation. The first and second terms on the right-hand side, which are in the form of boundary integrals, express the induced effect of the Dirichlet and Neumann boundary conditions.

For each time step t^{n+1} , the computational domain Ω_E coincides with the physical domain Ω only at $t = t^{n+1}$, and the boundary conditions and initial condition are given on the physical boundary Γ , and the physical domain Ω of time step $t = t^n$. However, the boundary and initial values are required to be imposed in integral terms of Equation (35) on the computational characteristics boundary Γ_E ($\Gamma_T \cup \Gamma_Q$), and the domain Ω_E of time step $t = t^n$. The region of the characteristic domain is determined by the method of characteristics as

$$\frac{d\bar{x}}{dt} = \bar{u} \quad (40)$$

$$\bar{x}^n = \bar{x}^{n+1} - \bar{u} \cdot dt \quad (41)$$

The higher-order fractional step technique, or the Runge–Kutta scheme if necessary, could be used to improve the accuracy of the integration with respect to the time domain.

The boundary element approach [6] is used to solve the boundary integral equation (35) and its associated boundary and initial conditions. Constant, or linear or quadratic shape functions can be used to discretize [6] the temporal and spatial domain respectively, as

$$\omega(\bar{x}, t) = F(t)\omega(\bar{x}, t^{n+1}), \quad F(t) = 1 \quad \text{at } t^n \leq t \leq t^{n+1} \quad \text{on } \Gamma_T \quad \text{and} \quad \Gamma_Q \quad (42)$$

$$q(\bar{x}, t) = F(t)q(\bar{x}, t^{n+1}), \quad F(t) = 1 \quad \text{at } t^n \leq t \leq t_k \quad \text{on } \Gamma_T \quad \text{and} \quad \Gamma_Q \quad (43)$$

$$\omega(\bar{x}, t^{n+1}) = \sum_{j=1}^N S_j(\bar{x})\omega(\bar{x}_j, t^{n+1}) \quad \text{at } t = t^{n+1} \quad \text{on } \Gamma_T \quad \text{and} \quad \Gamma_Q \quad (44)$$

$$q(\bar{x}, t^{n+1}) = \sum_{j=1}^N S_j(\bar{x})q(\bar{x}_j, t^{n+1}) \quad \text{at } t = t^{n+1} \quad \text{on } \Gamma_T \quad \text{and} \quad \Gamma_Q \quad (45)$$

$$\omega(\bar{x}, t) = \sum_{i=1}^M T_i(\bar{x})\omega(\bar{x}_i, t) \quad \text{at } t^n \leq t \leq t^{n+1} \quad \text{on } \Gamma_T \quad \text{and} \quad \Gamma_Q \quad (46)$$

where N is the number of the boundary nodes and M is the number of nodes of the discretization of the volume integral and S and T are all the corresponding shape functions for space. The use of constant elements for the temporal domain allows the analytic integral of time [6] in Equation (35).

After approaching the base point included in the integral equation (35) to the boundary nodes on Ω_E at $t = t^{n+1}$, and imposing the boundary conditions and initial conditions, a simultaneous equations system can be written in the matrix form as

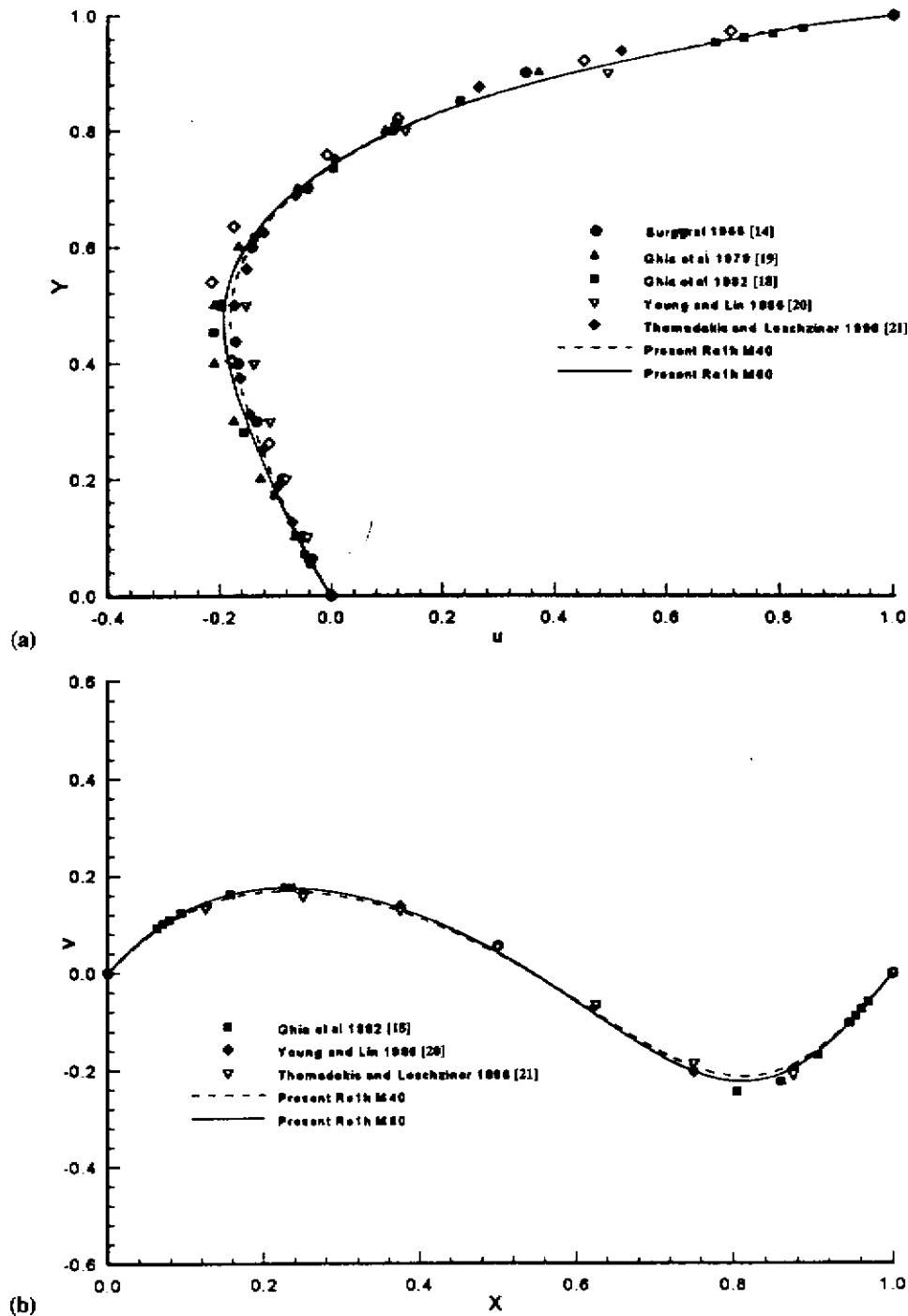
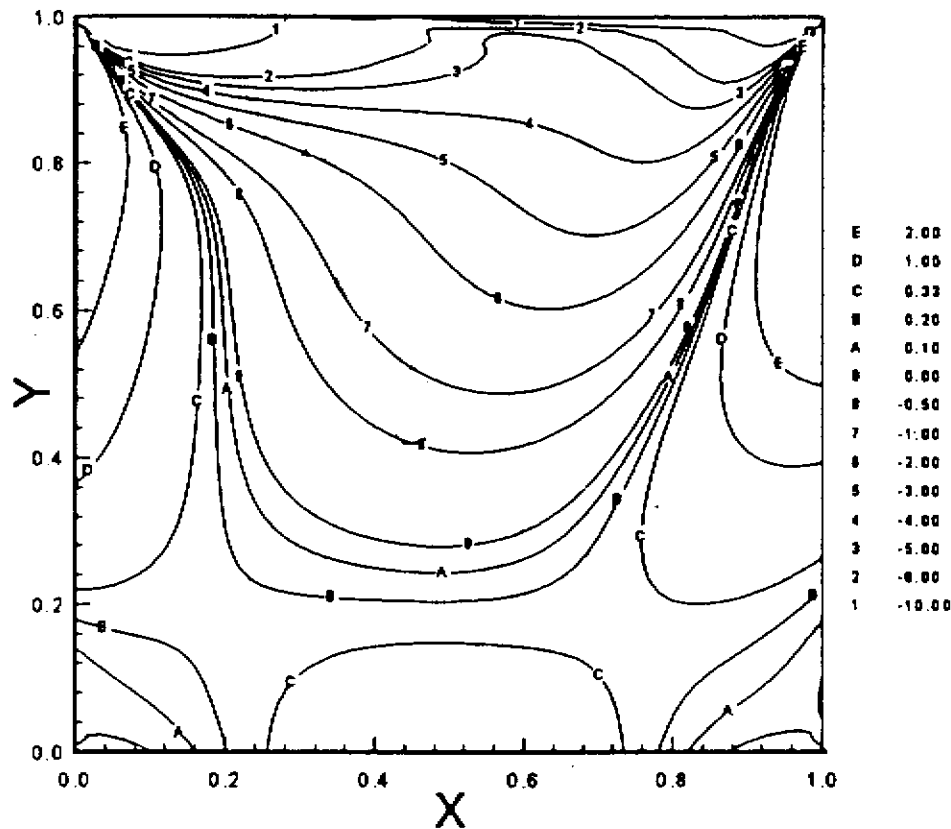


Figure 2. Profile of u (a) and v (b) along the cavity vertical and horizontal centerline of a square cavity for $Re = 100$.

Figure 3. Vorticity distribution for $Re = 100$.

$$[A]_{N \times L_1} \{\omega\}_{L_1 \times 1} + [B]_{N \times L_2} \{q\}_{L_2 \times 1} = \{\text{RHS}\}_{N \times 1} \quad (47)$$

in which L_1 and L_2 are the unknown values of ω and q respectively, and $L_1 + L_2 = N$. If the time difference is the same, the elements included in the matrices $[A]$ and $[B]$ will not be changed for every time step. Only the right-hand side vector $\{\text{RHS}\}$ should be evaluated for each time step due to the changes of the time-dependent boundary conditions and the solutions of the previous time step solutions.

3.3. Determination of streamfunction

The streamfunction distribution of the two-dimensional fluid flow is determined from the following formula:

$$\nabla^2 \psi = -\omega \quad (48)$$

where ψ is the streamfunction. Similar to the BEM formulation of velocity Poisson equations in Section 3.1, the boundary integral equation for Equation (48) can be written as

$$C_i \psi_i = \int_{\Gamma} \psi \frac{\partial \ln(r)}{\partial n} d\Gamma - \int_{\Gamma} \frac{\partial \psi}{\partial n} \ln(r) d\Gamma - \int_{\Omega} \omega \ln(r) d\Omega \quad (49)$$

After the vorticity distribution is determined by solving the vorticity transport equation by introducing the appropriate boundary conditions, the streamfunction distribution can be determined by solving the boundary integral equation (49).

4. SOLUTION PROCEDURE

As mentioned earlier, here an iterative scheme is used in the solution of the velocity-vorticity formulation of Navier-Stokes equations. In most of the incompressible viscous flow problems solved using Navier-Stokes equations, the most natural boundary condition arises when the velocity is prescribed all over the boundaries of the problem. The vorticity boundary conditions are seldom prescribed and hence should be determined iteratively from computations. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary conditions, which are used in the solution of the vorticity transport equation. The computational procedure adopted here includes the following iterative steps:

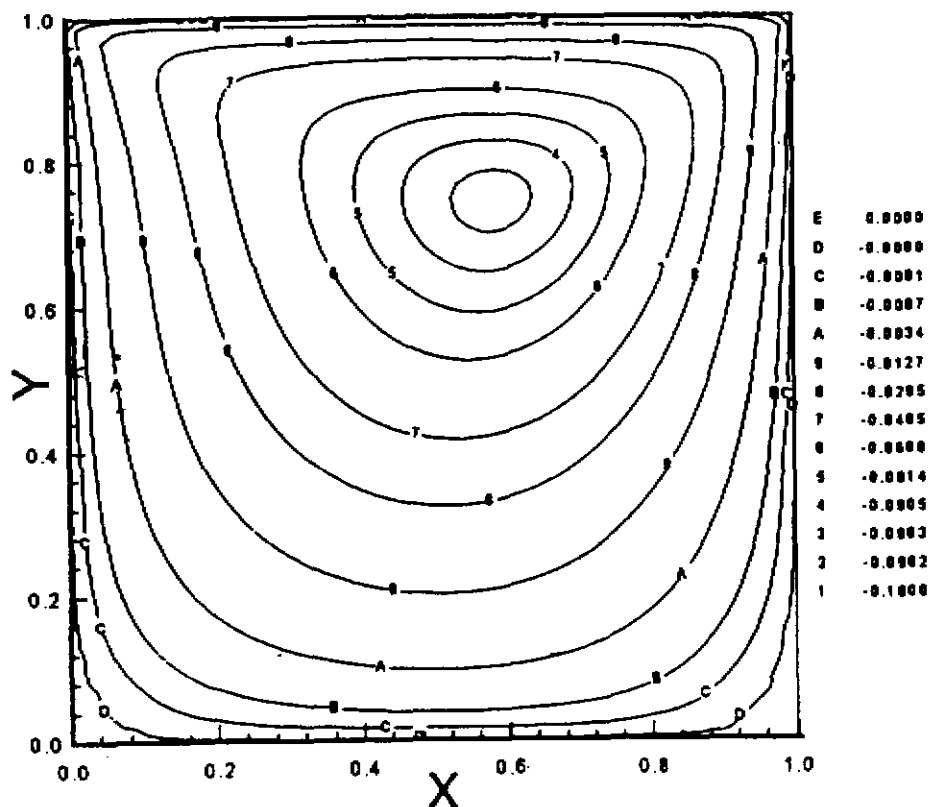


Figure 4. Streamfunction distribution for $Re = 100$.

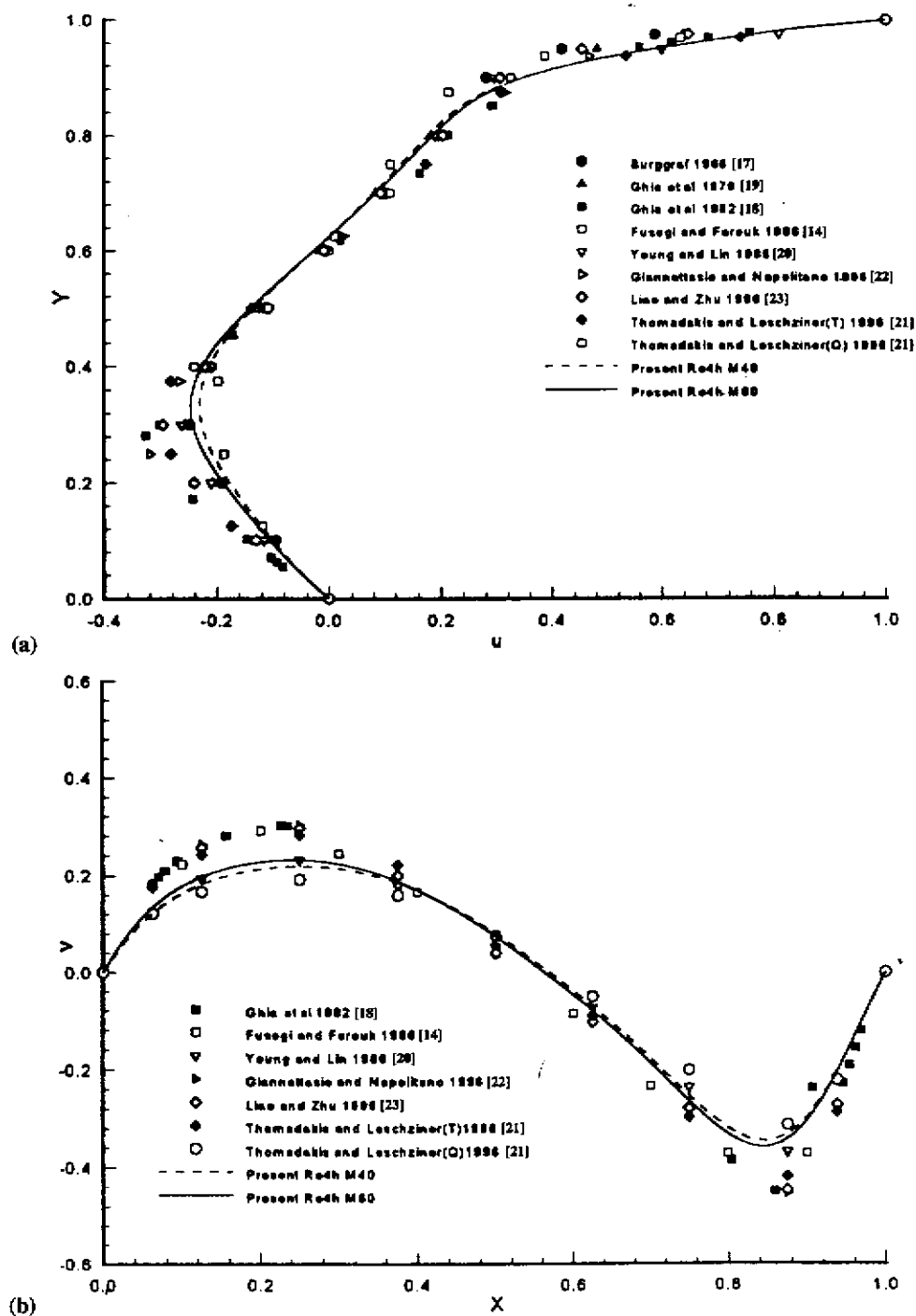


Figure 5. Profile of u (a) and v (b) along the cavity vertical and horizontal centerline of a square cavity for $Re = 400$.

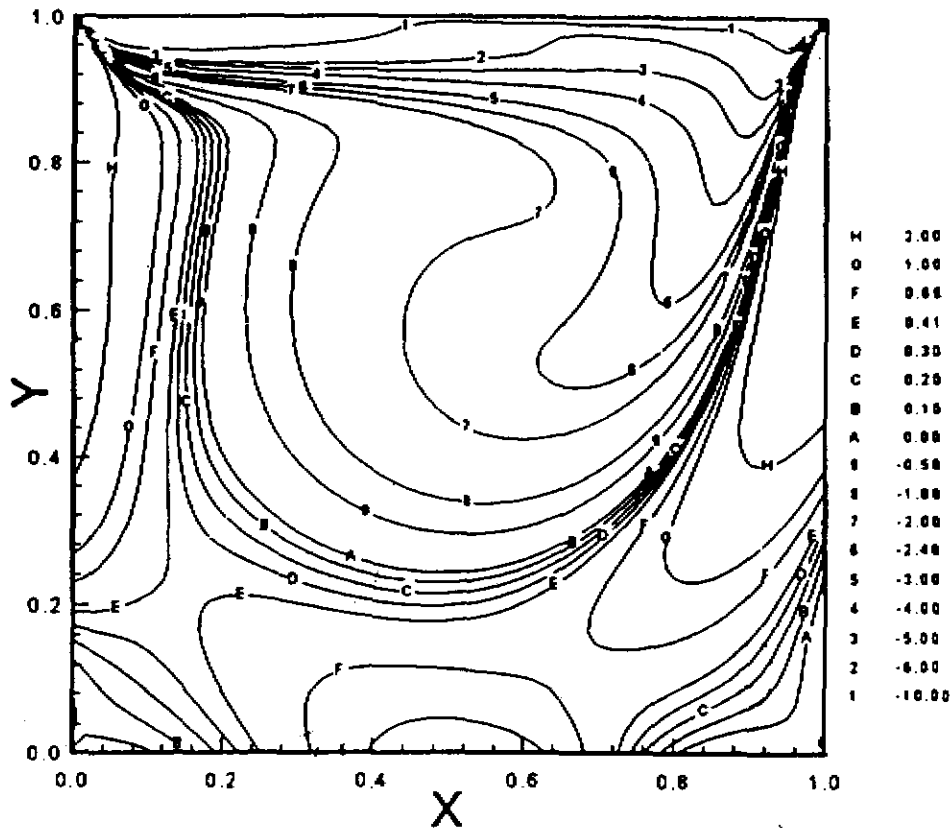


Figure 6. Vorticity distribution for $Re = 400$.

For the time step $n = 1$

1. Assume some initial values for vorticity distribution and derivatives, say zero.
2. Solution of the velocity Poisson equations using the BEM
 - Solve for the unknown boundary velocity or velocity flux values using Equations (9) and (10)
 - Calculate the velocity distribution and velocity derivatives at all nodal points
 - Determine the new vorticity boundary values using Equation (3)
3. Solution of the vorticity transport equations using the ELBEM
 - Solve for the unknown vorticity values throughout the domain using Equation (8)
 - Relax the vorticity values, if necessary
4. Check for convergence of the velocity and vorticity components in the present iteration, for example

$$\frac{|u_n^{k+1} - u_n^k|}{|u_n^k|} \leq 0.001$$

If convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to step 2.

5. In the successive time step, use the velocity and vorticity components from the previous time step as initial conditions and use the iterative procedure, steps 2–4. The procedure is repeated until the prescribed time step is reached.

In order to validate the self-consistency of the present formulation, calculations were made to ensure the satisfaction of mass balance conditions in the entire domain for all the computations. In all the calculations, mass balances were satisfied within 0.1 per cent.

For the unsteady computations, the time step was chosen with variations in Reynolds number and the mesh size, according to the condition given by Liu and Dane [16] as

$$\frac{1}{Re} \Delta t \left(\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right) \leq \frac{1}{2} \quad (50)$$

where Δx and Δy are the mesh size in the x - and y -Cartesian directions.

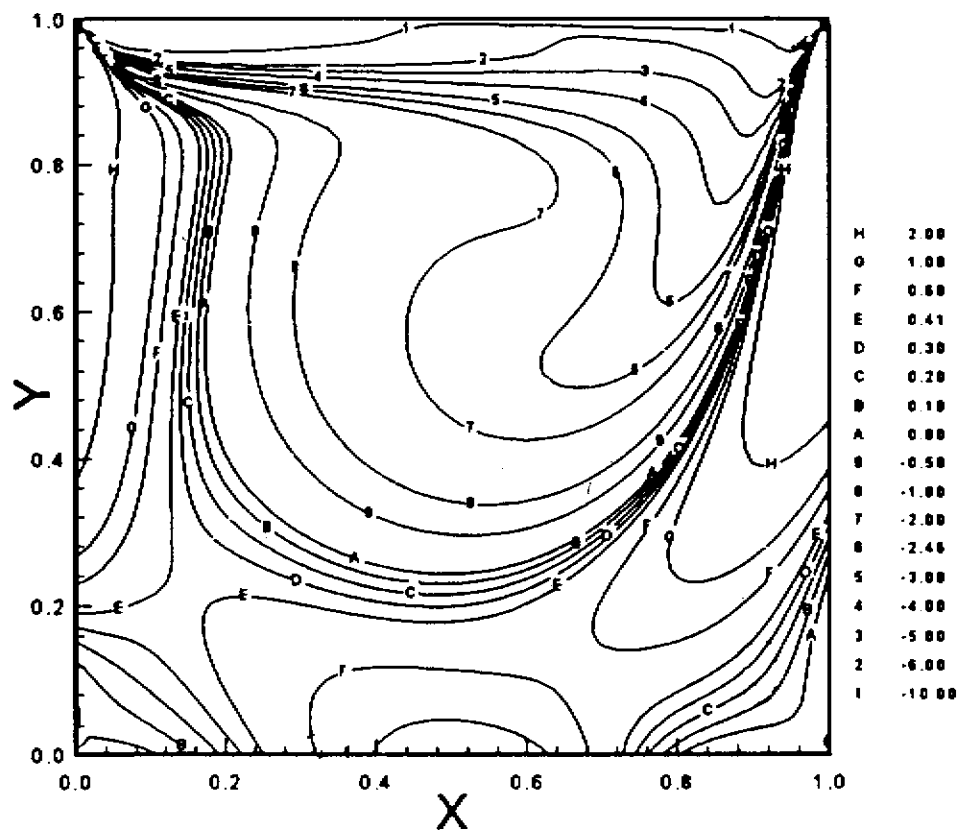


Figure 7. Streamfunction distribution for $Re = 400$.

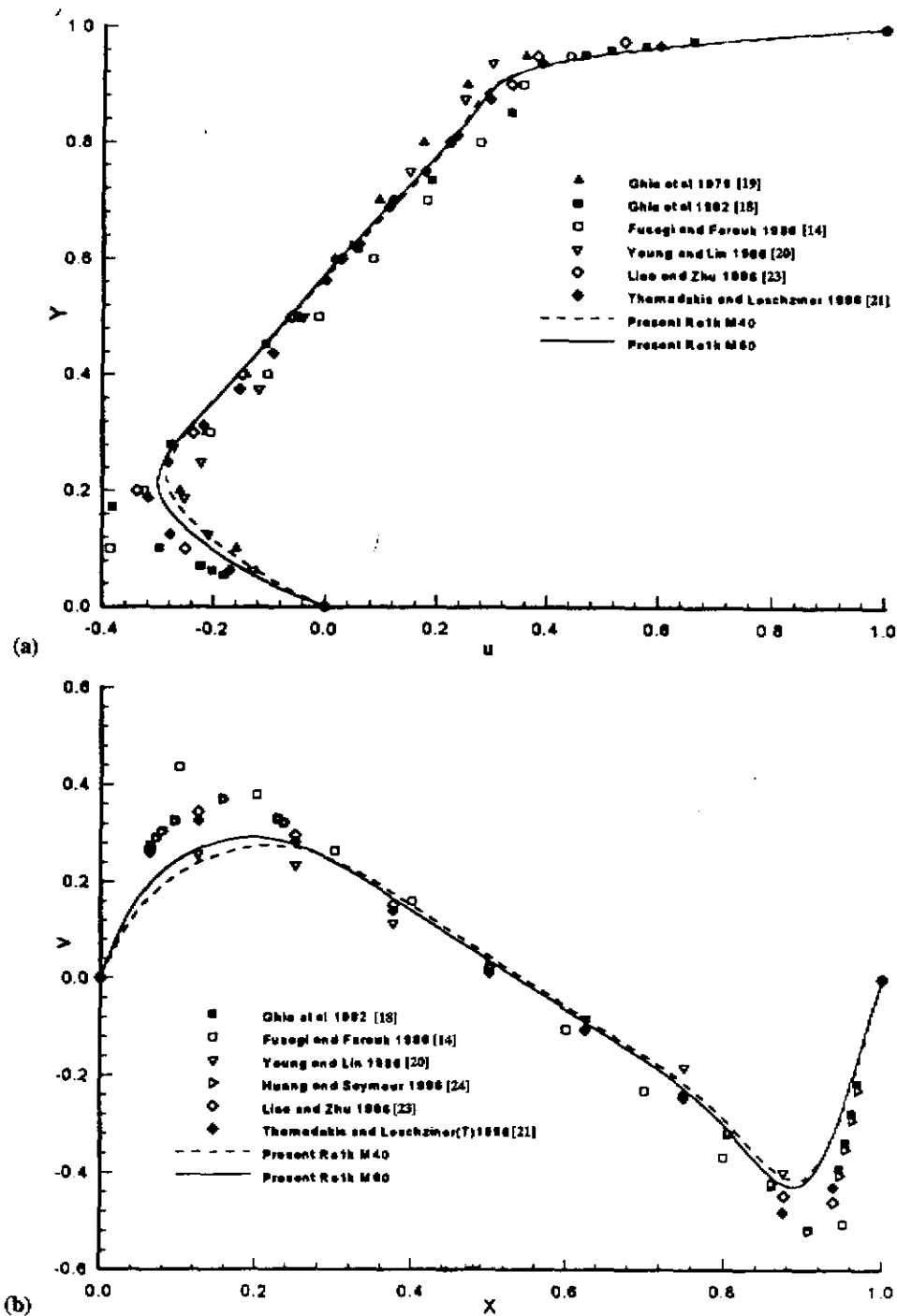


Figure 8. Profile of u (a) and v (b) along the cavity vertical and horizontal centerline of a square cavity for $Re = 1000$.

5. MODEL RESULTS AND DISCUSSIONS

The proposed ELBEM model has been applied on a test problem to verify the feasibility of the model. The test problem is the classical 'driven flow in a square cavity', for which many numerical model results are available in the literature. Present model results are compared with the results of a series solution and FDM, FEM and BEM models in two dimensions.

The model problem consists of a square cavity with a moving top lid with constant velocity, totally filled with an incompressible viscous fluid. In all the cases, the flow inside the cavity was initially at rest. No-slip and impermeability conditions were imposed on all walls, with the velocity at the upper wall set equal to unity. Due to the computational limitations (we used an IBM AIX workstation with 128 MB RAM), the present analysis is limited to a maximum computational mesh points of 60×60 (on the boundary as well as internal domain).

Four analyses have been presented here, for $Re = 100, 400, 1000$ and 2000 respectively. Although the computations were carried out in time, only steady state solutions are presented here. In all the cases, steady states are reached.

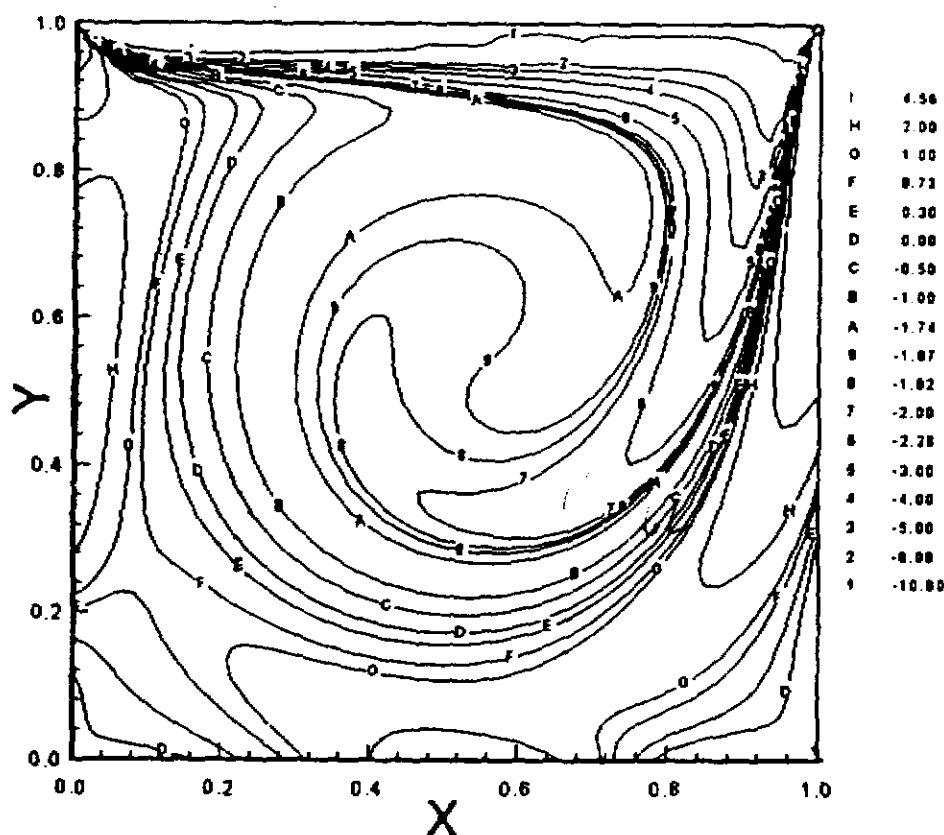


Figure 9. Vorticity distribution for $Re = 1000$.

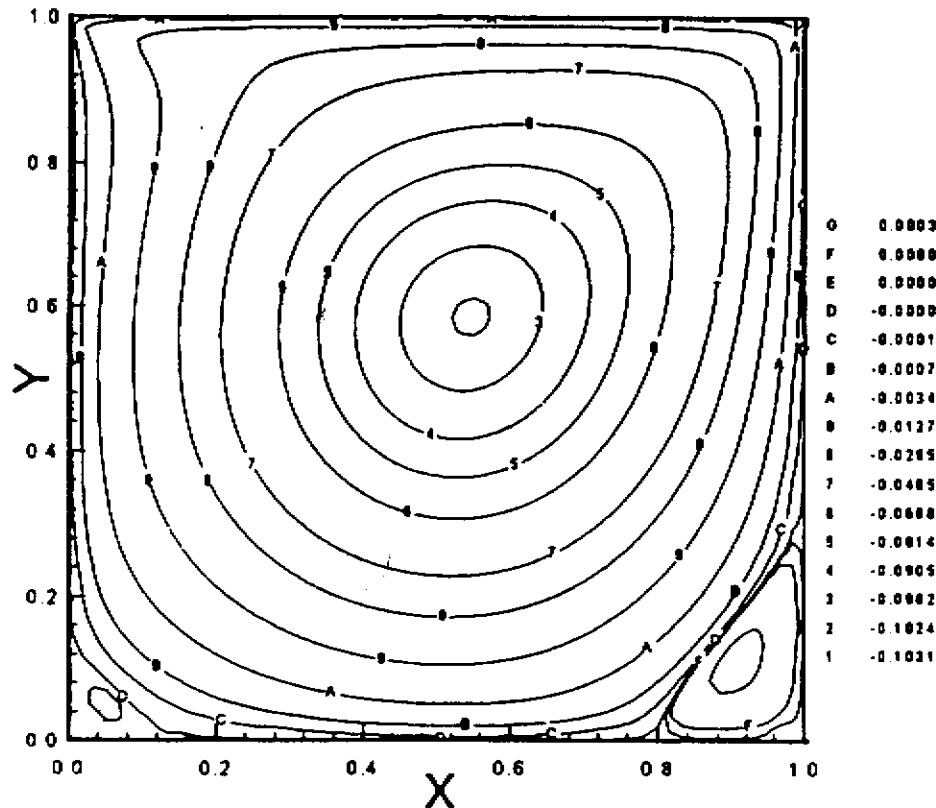


Figure 10. Streamfunction distribution for $Re = 1000$.

Figure 2 shows the u - and v -velocity profiles along the vertical and centerlines of the cavity for $Re = 100$. Two different grids of 40×40 and 60×60 uniform quadrilaterals have been used for the computations. Figure 3 shows the vorticity distribution along the domain and Figure 4 shows the profile of the streamfunction distribution along the domain. The velocity variations are compared with different models of Burgraff [17], Ghia *et al.* [18,19], Young and Lin [20] and Thomadakis and Leschziner [21]. The results mostly agree with all the model results. From Figure 2 it can be seen that for both computational mesh grids, the results are almost the same.

Figure 5 shows the u - and v -velocity profiles along the vertical and centerlines of the cavity for $Re = 400$ with two different grids of 40×40 and 60×60 uniform quadrilaterals. Figures 6 and 7 show the vorticity and streamfunction distributions respectively along the domain. The velocity variations are compared with different models of Burgraff [17], Ghia *et al.* [18,19], Fusege and Farouk [14], Young and Lin [20], Giannattasio and Napolitano [22], Liao and Zhu [23], and Thomadakis and Leschziner [21]. The results obtained are closer to the results of the FEM and the finite volume models. As is obvious from the figures, the small difference to other models can be attributed to the mesh size used in the present investigation.

As the Reynolds number increases, the sensitivity to the grid density becomes more obvious. For a higher Reynolds number, $Re = 1000$, Figure 8 shows the x -component velocity profile (u) and y -component velocity profile (v) on the vertical and horizontal centerline of the cavity. Figures 9 and 10 show the vorticity and streamfunction distributions respectively along the domain. Results of the analysis are again compared with the various models [14,18–21,23,24]. The present analysis is in good agreement with most of the models, bearing in mind that the maximum mesh density was only 60×60 . Further analysis has been carried out for a Reynolds number of 2000 using 60×60 mesh. Figures 11–13 show the vorticity, streamfunction and velocity distributions respectively along the domain.

The merit of the present model is that it provides the best way to treat the velocity–vorticity formulation for two-dimensional flow by the BEM. In general, the boundary conditions of vorticity are not known *a priori*, so that the solution of the vorticity transport equation is rather difficult. However, the BEM solution of the velocity Poisson equations together with the no-slip boundary conditions will automatically render the necessary vorticity boundary conditions directly as the normal derivatives of velocity, while solving the boundary integral equations. If numerical models like FDM and FEM are used in the solution of velocity

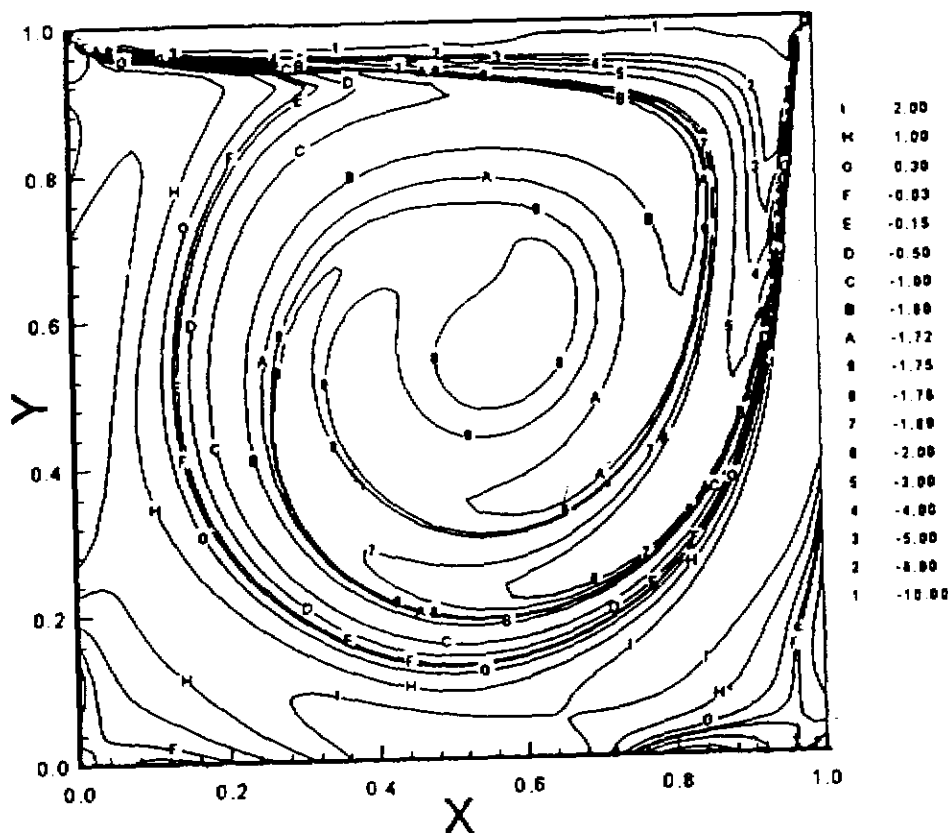


Figure 11. Vorticity distribution for $Re = 2000$.

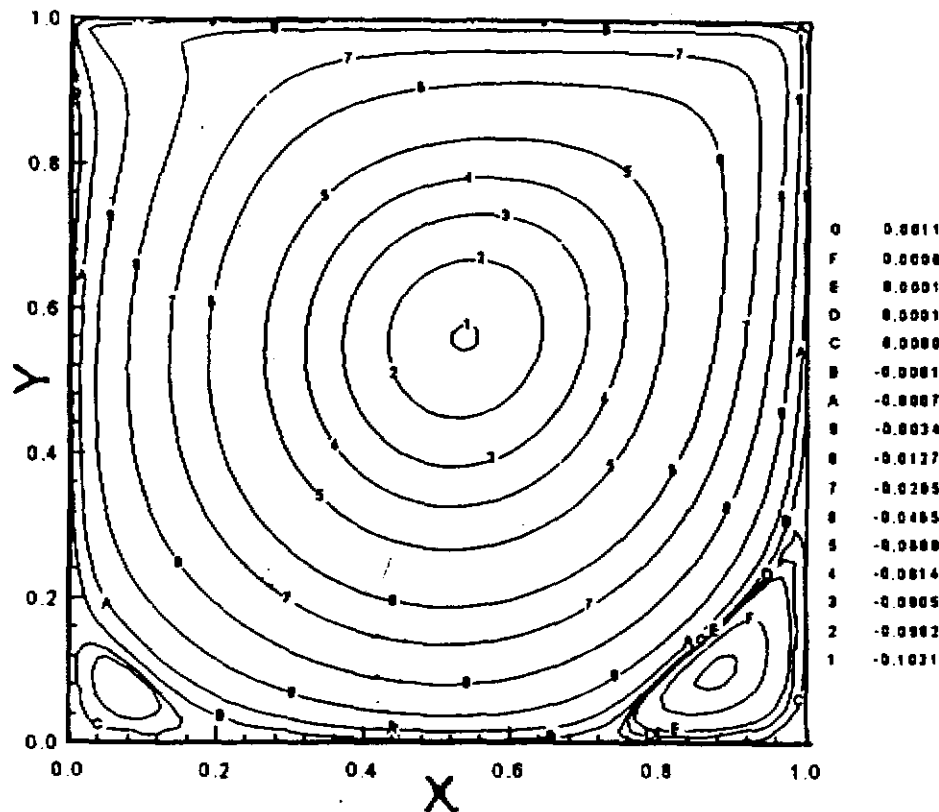


Figure 12. Streamfunction distribution for $Re = 2000$.

Poisson equations, then the boundary vorticity values have to be separately determined from the velocity distribution, which may reduce the accuracy in determining the vorticity boundary conditions for the solution of vorticity transport equation.

As the vorticity transport equation includes convective terms and time-dependent terms, the general BEM solution [5,6] of vorticity transport equation is very difficult. The ELBEM, proposed by combining the Eulerian-Lagrangian method and the BEM, has been proved to be a feasible method to solve advective-diffusion equations such as the vorticity transport equation [Young *et al.*]. Hence, the present model in which the velocity Poisson equations are solved using the BEM and the vorticity transport equation is solved using ELBEM and the iterative scheme combining both models provides the best way to treat the velocity-vorticity formulation for two-dimensional incompressible flow problems. This study demonstrates that even with a relatively coarse mesh, the solutions are very stable and fairly accurate as shown in the case study with different Reynolds numbers.

The approximate number of iterations required for the convergence at each time step vary from 50 to 500 depending on the value of the Reynolds number, time step and grid. Even though the CPU time for each calculation has not been separately found out, typical CPU time for the calculation varies from 1 to 6 h on an IBM AIX workstation for 60×60 mesh.

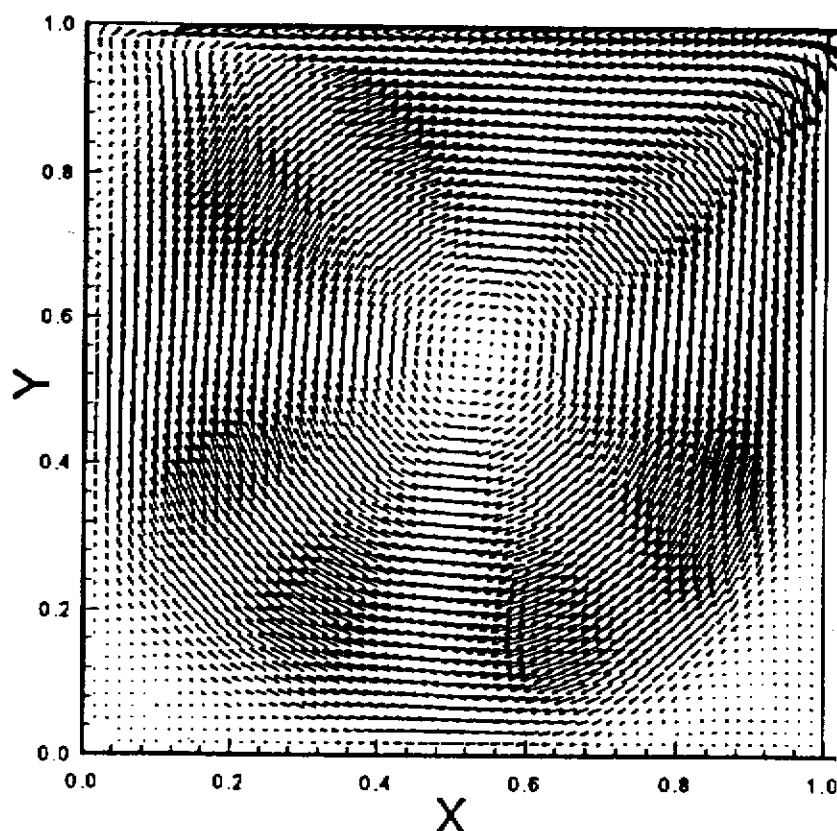


Figure 13. Profile of the flow vectors for $Re = 2000$.

Even though in the present analysis we have carried out the analysis up to a Reynolds number of 2000, the method can be further used for higher Reynolds number with a refined mesh, smaller time step and vorticity relaxation. The ELBEM has already been successfully implemented for three-dimensional diffusion and advection problems [25; Young DL, Her BC, Eldho TI. Boundary integral modeling of three-dimensional circulation and transport in stratified estuaries. *Journal of Engineering Mechanics, ASCE* 2000 (in press)]. Authors also have successfully implemented the velocity–vorticity formulation for the Stokes problem [26] and the Navier–Stokes problem [27] in three dimensions by a combined BEM and FEM scheme. Extension of the ELBEM model for three-dimensional Navier–Stokes equations in velocity–vorticity form will be presented in one of our future papers.

6. CONCLUDING REMARKS

An accurate Eulerian–Lagrangian BEM for solving the velocity–vorticity Navier–Stokes equations is proposed for the first time by the combination of the ELM and the BEM. The

Poisson-type velocity equations are solved using the general boundary integral technique with domain integration for the source terms and the vorticity boundary conditions are exactly determined. The vorticity transport equation is solved using the ELBEM on a transformed characteristic domain. By the combination of the ELM and the BEM, the BEM is made easier to handle the variable velocity field. Here the results of two-dimensional Navier–Stokes problems with low–medium Reynolds numbers in a typical square cavity flow are presented. A comparison with other numerical models demonstrates the feasibility of the present ELBEM model.

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BIEM MODELING OF 3D CIRCULATION AND TRANSPORT IN STRATIFIED ESTUARIES

By D. L. Young,¹ B. C. Her,² and T. I. Eldho³

ABSTRACT: Here the boundary integral equation method (BIEM) is used for 3D modeling of hydrodynamics and pollutant transport in stratified estuaries. The flow computations are made using a newly developed BIEM solution. The transport modeling has been done using an Eulerian-Lagrangian BIEM (ELBIEM) model. In ELBIEM, the advection part in the transport equation is treated by the concept of the Eulerian-Lagrangian scheme, which overcomes the limitation of traditional BIEM to deal with an arbitrary velocity field. The coupling of the 3D shallow water BIEM model and advection-diffusion ELBIEM model enables one to effectively deal with fluctuation of free surface and density stratification in an estuary. The main advantages of the BIEM model include reduction in computational dimensions, ease in discretization and data preparation, accurate free surface simulation, less numerical diffusion and dispersion problems, and direct flux solution at boundaries. The numerical simulation results are compared with other model results and found to be satisfactory. The illustrated case study shows the effectiveness of the model in the simulation of mass, momentum, and heat transfer due to air-water interaction in stratified estuary problems.

INTRODUCTION

The behavior of pollutant transport in the shallow, homogeneous, or stratified bodies of waters in estuaries, large lakes, and coastal oceans depends on the momentum transport in these flow fields. The important issues of water quantity and quality have led to an increasing interest in the large-scale motion and pollutant transport in shallow waters like estuaries. Because of the complexity of the equations that govern pollutant transport in shallow-water bodies, the only feasible approach to their solution is via 3D numerical models. The problems of numerical diffusion, dispersion, and oscillation, and demand of computer time and memory for simulation are the major challenges in the 3D numerical modeling.

A considerable amount of research on numerical modeling of the hydrodynamics and pollutant transport in shallow-water flow fields in 2D and 3D can be found in the literature. Most of these numerical models are based on the finite-difference method (FDM) or finite-element method (FEM). For the flow mechanics in shallow waters, mathematical models employing the linear barotropic hydrodynamic equations, based on the foundation of Ekman's model (1905), are widely used to describe the phenomena of hydrodynamic circulations [e.g., Liggett (1969), Gallagher et al. (1973), and Young and Liggett 1977].

Liggett and Hadjithodorou (1969) presented an algorithm of depth-averaged stream function using FDM for steady-state lake circulations by utilizing the analytical solutions of Wender (1957). This method was extended by Gallagher et al. (1973) for steady state using FEM and by Young and Liggett (1977) for transient flow problems using FEM in Laplace transform space. Although the stream function approach can evaluate the 3D flow field in the horizontal 2D computational domain, there are some disadvantages such as the implementation of complex boundary conditions. The finite Fourier-

transform approach (Liggett 1969) and the eigenfunction approach (Davies 1983; Lardner and Song 1992) also were applied to linear barotropic hydrodynamic equations. The eigenfunction approach needs to solve a series of equation systems, and it is difficult to determine the optimal number of eigenfunction expansions.

The boundary integral equation method (BIEM) is an alternative approach to the aforementioned methods for simulating wind-driven circulation in shallow-water flow fields. The main advantages of BIEM include reduction in computational dimensions, ease in discretization and data preparation, flexibility to deal with infinite domain problems, ease in dealing with the fluctuating free surface, and direct solution to flux at the boundaries. Despite all these advantages, only a very few studies using BIEM have been reported in the flow and transport analysis in estuaries. Iwasa and Tada (1988) researched BIEM solutions of lake circulation using a depth-averaged stream function approach with the help of the Laplace fundamental solution, which could not have wide range applications due to the use of the depth-averaged stream function approach and the simplified boundary conditions.

With all the advantages mentioned above, the BIEM technique has a large potential in the modeling of large-scale shallow-water flow fields. The main hindrance in the development of the BIEM model is the nonavailability of fundamental solutions for the corresponding governing equations, which are very much essential in the development of boundary integral equations. Recently Young et al. (two unpublished manuscripts, 1999) developed a 3D BIEM model for the Ekman-type shallow-water formulation (Ekman 1905), using newly derived fundamental solutions and boundary integral equations to simulate shallow-water flow fields. The developed BIEM model was verified with available analytical and numerical solutions and found to be feasible in the large-scale hydrodynamic modeling of shallow-water flow fields. These BIEM models, extended for stratified shallow-water flow fields, are used here for the determination of hydrodynamics of stratified estuaries.

While solving the parabolic-type pollutant transport equations in estuaries, the numerical diffusion and dispersion are the two major problems of concern. The popular methods such as the upwind FDM (Sharif and Busnaina 1988) and upwind FEM (Heinrich et al. 1977) work well only for the problems in which the diffusion effect dominates. Eulerian-Lagrangian method (ELM) is a widely used scheme for the pollutant transport modeling. The ELM combines aspects of Eulerian and Lagrangian approaches so as to merge the simplicity of a fixed Eulerian grid with the computational power of the Lagrangian

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method in deformed coordinates (Neuman 1981). In the transport modeling using ELM, the advection part is solved by the Lagrangian method, which can be computed independently at each time step by the method of characteristics applied to a grid fixed domain. The remaining diffusion part can be solved by FEM (Neuman 1984), FDM (Li 1991) or BIEM (Young et al. 1999b) on a separate grid. The influence of the advection is projected from one grid to another by local interpolation.

In the present study, an accurate Eulerian-Lagrangian BIEM (ELBIEM) is used for the pollutant transport in estuaries. The pollutant transport equations are solved using the ELBIEM on a transformed characteristic domain. Based on the concept of ELM, the formulation of ELBIEM and its associated fundamental solution is obtained for pollutant transport equations. By the combination of ELM and BIEM, the ELBIEM is made easy to handle the variable velocity field.

The linkage of the 3D shallow-water BIEM model and the advection-diffusion ELBIEM model enables one to deal with the fluctuation of free surface and density stratification in an estuary by maintaining all the advantages of BIEM. The feasibility and accuracy of the model has been demonstrated in comparison with other model results.

MATHEMATICAL FORMULATION

In the present study, hydrodynamics of the estuary are derived from the shallow-water flow field described by the linear barotropic Ekman-type model (Ekman 1905; Welander 1957). The governing hydrodynamics equations can be described in terms of momentum equations and continuity equation as follows (Liggett 1969, 1994):

$$\frac{\partial \mathbf{u}}{\partial t} - f\mathbf{v} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} - \frac{1}{\rho_0} \frac{\partial p'}{\partial x} + \nu \frac{\partial^2 \mathbf{u}}{\partial x^2} \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + f\mathbf{u} = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} - \frac{1}{\rho_0} \frac{\partial p'}{\partial y} + \nu \frac{\partial^2 \mathbf{v}}{\partial y^2} \quad (2)$$

$$0 = -\frac{1}{\rho} \left(\frac{\partial p}{\partial z} + \frac{\partial p'}{\partial z} \right) - g \quad (3)$$

$$\frac{\partial \mathbf{u}}{\partial x} + \frac{\partial \mathbf{v}}{\partial y} + \frac{\partial \mathbf{w}}{\partial z} = 0 \quad (4)$$

where $\rho = \rho_0 + \rho'$, $\rho' \ll \rho$; ($\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$ = velocity vectors defined in the Cartesian coordinate system, x , y , and z , respectively; p = pressure for homogeneous water; p' = pressure fluctuations due to the density variations = $\int_z^0 \rho' dz$, where $\rho' = \rho'/\rho_0$; η = free surface position; t = time; ρ = fluid density; ρ' = density deviation from the standard water density due to stratification; ρ_0 = homogeneous water density; g = acceleration due to gravity; ν = eddy viscosity dependent on the turbulent motion of the flow; and $f = 2\Omega \sin \theta$ = Coriolis parameter, with θ and Ω representing latitude of fluid element and angular velocity of the earth, respectively.

The governing equation for transport phenomena describing the unsteady convective diffusion, assuming constant eddy diffusivity, can be expressed (Liggett 1994)

$$\frac{\partial T}{\partial t} + \mathbf{u} \frac{\partial T}{\partial x} + \mathbf{v} \frac{\partial T}{\partial y} + \mathbf{w} \frac{\partial T}{\partial z} = K^T \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + Q, \quad (5)$$

where T = temperature (or pollutant concentration C or salinity s); K^T = eddy diffusivity; Q = source or sink term of temperature or concentration; and t = time. With respect to temperature and salinity variations, the density variation ρ is expressed as (Bloss et al. 1988) $\rho = \rho_0 [1 - \{7(T - T_0)^2 - 750s\}10^{-6}]$, where $\rho_0 = 999.972 \text{ kg/m}^3$ at $T_0 = 4^\circ\text{C}$; T = temperature in degrees Celsius, and s = salinity in parts per thousand.

To observe the motion with a shorter or longer period hydrodynamics calculations, the timescale is chosen as $1/f$. The above equations are nondimensionalized through the redefinition of the variables as follows (Liggett 1969, 1994): $x^* = x/L$, $y^* = y/L$, $z^* = z/D$, $\mathbf{u}^* = fL\mathbf{u}/(gD)$, $\mathbf{v}^* = fL\mathbf{v}/(gD)$, $\mathbf{w}^* = fL^2\mathbf{w}/(gD^2)$, $t^* = ft$, $h^* = h/D$, $p^* = p/(\rho_0 gD)$, $p'^* = p'/(\rho_0 gL)$, $T^* = T/T_0$, $K^{T*} = K^T/(fL^2)$, and $K = F^2 K^T$. In these definitions D is the typical vertical dimension used to normalize depth, L is the typical horizontal dimension used to normalize the horizontal dimensions, h is the normalized depth of the flow field and F is the Froude number $= fL/(gD)^{1/2}$. Dropping the asterisk from the dimensionless variables in the following equation for brevity, the nondimensional governing partial differential equations for (1)–(4) can be rewritten

$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{v} = -\frac{\partial p}{\partial x} - \frac{\partial p'}{\partial x} + E_k \frac{\partial^2 \mathbf{u}}{\partial x^2} \quad (1)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{u} = -\frac{\partial p}{\partial y} - \frac{\partial p'}{\partial y} + E_k \frac{\partial^2 \mathbf{v}}{\partial y^2} \quad (2)$$

$$0 = -\frac{\partial p}{\partial z} - \frac{\partial p'}{\partial z} - 1 \quad (3)$$

$$\frac{\partial \mathbf{u}}{\partial x} + \frac{\partial \mathbf{v}}{\partial y} + \frac{\partial \mathbf{w}}{\partial z} = 0 \quad (4)$$

where E_k = Ekman number, i.e., $E_k = \nu/fD^2$. To determine the hydrodynamics of an estuary or to find the velocity distribution ($\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$) and pressure variation, equations (6)–(9) are solved subject to the appropriate initial and boundary conditions.

The nondimensional governing partial differential equation for (5) can be rewritten

$$\frac{\partial T}{\partial t} + \mathbf{u} \frac{\partial T}{\partial x} + \mathbf{v} \frac{\partial T}{\partial y} + \mathbf{w} \frac{\partial T}{\partial z} = K \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + Q, \quad (10)$$

In (10), the nondimensional time parameter used is $t^* = gDt/(fL^2)$.

For the flow hydrodynamics, the initial conditions are expressed as follows:

$$\mathbf{u}(x, y, z, t) = \mathbf{u}_0; \quad \mathbf{v}(x, y, z, t) = \mathbf{v}_0 \quad (11a,b)$$

$$\mathbf{w}(x, y, z, t) = \mathbf{w}_0; \quad \eta(x, y, t) = \eta_0 \quad (11c,d)$$

at $t = 0$. If flow starts from rest, $\mathbf{u}_0$, $\mathbf{v}_0$, $\mathbf{w}_0$, and η_0 are all zero.

For the flow hydrodynamics, boundary conditions are expressed as follows:

Bottom boundary conditions

$$\mathbf{u}(x, y, -h, t) = 0; \quad \mathbf{v}(x, y, -h, t) = 0 \quad (12a,b)$$

$$\mathbf{w}(x, y, -h, t) = 0 \quad (12c)$$

$$\frac{\partial \mathbf{u}}{\partial z}(x, y, -h(x, y), t) = \Delta_{xb}(x, y, t) \quad (13a)$$

$$\frac{\partial \mathbf{v}}{\partial z}(x, y, -h(x, y), t) = \Delta_{yb}(x, y, t) \quad (13b)$$

Free surface dynamic boundary conditions are imposed in terms of wind shear stress

$$\frac{\partial \mathbf{u}}{\partial z}(x, y, \eta, t) = \Delta_x(x, y, t) \quad (14a)$$

$$\frac{\partial \mathbf{v}}{\partial z}(x, y, \eta, t) = \Delta_y(x, y, t) \quad (14b)$$

Free surface kinematic boundary condition is

$$\frac{\partial \eta}{\partial t} = \frac{1}{F^2} w, \quad \text{at } z = \eta \quad (15)$$

reline boundary conditions can be applied to the BIEM

$$u(x, y, z, t) = u_i; \quad v(x, y, z, t) = v_i \quad (16a,b)$$

$$w(x, y, z, t) = w_i; \quad \bar{U}(x, y, z, t) \cdot \bar{n} = \bar{U}_i \quad (16c,d)$$

re $\bar{U}$ = depth-averaged velocity; and $\bar{n}$ = unit outward nor-

vector.
or the transport equation [(10)], the initial condition, usu-
prescribed temperature or concentration, is described
throughout the domain at some initial time as $T = T_i(\bar{x})$, in Ω
= 0, and two common types of boundary conditions pre-
ceded are

$$T = T_0(t) \quad \text{on } \Gamma, \quad (17a)$$

$$q = -K \frac{\partial T}{\partial n} + (\bar{u}T) \cdot \bar{n} = q_0(t) \quad \text{on } \Gamma_q \quad (17b)$$

re $0 < t$; Ω = flow domain with a boundary $\Gamma(\Gamma = \Gamma_f \cup \Gamma_q)$;
given velocity field; q = normal flux; $-K\partial T/\partial n$ = diffusive
and $(\bar{u}T) \cdot \bar{n}$ = convective flux.

o construct a BIEM model for transient-flow problems,
the fully implicit finite-difference form of the time deriva-
e for (6)–(9) is used. The implicit type of governing equa-
s are represented as follows:

$$v^{n+1} - v^{n+1} - E_t \left(\frac{\partial^2 u}{\partial z^2} \right)^{n+1} = - \left(\frac{\partial p}{\partial x} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Su^n \quad (18)$$

$$u^{n+1} + u^{n+1} - E_t \left(\frac{\partial^2 v}{\partial z^2} \right)^{n+1} = - \left(\frac{\partial p}{\partial y} \right)^{n+1} - \left(\frac{\partial p'}{\partial y} \right)^{n+1} + Sv^n \quad (19)$$

$$0 = - \left(\frac{\partial p}{\partial z} \right)^{n+1} - \left(\frac{\partial p'}{\partial z} \right)^{n+1} - 1 \quad (20)$$

$$\left(\frac{\partial u}{\partial x} \right)^{n+1} + \left(\frac{\partial v}{\partial y} \right)^{n+1} + \left(\frac{\partial w}{\partial z} \right)^{n+1} = 0 \quad (21)$$

hich $S = 1/\Delta t$; Δt = time interval; n = present time level;
 $n + 1$ = advanced time level. The variables of n th time
are known, whereas $n + 1$ step variables are unknown.

BOUNDARY INTEGRAL FORMULATION

BIEM Formulation for Hydrodynamics Simulation

ne governing equations [(18) and (19)] can be converted
boundary integral equations by using Green's theorem and
integration-by-parts method (Wang 1994; Young et al., two
ublished manuscripts, 1999)

$$\begin{aligned} \bar{x} = \int_{\Omega_0} \left\{ \hat{u}_x \left[- \left(\frac{\partial \eta}{\partial x} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Su^n \right] \right. \\ \left. + \hat{v}_x \left[- \left(\frac{\partial \eta}{\partial y} \right)^{n+1} - \left(\frac{\partial p'}{\partial y} \right)^{n+1} + Sv^n \right] \right\} d\Omega_0 \\ - \int_{\Gamma_0} \left\{ u^{n+1} \left[\left(E_t \frac{\partial \hat{u}_x}{\partial z} \bar{k} \right) \cdot \bar{n} \right] + v^{n+1} \left[\left(E_t \frac{\partial \hat{v}_x}{\partial z} \bar{k} \right) \cdot \bar{n} \right] \right\} d\Gamma_0 \\ + \int_{\Gamma_0} \left\{ \hat{u}_x \left[\left(E_t \frac{\partial u^{n+1}}{\partial z} \bar{k} \right) \cdot \bar{n} \right] + \hat{v}_x \left[\left(E_t \frac{\partial v^{n+1}}{\partial z} \bar{k} \right) \cdot \bar{n} \right] \right\} d\Gamma_0 \end{aligned} \quad (22)$$

$$\begin{aligned} v^{n+1}(\bar{x}) = \int_{\Omega_0} \left\{ \hat{u}_y \left[- \left(\frac{\partial \eta}{\partial x} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Su^n \right] \right. \\ \left. + \hat{v}_y \left[- \left(\frac{\partial \eta}{\partial y} \right)^{n+1} - \left(\frac{\partial p'}{\partial y} \right)^{n+1} + Sv^n \right] \right\} d\Omega_0 \\ - \int_{\Gamma_0} \left\{ u^{n+1} \left[\left(E_t \frac{\partial \hat{u}_y}{\partial z} \bar{k} \right) \cdot \bar{n} \right] + v^{n+1} \left[\left(E_t \frac{\partial \hat{v}_y}{\partial z} \bar{k} \right) \cdot \bar{n} \right] \right\} d\Gamma_0 \\ + \int_{\Gamma_0} \left\{ \hat{u}_y \left[\left(E_t \frac{\partial u^{n+1}}{\partial z} \bar{k} \right) \cdot \bar{n} \right] + \hat{v}_y \left[\left(E_t \frac{\partial v^{n+1}}{\partial z} \bar{k} \right) \cdot \bar{n} \right] \right\} d\Gamma_0 \end{aligned} \quad (23)$$

where Ω_0 = domain; Γ_0 = boundary of the domain for the base
point in which the point force or the point source acts;
 $\hat{u}_x, \hat{v}_x, \hat{u}_y,$ and $\hat{v}_y$ = fundamental solutions or free space
Green's functions.

The advanced time level flow variables on the left-hand side
of the integral equations are thus influenced by the effects of
free surface fluctuations and the inertial effect contained in the
volume integral terms. The boundary integral parts include the
velocity boundary condition effect and shear stress boundary
condition effects.

To obtain the fundamental solutions of (22) and (23), the
Fourier-transform method is applied (Bracewell 1986; Wang
1994; Young et al., two unpublished manuscripts, 1999). The
coupled differential adjoint operators are transformed into a
symbolic algebraic system in the Fourier space first, which is
solved by the matrix inversion. Each element of the inverse
matrix illustrates the resulting influence of the velocity com-
ponent and pressure due to a point force and point source in
the Fourier space. Then the inverse Fourier transforms are de-
rived by the Cauchy's integral formula, the residue theorem,
the convolution law, and the mathematical tables for the ele-
mentary parts of an inverse matrix.

Derived fundamental solutions due to the contribution of the
 x -directional point force are

$$\hat{u}_x = \frac{\delta(x_0 - x)\delta(y_0 - y)}{2\sqrt{2E_t(S^2 + 1)}} \exp(-C_1)[C_3 \cos C_2 - C_4 \sin C_2] \quad (24)$$

$$\hat{v}_x = \frac{\delta(x_0 - x)\delta(y_0 - y)}{2\sqrt{2E_t(S^2 + 1)}} \exp(-C_1)[C_4 \cos C_2 + C_3 \sin C_2] \quad (25)$$

Derived fundamental solutions due to the contributions of the
 y -directional point force are

$$\hat{u}_y = - \frac{\delta(x_0 - x)\delta(y_0 - y)}{2\sqrt{2E_t(S^2 + 1)}} \exp(-C_1)[C_4 \cos C_2 + C_3 \sin C_2] \quad (26)$$

$$\hat{v}_y = \frac{\delta(x_0 - x)\delta(y_0 - y)}{2\sqrt{2E_t(S^2 + 1)}} \exp(-C_1)[C_3 \cos C_2 - C_4 \sin C_2] \quad (27)$$

The parameters $C_1, C_2, C_3,$ and C_4 are defined

$$C_1 = C_3 \frac{|z - z_0|}{\sqrt{2E_t}}, \quad C_2 = C_4 \frac{|z - z_0|}{\sqrt{2E_t}} \quad (28a,b)$$

$$C_3 = \sqrt{S + \sqrt{1 + S^2}}, \quad C_4 = \sqrt{-S + \sqrt{1 + S^2}} \quad (28c,d)$$

where the variables $x_0, y_0,$ and z_0 = coordinates of base point
in which point force or point source acts; the variables $x, y,$
and z = coordinates of any field point in which the effect of
point action is concerned; the function δ = Dirac delta func-
tion, indicating the point action; and $S = 1/\Delta t$.

It is well known that the fundamental solution is the influ-
ence function of the physical system. Within the obtained so-
lutions [(24)–(27)], the exponential functions exhibit the de-
caying behavior caused by the turbulent shear stress. The
trigonometric functions indicate the spirallike property caused

by the Coriolis force. The Dirac delta functions express the unpropagated momentum transport due to the fundamental assumption of Ekman's model for the neglect of horizontal momentum transport. The properties of fundamental solutions all satisfy the mathematical requirement of Green's functions (Wang 1994; Young et al., two unpublished manuscripts, 1999).

The BIEM model is formulated by substituting fundamental solutions into boundary integral equations. The velocity in the vertical direction w is found from the continuity equation after solving u and v components. The problem is solved by letting the base point approach to each boundary node in sequence, finding the unknown variables on each boundary node, and then determining the field point from the solved boundary variables.

The free surface kinematic boundary conditions and the continuity equation are combined for free surface evaluation

$$\frac{\partial \eta}{\partial t} = -\frac{1}{F^2} \left[\frac{\partial}{\partial x} \int_{-h}^{\eta} u \, dz + \frac{\partial}{\partial y} \int_{-h}^{\eta} v \, dz \right] \quad (29)$$

Using a finite-difference scheme, the free surface position for the advanced $(n+1)$ step can be calculated from

$$\eta^{n+1} = \eta^n - (\Delta t) \frac{1}{F^2} \left[\frac{\partial}{\partial x} \int_{-h}^{\eta^{n+1}} u^{n+1} \, dz + \frac{\partial}{\partial y} \int_{-h}^{\eta^{n+1}} v^{n+1} \, dz \right] \quad (30)$$

The boundary condition on the shoreline is the usual no-flux condition. Because the unknown free surface position is contained in the integrals of (30) and is necessary for the evaluation of the velocity for the advanced step, a Picard's iteration method in the implicit scheme is used here, with the following steps:

1. Evaluate the flow field— u_i^{n+1} and v_i^{n+1} —for the i th iteration using the velocity and free surface elevation of the previous $i-1$ th iteration.
2. Compute the free surface elevation for this iteration

$$\bar{\eta}^{n+1} = \eta^n + (\Delta t/2)[F(u_i^{n+1}, v_i^{n+1}) + F(u_i^{n+1}, v_i^{n+1})];$$

$$F(u, v) = -\frac{1}{F^2} \left[\frac{\partial}{\partial x} \int_{-h}^{\eta} u \, dz + \frac{\partial}{\partial y} \int_{-h}^{\eta} v \, dz \right] \quad (31)$$

3. Compute the maximum euclidean norm of the velocity field

$$E = \max(|u_i^{n+1} - u_{i-1}^{n+1}|^2 + |v_i^{n+1} - v_{i-1}^{n+1}|^2)^{1/2}$$

4. If $E < \epsilon$ then stop the iteration, otherwise repeat Steps 1–3 for the next cycle of iteration. The symbol ϵ is used for the convergence criterion for the iterative procedure.

ELBIEM Formulation for Transport Simulation

Considering the pollutant transport equation [(10)], owing to the Eulerian-Lagrangian concept, the computational domain is now chosen along a characteristic domain and the convective diffusion equation is rewritten by a hydrodynamic derivative

$$\frac{DT}{Dt} = K \nabla^2 T + Q, \quad \text{in } \Omega_E \quad (32)$$

subject to the initial condition, $T = T_0(\bar{x})$, in Ω_E at $t = 0$ and boundary conditions

$$T = T_0(t) \quad \text{on } \Gamma_T \quad (33a)$$

$$q = -K \frac{\partial T}{\partial n} = q_0(t) \quad \text{on } \Gamma_Q \quad (33b)$$

where $0 < t$; the hydrodynamic derivative is defined as D/Dt

$= \partial/\partial t + \bar{u} \cdot \nabla$; Ω_E = characteristic domain with a boundary $\Gamma_E (= \Gamma_T \cup \Gamma_Q)$; and $\bar{u}$ = velocity vectors u , v , and w . The region of the characteristic domain is determined by the method of characteristics

$$\frac{d\bar{x}}{dt} = \bar{u}; \quad \bar{x}_{k-1} = \bar{x}_k - \bar{u} \cdot dt \quad (34)$$

Now using Green's second identity, the boundary integral equations can be derived on the characteristic domain

$$\begin{aligned} \alpha(\bar{x}_i, t_k) T(\bar{x}_i, t_k) &= \int_{\Omega_E} \hat{T}(\bar{x}_i, t_k; \bar{x}, t_{k-1}) T(\bar{x}, t_{k-1}) \, d\Omega_E \\ &- \int_{t_{k-1}}^{t_k} \int_{\Gamma_E} \hat{T}(\bar{x}_i, t_k; \bar{x}, t) q(\bar{x}, t) \, d\Gamma_E \, dt \\ &+ \int_{t_{k-1}}^{t_k} \int_{\Gamma_E} \hat{q}(\bar{x}_i, t_k; \bar{x}, t) T(\bar{x}, t) \, d\Gamma_E \, dt \\ &+ \int_{t_{k-1}}^{t_k} \int_{\Omega_E} \hat{T}(\bar{x}_i, t_k; \bar{x}, t) Q(\bar{x}, t) \, d\Omega_E \, dt \end{aligned} \quad (35)$$

in which α = Cauchy principal value; k indicates current time step; $\bar{x}_i$ = position vector of base point; $\bar{x}$ = any field point; and $q(\bar{x}, t) = -K \partial T / \partial n$; $\hat{q}(\bar{x}, t) = -K \partial \hat{T} / \partial n$, where n = unit outward normal; and $\hat{T}$ = associated fundamental solution.

The associated fundamental solution $\hat{T}$ satisfies the source varying formally adjoint operator of the governing equation [(32)] (without source or sink term). That is

$$\frac{D\hat{T}}{Dt} - K \nabla^2 \hat{T} = \delta(\bar{x} - \bar{x}_i) \delta(t - t_k) \quad (36)$$

Now the fundamental solutions can easily be derived for the 3D problems (Carslaw and Jaeger 1959; Brebbia et al. 1984)

$$\hat{T}(\bar{x}, t; \bar{x}_i, t_k) = \left[\frac{1}{[4\pi K(t - t_k)]^{3/2}} \exp[-r^2/4K(t - t_k)] \right] \quad (37)$$

where $r = |\bar{x} - \bar{x}_i|$ = Cartesian distance between the base point and any field point.

The integral equation [(35)] implies that the boundary conditions and initial conditions are treated as a continuous distribution of the impulse acting on the domain boundary. For each time step t_k , the computational domain Ω_E coincides with physical domain Ω only at $t = t_k$, and boundary conditions and initial conditions are given on the physical boundary Γ and the physical domain Ω of time step $t = t_{k-1}$. However the boundary and initial values are required to be imposed in integral terms of (35) on the computational characteristics boundary $\Gamma_E (\Gamma_T \cup \Gamma_Q)$ and the domain Ω_E of time step $t = t_{k-1}$.

Without using the traditional backward-tracking interpolation procedure, a forward-tracking method is used to evaluate the prescribed boundary condition and the last time step solution for the characteristic domain in this study. Thus, because the important information of the flow field can be transferred from the last time step, the error arising from the interpolation procedure can be reduced.

The boundary integral approach (Brebbia et al. 1984) is used to solve the boundary integral equation [(35)] with the associated boundary and initial conditions. Here constant shape function is used to discretize the temporal and spatial domain, which allows the analytical integration of time in (35). After approaching the base point included in the integral equation [(35)] to the boundary nodes on Ω_E at $t = t_k$ and imposing initial and boundary conditions, a simultaneous equations system is written and solved for the unknowns. The details of the

ment properties, interpolation functions, time integration, and equation system formation used here are described in Ebbia et al. (1984), which is not repeated here. The above discussed ELBIEM model has been found to be very stable and efficient for advection-diffusion problems with large Peclet numbers (above 5 and infinity, for a pure advection case) and Courant numbers (above 0.5) (Young et al. 1999b).

NUMERICAL SIMULATION PROCEDURE

The flow hydrodynamics and pollutant transport in estuaries are determined by linking the BIEM hydrodynamics model and the ELBIEM transport model. The following numerical simulation procedure has been used in the model development:

1. Input initial and boundary conditions for flow hydrodynamics and pollutant transport.
2. Compute the initial effect, boundary condition effect, density gradient, and pressure effect in the hydrodynamics equations.
3. Solve the boundary integral equations for unknown velocity u and v on the boundaries.
4. Calculate field (or interior) velocities u and v using the integral equations.
5. Compute the vertical velocity component w from the continuity equation.
6. Compute the free surface elevation from (30) for this time step.
7. Solve the transport equation by the ELBIEM scheme to get the temperature or concentration C variation, using the initial conditions, boundary conditions, and the calculated velocity distributions, on the boundaries of the domain.
8. Calculate field distributions of the temperature (or C) by using the integral equations.
9. Repeat Steps 2–8 for the next cycle of computation.

The time interval is a parameter included in fundamental solutions in the BIEM model; hence, use of a large time interval is possible without many numerical diffusions and dispersion problems. However a stability condition of $((gD)^{1/2} \Delta t / fL\Delta x) < 1$ is enforced in the present model, especially in calculation of free surface position, where D and L are characteristic depth and length, respectively, Δt is time interval, and Δx is mesh size.

MODEL VERIFICATION AND CONVERGENCE ANALYSIS

The BIEM hydrodynamics model mentioned here has been verified with analytical and other numerical schemes like FDM and FEM (Wang 1994; Young and Wang 1995a,b; Young et al., unpublished manuscript, 1999). Here a comparison with an analytical Ekman's spiral solution (Ekman 1905; Welander 1957) for an infinite extensive hypothetical ocean having a finite depth is briefly described. The shallow-water flow field to be simulated is driven by uniform, southern wind blowing from rest over the whole ocean. The simulation is carried out until a steady state has been achieved. Initially, the velocity field is assumed to be zero throughout the domain. The boundary conditions prescribed are a no-slip bottom condition, $\Delta_x = 0$, and $\Delta_y = fL\tau/\rho g$. It is assumed that the characteristic depth of the ocean $D = 80$ m; characteristic length $L = 1.25 \times 10^5$ m; $\rho = 980$ cm/s²; $\nu = 200$ cm²/s; $f = 0.0001$ rad/s; $\Delta t = 0.02$; and wind shear stress $\tau = 1$ cm²/s². Analyses have been carried out for various dimensionless depths— $h = 1.0, 0.6$, and 0.2 —and the solutions at steady state have been found. Table 1 shows a comparison of the free surface velocities of the BIEM solutions with the analytical solutions (Ekman 1905; Welander

1957). Good agreement is observed between the results. More detailed comparisons of the hydrodynamics BIEM model (including free surface variations) with other analytical solutions and numerical solutions of FDM and FEM are described in Young and Wang (1995a,b) and Young et al. (unpublished manuscript, 1999).

The ELBIEM model for the 3D pollutant transport has been compared with some exact solutions for the diffusion-advection problem, before solving the coupled hydrodynamics and transport problems. The diffusion-advection problem in comparison with the exact solutions is used for the purpose of the convergence analyses of the model parameters of mesh size and number of Gaussian points used for integration.

For the verification of the ELBIEM transport model and the convergence analysis, a unit cubic domain with a unit concentration on one side and zero concentration on the opposite side is considered. The concentration flux is assumed zero on all other faces, and $K = 1$. Initially, zero concentration is assumed throughout the domain. To test the effect of the mesh on the solution, a convergence analysis is carried out with the BIEM discretization of $2 \times 2 \times 2, 6 \times 6 \times 6, 8 \times 8 \times 8, 10 \times 10 \times 10, 12 \times 12 \times 12, 14 \times 14 \times 14$, and $16 \times 16 \times 16$.

Fig. 1 shows the concentration variation for various time steps in comparison with the derived exact solution and the ELBIEM solution for the different meshes for the diffusion-advection problem (nondimensional velocity $u = 1, v = 0$, and $w = 0$). The results show good agreement with the exact solutions. The effect of the mesh in the solution is very clear. With a BIEM discretization of $16 \times 16 \times 16$, reasonably comparable results with the exact solution is obtained. One convergence analysis for the number of Gaussian quadrature

TABLE 1. Comparison of BIEM Solutions and Analytical Solutions for Ekman's Spiral Problem with Various Depths

Depth, h (1)	Analytical (2)	BIEM (3)	Relative error (%) (4)
(a) u			
1.0	0.00079674	0.00079698	0.03
0.6	0.00080899	0.00080829	0.09
0.2	0.00043046	0.00043039	0.01
(b) v			
1.0	0.00079780	0.00079890	0.14
0.6	0.00078286	0.00078373	0.11
0.2	0.00105587	0.00105582	0.00

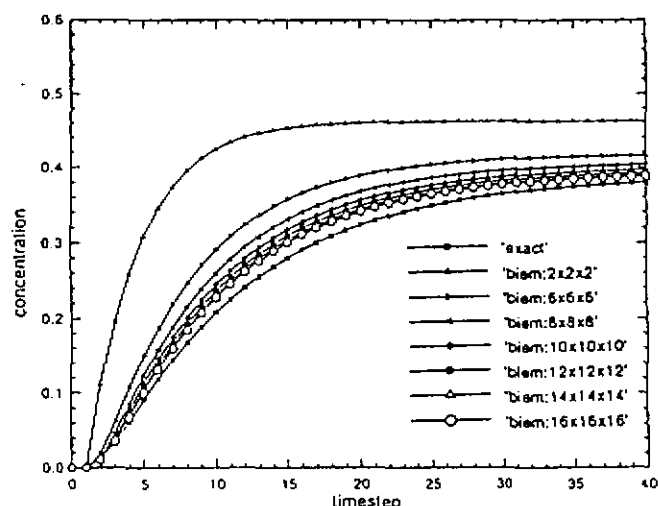


FIG. 1. Comparison of Concentration Variation with Exact Solution and Mesh Sensitivity (Advection-Diffusion Problem)

points, optimal for numerical integration, also has been carried out for Points 3, 4, 8, and 10 with a mesh of $4 \times 2 \times 2$. The results with 8 and 10 Gaussian points are almost the same; hence, 8-point Gaussian quadrature integration is used for further analysis. Further verification of the 3D transport model is described in Young et al. (1999a).

RESULTS AND DISCUSSION

Thermal stratification is widely believed to exert an important influence on large-scale shallow-water flow fields of lakes, estuaries, and oceans through its effect on density variations and other physical factors. There exists a stratified temperature profile through the depth of the water body. Although the problem to be solved is that of the vertical temperature profiles, there is an action of the wind shear and this renders the problem 3D. Here one analyzes the stratification and circulation in a large-scale shallow-water flow field with thermal effects and wind shear effects.

To test the capability of the combined BIEM flow and transport model, the flow pattern and temperature distribution due to wind effect in a shallow water basin is considered. The parameters for this case study are taken from Davies (1983). The closed rectangular basin considered has dimensions and rotation representative of the North Sea. A rectangular basin (400×800 km) with a flat bottom (65 m) and slip bottom boundary conditions is considered for simulation. The following physical parameters are chosen: $\nu = 650 \text{ cm}^2/\text{s}$, $f = 0.00012222 \text{ rad/s}$, $\tau_{yy} = -14.63414634 \text{ cm}^2/\text{s}^2 =$ shear stress in the y -direction, $\Delta t = 409 \text{ L/s}$; and the coefficient of the linear bottom friction is 0.2 cm/s . Here a mesh of $10 \times 20 \times 10$ is considered for the computations. As far as the transport boundary conditions are considered, except where there is heat transfer on the air-sea interface, the sides are all insulated. The initial temperature throughout the domain is assumed to be 20°C .

Two cases of combinations of physical conditions in the problem are considered. In the first case there is no wind shear, but in the second case wind shear is allowed. In both cases, heat transfer is allowed and moving free surface domain is considered.

Case 1

Here one considers the domain without any wind shear, but temperature transfer is allowed to the domain (heating) and from the domain (cooling). Because no wind shear is imposed, current is generated by the convective heat transfer only. Heat-

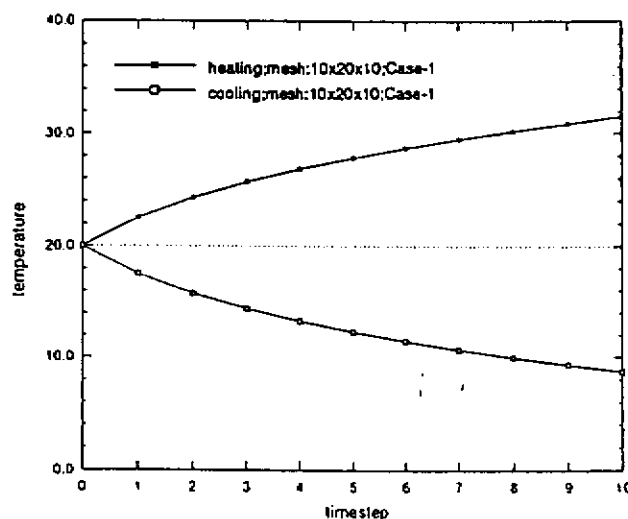


FIG. 2. Response of Temperature at Free Surface—Case 1

ing and cooling processes can easily be simulated, as shown in Fig. 2 for the free surface and in Fig. 3 for the domain depth.

For further analysis, one considers the cooling cycle only. Under the unstable density stratification, the phenomenon of overturn is observed. Figs. 4(a and b) show the density and velocity distribution, respectively, at the profile of $x = 0.5$ for a time step of 50. Figs. 5(a and b) illustrate the density and velocity distributions, respectively, at the profile of $y = 1.0$. Figs. 6(a and b) exhibit the density and velocity distributions, respectively, at the profile of $z = -0.5$ for a time step of 50. The 3D features of the current structure are vividly illustrated in the simulation.

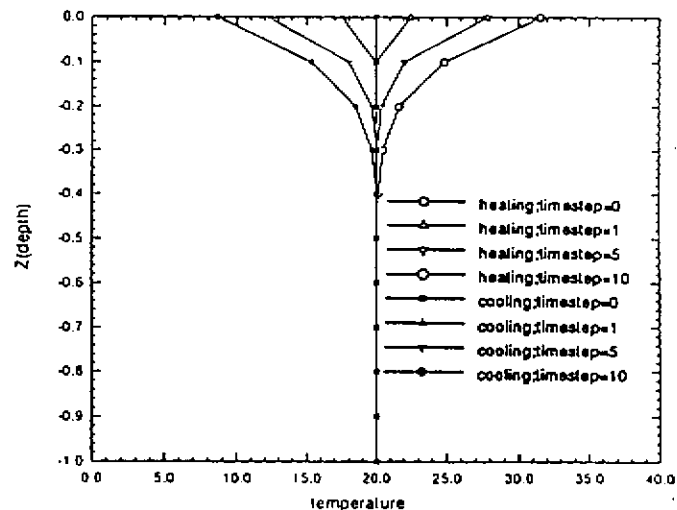


FIG. 3. Response of Temperature through Depth—Case 1

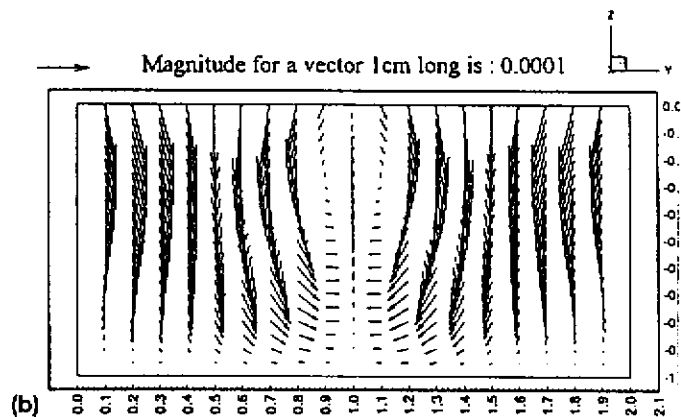
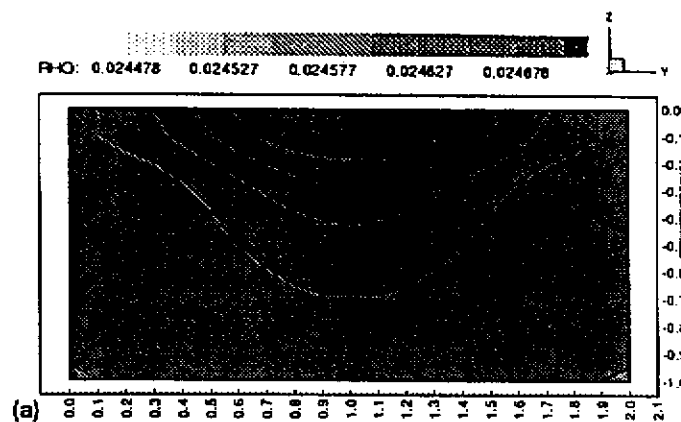
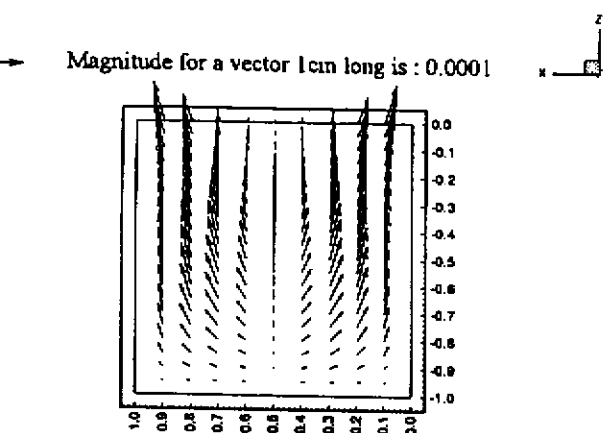
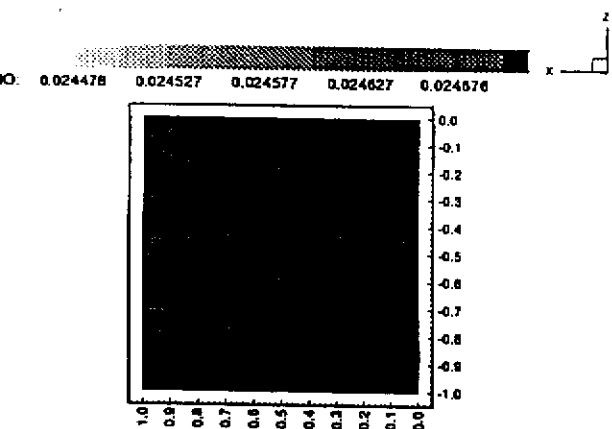
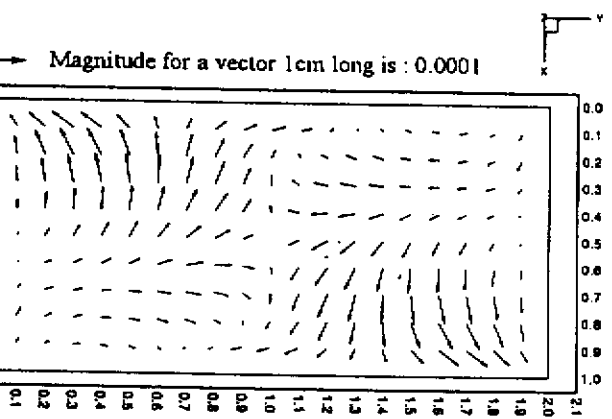
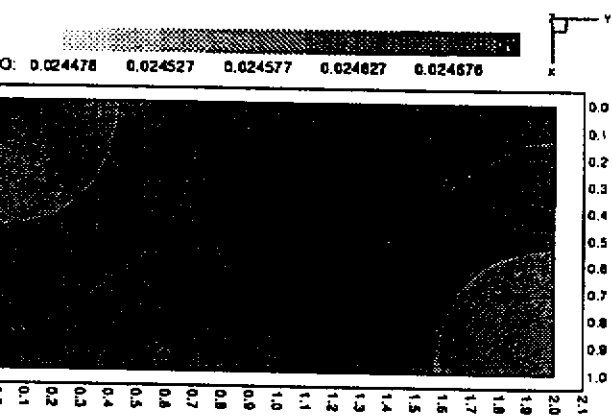


FIG. 4. At $x = 0.5$, Cooling without Wind Shear, Time Step = 50 (a) Density Distribution; (b) Velocity Distribution



5. At $y = 1.0$, Cooling without Wind Shear, Time Step = 50: (a) Density Distribution; (b) Velocity Distribution



6. At $z = -0.5$, Cooling without Wind Shear, Time Step = 50: (a) Density Distribution; (b) Velocity Distribution

As obvious from Fig. 3, in the heating process of the stratified shallow-water body, the thermal structure manifests a well-mixed warm upper layer (epilimnion) separated by a zone of intense temperature gradient (metalimnion) from a relatively colder layer (hypolimnion). As can be seen in Figs. 4–6, the thermal stratification plays an important role in the circulation and distribution of density. As in Figs. 4(a and b), the cooling effects produce strong density differences that lead to an “overturning” of water masses from top to bottom.

Case 2

Here one considers the domain with wind shear, and heat transfer also is allowed from the domain. Figs. 7(a and b) show the density and velocity distributions, respectively, at the profiles of $x = 0.4$ for a time step of 100. Figs. 8(a and b) show the density and velocity distributions, respectively, at the profiles of $y = 1.0$ for a time step of 100. Figs. 9(a and b) show the density and velocity distributions, respectively, at the profiles of $z = -0.5$ for a time step of 100. Due to the consideration of heat transfer at the air-water interface, the density stratification is manifest as far as wind-driven circulation is concerned. The density stratification caused the the heat transfer has a strong impact on the flow pattern. The flow patterns and streamlines for the $x = 0.4$ profile for the homogeneous water body are depicted in Figs. 10(a and b), respectively. The streamlines for the $x = 0.4$ profile for the stratified water body are shown in Fig. 11. The stratified case exhibits the phenomenon of multiple circulation gyres and thermocline. The stratified water body also shows the existence of secondary currents. As can be seen in Fig. 7(b), the maximum wind-driven current was observed to be close to the surface and the maximum return current was found to be near the thermocline. Below the metalimnion, an almost stagnant current opposite to the wind direction also is observed.

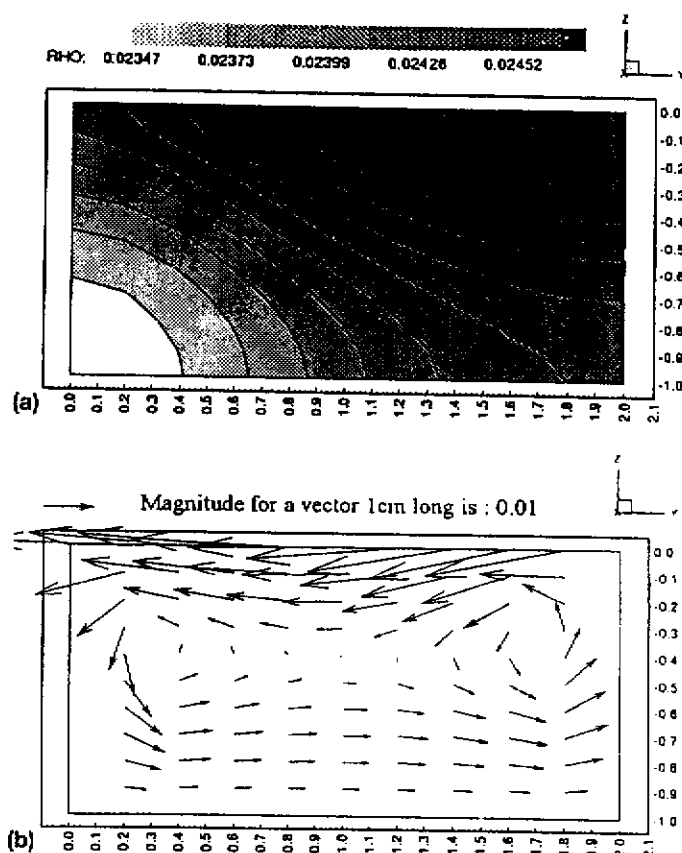


FIG. 7. At $x = 0.4$, Cooling with Surface Wind Shear, Time Step = 100: (a) Density Distribution; (b) Velocity Distribution

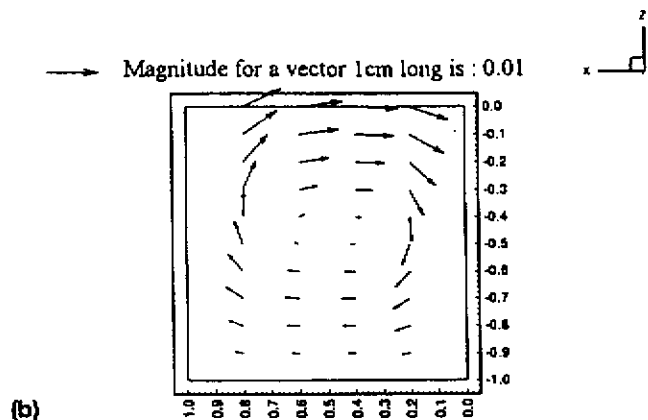
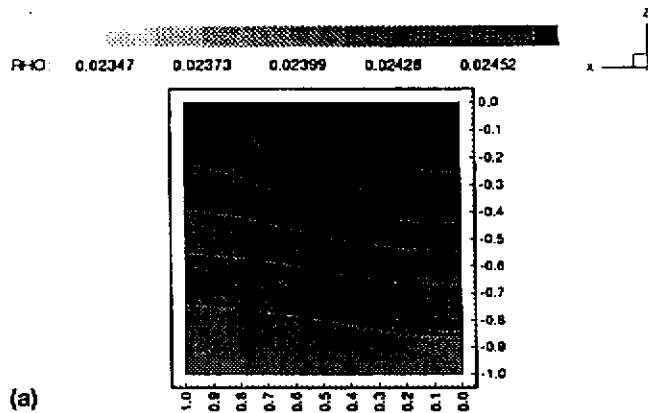


FIG. 8. At $y = 1.0$, Cooling with Surface Wind Shear, Time Step = 100: (a) Density Distribution; (b) Velocity Distribution

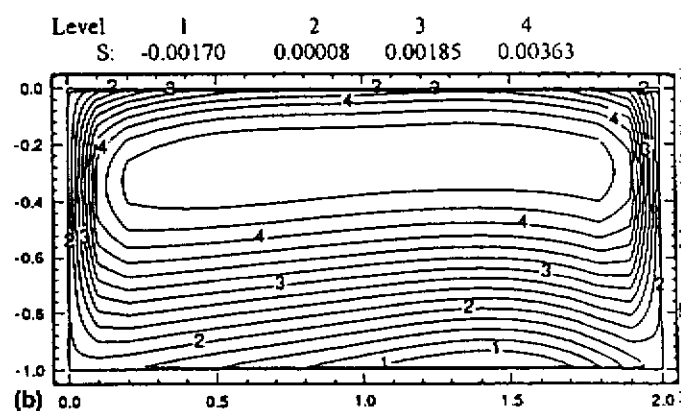
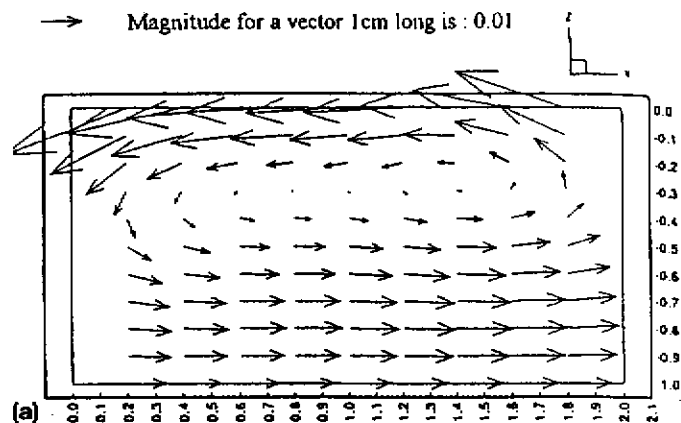


FIG. 10. At $x = 0.4$ for Homogeneous Shallow Water Bodies—Case 2: (a) Flow Pattern; (b) Streamlines

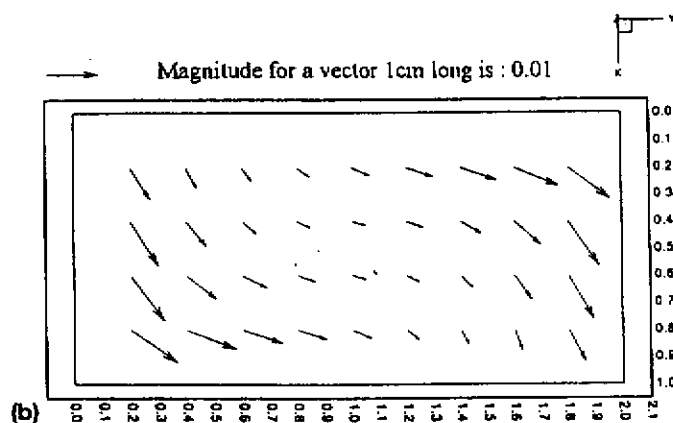
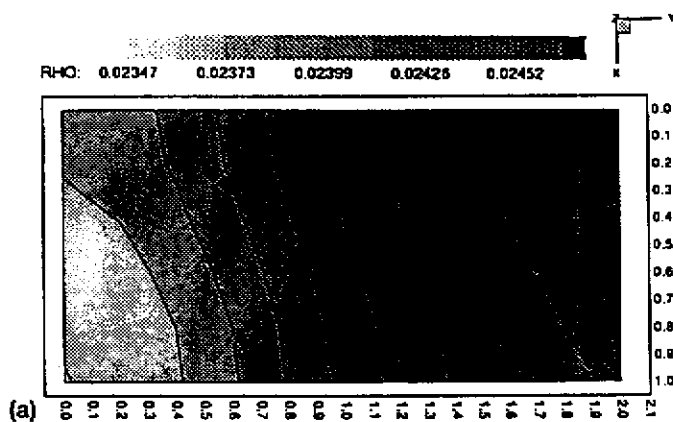


FIG. 9. At $z = -0.5$, Cooling with Surface Wind Shear, Time Step = 100: (a) Density Distribution; (b) Velocity Distribution

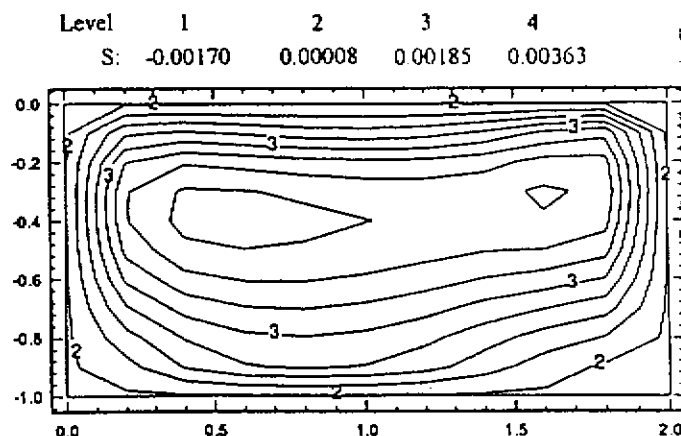


FIG. 11. Streamlines at $x = 0.4$ for Stratified Shallow Water bodies—Case 2

As can be seen in Figs. 10(a and b), 7(b), and 11, a comparison of the flow fields for the homogeneous and stratified cases shows some interesting phenomena. The homogeneous flow field is very simple, and there is only one circulating gyre in the whole water body after the long action of the wind shear stress. The stratified flow field is very complex and clearly two circulating gyres and also the phenomenon of overturn can be observed. It is clear that the wind stress is the main mechanism for the surface current and penetrates less deeply in the stratified case than in the homogeneous case. The thermal flux at the surface contributes mainly to the interior of the shallow water body. When the shallow-water flow field is stratified, the wind-induced drift is confined to the upper layers, with the maximum return current occurring near the thermocline.

A comparison between Figs. 4–6 and 7–9 illustrates the difference of circulation patterns and density distribution with

wind shear effects and with wind shear effects, having heat transfer effects in both cases. As obvious, due to wind action, circulation becomes more prominent and density stratification is more complex.

The present study is an attempt to gain some insight into the complex problem of circulation and transport in a stratified shallow-water flow field by using BIEM. The model is used to examine the heat transfer effects and wind stress effects on induced circulation, thermal composition, and density distribution within a homogeneous and stratified shallow-water flow field. Although no quantitative comparisons of the present results were made with other model results due to difference in approaches and problems considered, the qualitative behavior of the solutions obtained are similar to those observed by Lee and Liggett (1970), Liggett and Lee (1971), Lee (1972), and Young et al. (1976). Using the coupled hydrodynamics and pollutant transport BIEM model, although here the analysis of flow pattern, density and temperature distribution due to wind effect, and heat transfer in a stratified shallow water basin was presented, the model can be easily used in the pollutant or pollutant transport analysis in large-scale shallow-water flow fields such as homogeneous or stratified estuaries, lakes, and oceans.

CONCLUDING REMARKS

In this study, a 3D BIEM model was presented for the hydrodynamics and pollutant transport in stratified estuaries. The main advantages of the presented BIEM model include reduction in computational dimensions, ease in discretization and data preparation, accurate free surface simulation, ease in dealing with irregular boundary problems, less numerical diffusion in dispersion problems, and direct flux solution at boundaries. The model consists of two submodels: the flow equation solved by the 3D Ekman's shallow-water theory using BIEM, and the temperature or pollutant concentrations are solved by the 3D advection diffusion equation using ELBIEM. In the 3D BIEM model, the free surface variations are accurately simulated as the computational domain can easily be moved about to follow the free surface fluctuations. For pollutant transport simulation, with the ELBIEM model, the numerical dispersion and diffusion problems can be reduced. Numerical simulations of the model for various case studies have shown good agreement with some analytical and other numerical solutions. The present model is able to handle both homogeneous and stratified environments under the air-sea interaction at the water surface to consider the mass, momentum, and heat transfers.

ACKNOWLEDGMENTS

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APPENDIX II. NOTATION

The following symbols are used in this paper:

- D = typical depth;
 F = Froude number;
 f = Coriolis parameter;
 g = acceleration due to gravity;
 h = local depth;
 K = eddy diffusivity;
 L = typical length of domain;
 n = unit outward normal;
 p = pressure;
 p' = pressure fluctuation due to density variation;
 Q_s = source or sink;

T = temperature distribution;
 t = time;
 u, v, w = velocity vectors in x -, y -, and z -directions, respectively;
 Δt = time interval;
 δ = Dirac delta function;

η = free surface;
 θ = latitude of fluid element;
 ν = eddy viscosity;
 ρ, ρ_0 = fluid density and water density, respectively;
 ρ' = density deviation from standard water density; and
 τ = wind shear stress.

A6. Young, D.L., Liu, Y.H., and Eldho, T.I., 2000, " A Combined BEM-FEM Model for the Velocity-Vorticity Formulation of Navier-Stokes Equations in Three-dimensions", International Journal of Engineering Analysis with Boundary Elements, Vol.24/4 ,pp. 307-316.(SCI)

A combined BEM–FEM model for the velocity–vorticity formulation of the Navier–Stokes equations in three dimensions

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Abstract

This paper describes a combined boundary element and finite element model for the solution of velocity–vorticity formulation of the Navier–Stokes equations in three dimensions. In the velocity–vorticity formulation of the Navier–Stokes equations, the Poisson type velocity equations are solved using the boundary element method (BEM) and the vorticity transport equations are solved using the finite element method (FEM) and both are combined to form an iterative scheme. The vorticity boundary conditions for the solution of vorticity transport equations are exactly obtained directly from the BEM solution of the velocity Poisson equations. Here the results of medium Reynolds number of up to 1000, in a typical cubic cavity flow are presented and compared with other numerical models. The combined BEM–FEM model are generally in fairly close agreement with the results of other numerical models, even for a coarse mesh. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Velocity–vorticity formulation; Navier–Stokes equations; Boundary elements; Finite elements

1. Introduction

Three formulations are well known for the solution of the incompressible Navier–Stokes equations in terms of: primitive variables of pressure and velocity, velocity–stream function and velocity–vorticity. The first two formulations have been thoroughly investigated by various researchers for two- (2D) and three-dimensional (3D) problems using various numerical methods like finite difference (FDM), finite elements (FEM) and boundary element methods (BEM) (e.g. [1–3]). The third formulation in terms of velocity and vorticity also has been explained in the last decade in two and three dimensions using various numerical schemes like FDM [4], FEM [5] and BEM [6].

For the solution of inertial and non-inertial unsteady incompressible viscous flows, numerical solution based on velocity–vorticity Navier–Stokes equations has been pioneered by Fasel [7]. Many researchers successively used the velocity–vorticity formulation for the calculations of 2D and 3D steady and unsteady flows. In most investigations, the governing equations have been written as a system of parabolic and Poisson type equations for the components of the vorticity and velocity fields, respectively. The main

advantage of this formulation includes the numerical separation of the kinematic and kinetic aspects of the fluid flow from the pressure computation, which is determined afterwards from the known velocity and vorticity fields.

The theoretical potentials of FEM [8] and BEM [3] have been adequately exposed for the solution of the Navier–Stokes equations by various researchers. In this paper, an effort has been made to combine the well-known BEM and FEM techniques for solving the velocity–vorticity form of the Navier–Stokes equations in three dimensions. In the present model, the vorticity transport equations in the velocity–vorticity formulation of the Navier–Stokes equations are approximated using a standard Galerkin finite element technique [9] and combined with velocity–vorticity Poisson type equations, which are solved using a standard boundary–domain integral method [10]. The vorticity boundary conditions are exactly obtained by the BEM solution of the Poisson equations. An iterative scheme is employed in the solution of the system of equations after the numerical discretization using BEM and FEM.

The robustness and accuracy of the combined BEM–FEM model has been demonstrated using the well-known model problem of flow in a driven cubic cavity. The cavity flow problem is of continuing interest because it offers a relatively simple model on which numerical techniques may be examined and verified with other numerical

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schemes. Using the combined BEM–FEM model, even for a coarse mesh, accurate results comparable with other models using fine meshes in literature, are obtained for Reynolds number up to 1000.

After presenting the governing equations, the numerical formulation using BEM and FEM are briefly described. Then the solution procedure and numerical results for 3D driven cavity flow problems are provided, followed by a few concluding remarks.

2. Governing equations

Considering a connected fixed domain Ω with boundary Γ occupied by incompressible Newtonian fluid, the governing equations for mass and linear momentum transport can be written as [11]

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{Re} \nabla^2 \bar{u} \quad (1)$$

$$\nabla \cdot \bar{u} = 0 \quad (2)$$

where $\bar{u}$ is the velocity vector, p is the pressure, Re is the Reynolds number and t is the time. Eqs. (1) and (2) represent the Navier–Stokes equations in the pressure–velocity formulation.

The vorticity vector $\bar{\omega}$ can be expressed as:

$$\bar{\omega} = \nabla \times \bar{u} \quad (3)$$

By taking the curl of both sides of Eq. (1) and using Eqs. (2) and (3), we can obtain the vorticity transport equation as:

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{Re} \nabla^2 \bar{\omega} \quad (4)$$

By taking the curl of Eq. (3) and using Eq. (2) we get,

$$\nabla^2 \bar{u} = -\nabla \times \bar{\omega} \quad (5)$$

which is vector form of Poisson's equation for $\bar{u}$.

Eqs. (4) and (5) with $\bar{u}$ and $\bar{\omega}$ as velocity and vorticity vectors are known as velocity–vorticity formulation of the Navier–Stokes equations and can replace Eqs. (1) and (2) in which $\bar{u}$ and p are variables.

We seek a solution in the domain Ω which satisfies the initial conditions,

$$\bar{u} = \bar{u}_0; \quad \bar{\omega} = \nabla \times \bar{u}_0 \quad \text{at } t = 0 \quad (6)$$

and the boundary conditions,

$$\bar{u} = \bar{u}_F; \quad \bar{\omega} = (\nabla \times \bar{u})|_{\Gamma} \quad \text{at } t \geq 0 \quad (7)$$

on the boundary Γ of Ω .

If (u, v, w) are the velocity vectors and (ξ, η, ζ) are the vorticity vectors, then from Eq. (4), the three vorticity

transport equations can be written as:

$$\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z}$$

$$= \xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} + \frac{1}{Re} \nabla^2 \xi$$

$$\frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + v \frac{\partial \eta}{\partial y} + w \frac{\partial \eta}{\partial z}$$

$$= \xi \frac{\partial v}{\partial x} + \eta \frac{\partial v}{\partial y} + \zeta \frac{\partial v}{\partial z} + \frac{1}{Re} \nabla^2 \eta$$

$$\frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} + w \frac{\partial \zeta}{\partial z}$$

$$= \xi \frac{\partial w}{\partial x} + \eta \frac{\partial w}{\partial y} + \zeta \frac{\partial w}{\partial z} + \frac{1}{Re} \nabla^2 \zeta$$

Eq. (5) can be written as

$$\nabla^2 u = -\frac{\partial \zeta}{\partial y} + \frac{\partial \eta}{\partial z}$$

$$\nabla^2 v = \frac{\partial \zeta}{\partial x} - \frac{\partial \xi}{\partial z}$$

$$\nabla^2 w = -\frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y}$$

The solution of vorticity transport Eqs. (8)–(10) in combination with Poisson equations (11)–(13) with initial and boundary conditions, gives the velocity and vorticity distribution all over the domain concerned time step.

3. Numerical formulation

As mentioned earlier, in the solution of the velocity–vorticity formulation of the Navier–Stokes equation using the combined BEM–FEM formulation, the vorticity transport equations (Eqs. (8)–(10)) are solved using the Poisson type velocity equations (Eqs. (11)–(13)) solved using BEM. In this section, the numerical formulation for both BEM and FEM are briefly described.

3.1. Boundary element formulation

Consider the Poisson type velocity equation in u Eq. (5),

$$\nabla^2 u = b(\bar{\omega})$$

with velocity boundary conditions as

$$u = \bar{u}_0 \text{ on } \Gamma_1; \quad q_0 = \frac{\partial \bar{u}_0}{\partial n} \text{ on } \Gamma_2$$

where n is the unit outward normal vector. In the model, an iterative scheme is used such that the right

side of Eq. (14) is known in the current iteration and the time step from the previous step by solving the vorticity transport equation (Eq. (4)).

A weighting function u^* can now be introduced such that it has continuous first derivatives within Ω . The following weighted residual statement can now be written:

$$\int_{\Omega} (\nabla^2 u - b) u^* d\Omega = \int_{\Gamma_2} (q - \bar{q}_0) u^* d\Gamma - \int_{\Gamma_1} (u - \bar{u}_0) q^* d\Gamma \quad (16)$$

where $q = \partial u / \partial n$ and $q^* = \partial u^* / \partial n$.

Let u^* be the fundamental solution of the Laplace equation in three dimensions, represented as $u^* = 1/(4\pi r)$, where r is the distance from the collocation point (k) to other field points (i) given as:

$$r = \sqrt{(x_k - x_i)^2 + (y_k - y_i)^2 + (z_k - z_i)^2} \quad (17)$$

Now applying Green's second identity theorem to Eq. (16) and using the standard boundary element procedure [10], we can get the boundary integral equation as

$$C_i u_i + \int_{\Gamma} u q^* d\Gamma + \int_{\Omega} b u^* d\Omega = \int_{\Gamma} q u^* d\Gamma \quad (18)$$

where C_i is Green's constant which can be calculated by surrounding the boundary point i by a small sphere of radius ϵ and taking each term in Eq. (18) in the limit as $\epsilon \rightarrow 0$. Generally C_i can be represented as $\theta/4\pi$ where θ is the internal solid angle at point i in radians.

In Eq. (18), we have boundary integrals and volumetric-domain integrals. In the present model, the domain integration is carried out by subdividing the domain into a series of internal cells, on each of which a numerical integration is performed. Here 2D isoparametric quadrilateral linear elements are used for the boundary discretization and 3D isoparametric quadrilateral cells are used for the internal discretization. The details of the element properties, shape functions, coordinate transformation and numerical integration used here are described in Brebbia et al. [10] which is not repeated here.

If the domain is discretized into M internal cells, then the domain integral can be written as

$$D_i = \int_{\Omega} b u^* d\Omega = \sum_{e=1}^M \left[\sum_{k=1}^{NI} w_k (b u^*)_k \right] \Omega_e \quad (19)$$

where the integral has been approximated by a summation over different cells (e varies from 1 to M), w_k are the Gauss integration weights, the function $(b u^*)_k$ needs to be evaluated at integration points k on each cell (k varies from 1 to NI , where NI is the total number of integration points on each cell) and Ω_e is the volume of cell e . The term D_i is the result of the numerical integration and is different for each position i of the boundary nodes.

Assuming that the boundary of the domain is discretized

into NE isoparametric quadrilateral linear elements with N nodes, Eq. (18) can be discretized and written in matrix form as

$$C_i u_i + \sum_{j=1}^N \bar{H}_{ij} u_j + D_i = \sum_{j=1}^N G_{ij} q_j \quad (20)$$

Combining the effect of the constant term C with the $\bar{H}$ matrix, we can write the system of matrix as

$$H u + D = G q \quad (21)$$

In Eq. (21), the boundary conditions are introduced and the known values are taken to the right-hand side to form a system of linear equations of the form

$$A X = F \quad (22)$$

where X is a vector of unknown boundary values of u and q , and F is a known vector. Eq. (22) is solved using the Gauss elimination scheme and all the boundary values will be then known. Once this is done, it is possible to calculate internal values of u or its derivatives. The values of u are calculated at any internal point using the Eq. (18) that can be written in condensed form as:

$$u_i = \int_{\Gamma} q u^* d\Gamma - \int_{\Gamma} u q^* d\Gamma - \int_{\Omega} b u^* d\Omega \quad (23)$$

The same discretization is used for the boundary integrals, i.e.

$$u_i = \sum_{j=1}^N G_{ij} q_j - \sum_{j=1}^N \bar{H}_{ij} u_j - D_i \quad (24)$$

where i is an internal point.

The values of the internal fluxes in the Cartesian directions are calculated by carrying out derivatives on Eq. (23), i.e.

$$(q_x)_i = \left(\frac{\partial u}{\partial x} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial x} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial x} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial x} d\Omega$$

$$(q_y)_i = \left(\frac{\partial u}{\partial y} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial y} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial y} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial y} d\Omega$$

$$(q_z)_i = \left(\frac{\partial u}{\partial z} \right)_i = \int_{\Gamma} q \frac{\partial u^*}{\partial z} d\Gamma - \int_{\Gamma} u \frac{\partial q^*}{\partial z} d\Gamma - \int_{\Omega} b \frac{\partial u^*}{\partial z} d\Omega \quad (25)$$

Notice that the derivatives are carried out only on the fundamental solution u^* and q^* as we are computing the variations of flux around the point i .

The main advantage of using BEM in the solution of the velocity Poisson equation is the exact determination of the

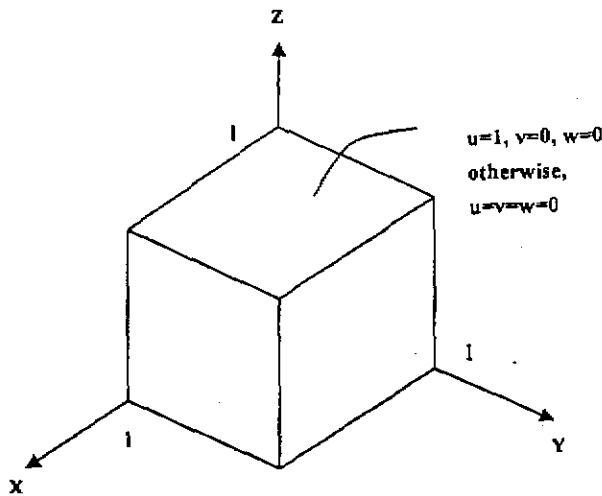


Fig. 1. Model problem with boundary conditions.

vorticity boundary conditions. The vorticity boundary conditions that are essential to solve the vorticity transport equations are directly obtained as the velocity normal derivative from the solution of Eq. (18).

3.2. Finite element formulation

Consider one of the vorticity transport equations in ξ as

$$\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} - \xi \frac{\partial u}{\partial x} - \eta \frac{\partial u}{\partial y} - \zeta \frac{\partial u}{\partial z} - \frac{1}{Re} \nabla^2 \xi = 0 \quad (26)$$

Using the method of weighted residuals and the Galerkin criterion [9], Eq. (26) can be written as

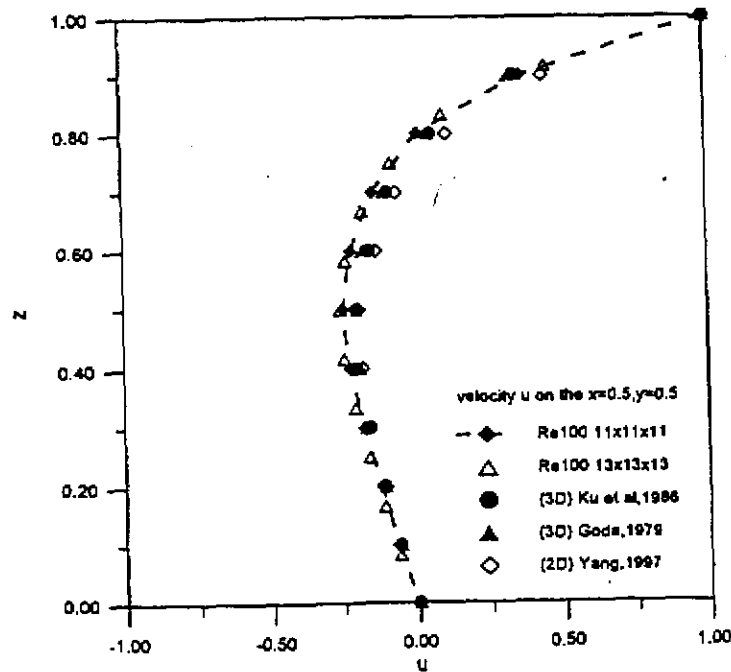
$$0 = \iiint_V N_i \left(\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} - \xi \frac{\partial u}{\partial x} - \eta \frac{\partial u}{\partial y} - \zeta \frac{\partial u}{\partial z} - \frac{1}{Re} \left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2} \right) \right) dV \quad (27)$$

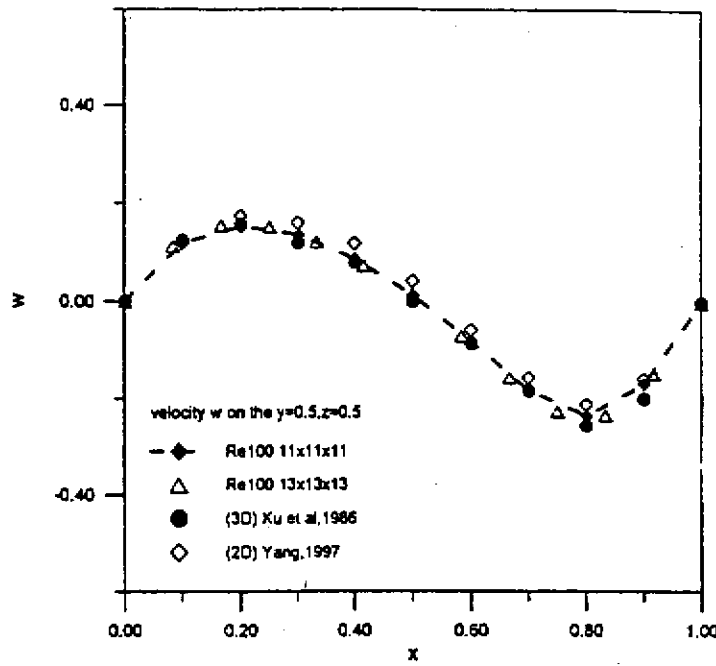
where $N_i = N_i(x, y, z)$ is the shape function. Approximating ξ using the shape function as

$$\xi = \xi(x, y, z, t) = \sum N_i(x, y, z) \bar{\xi}_i(t) \quad (28)$$

and using a time integration for the time derivative of ξ , Eq. (27) can be written as

$$\begin{aligned} 0 = & \sum \iiint_V N_i N_j \bar{\xi}_j' dV \\ & + \sum \iiint_V \left(u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z} \right) \bar{\xi}_j dV \\ & - \sum \iiint_V N_i \left(\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} \right) dV \\ & - \sum \iint_{S_e} q_n N_i dA + \frac{1}{Re} \sum \iiint_V \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) \bar{\xi}_j dV \end{aligned} \quad (29)$$

Fig. 2. Velocity profile (u) on the vertical centerline of a cubic cavity for $Re = 100$.

Fig. 3. Velocity profile (w) on the horizontal centerline of a cubic cavity for $Re = 100$.

where

$$q_n = \frac{\partial \xi}{\partial x} n_x + \frac{\partial \xi}{\partial y} n_y + \frac{\partial \xi}{\partial z} n_z$$

Eq. (29) can be written in the form

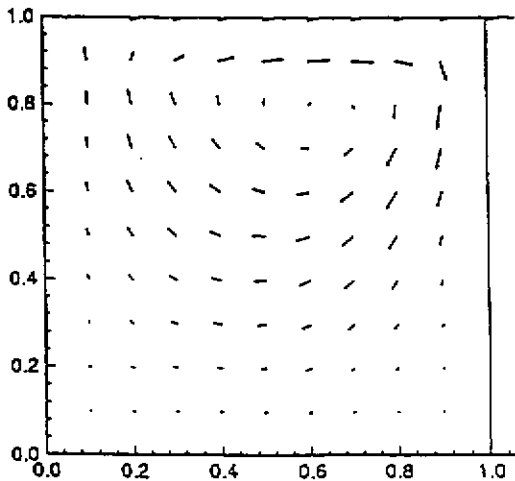
$$\sum [M^e](\xi') + [L^e](\xi) - [R^e] - [Q^e] + \frac{1}{Re}[K^e](\xi) = 0 \quad (30)$$

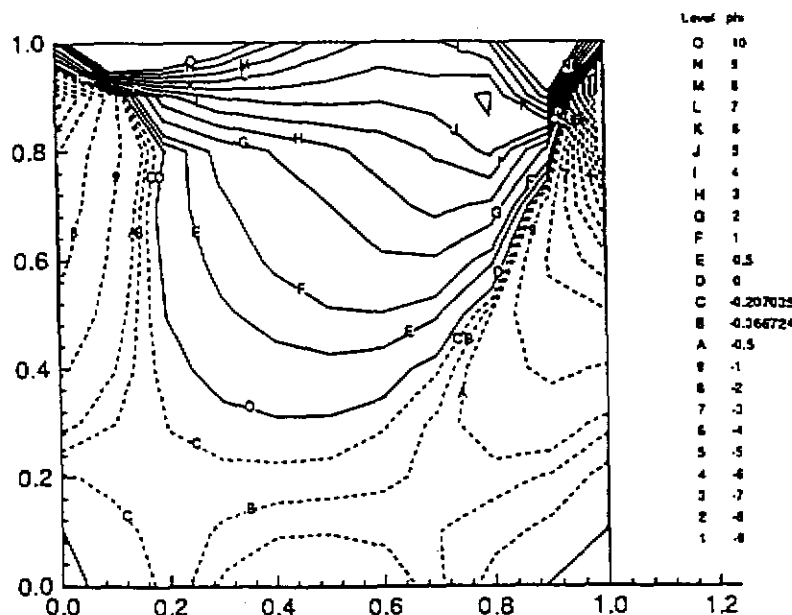
where

$$\begin{aligned} M_{ij}^e &= \iiint_{V^e} N_i N_j dV; \\ L_{ij}^e &= \iiint_{V^e} \left(u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z} \right) dV; \\ R_i^e &= \iiint_{V^e} N_i \left(\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} \right) dV; \\ Q_i^e &= \iint_S q_n N_i dA; \\ K_{ij}^e &= \iiint_{V^e} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) dV \end{aligned} \quad (31)$$

Here isoparametric quadrilateral linear elements are used for the 3D discretization. The details of the interpolation functions, integration and formation of the conductance matrix are described by Reddy [9]. For the solution of the vorticity transport equations, an iterative algorithm is used in which it is assumed that at the current time step, the values of u , v , w , η , ξ , $\partial u/\partial x$, $\partial v/\partial y$ and $\partial w/\partial z$ are known from the previous step. Using a difference scheme to approximate the time derivative of ξ between time steps $(n+1)$ and n as $\{\xi'\} = (\{\xi_{n+1}\} - \{\xi_n\})/\Delta t$ and putting $\{\xi_n\} = \{\xi\}$, we can write the final system of equations in matrix form as

$$\begin{aligned} [M^e]\{\xi_{n+1}\} &= [M^e]\{\xi_n\} - \Delta t[L^e](\xi_n) \\ &\quad + \Delta t[R^e] + \Delta t[Q^e] - \frac{\Delta t}{Re}[K^e](\xi_n) \end{aligned} \quad (32)$$

Fig. 4. Profile of the flow vectors in the $y = 1/2$ plane for $Re = 100$.

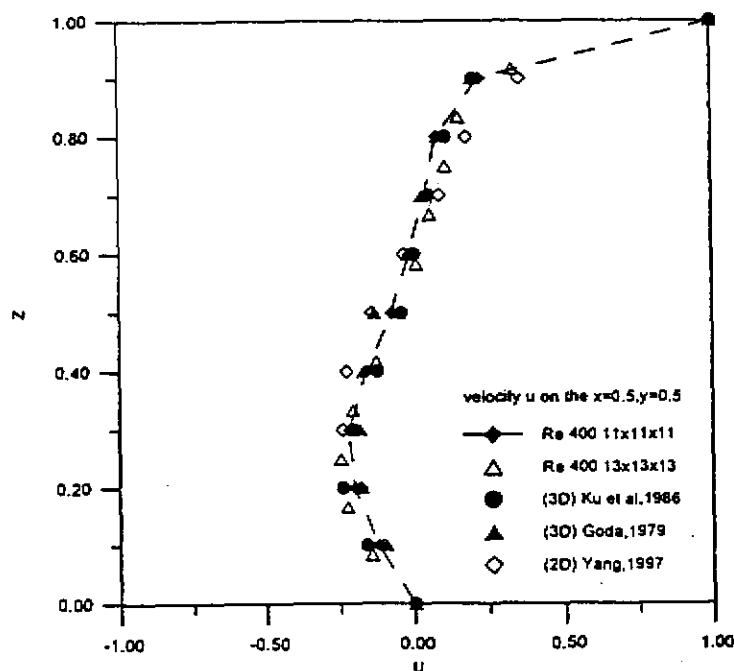
Fig. 5. Vorticity profile (η) in the $y = 1/2$ plane for $Re = 100$.

Here the vorticity boundary conditions obtained from the solution of velocity Poisson equations by BEM is used and the system of equations are solved to find the unknown values of ξ . The derivatives of ξ in Cartesian coordinates are also found which is used in the Poisson equation for the successive iterations and time steps. Here a second order Runge–Kutta (RK) method is used to relax the vorticity values in each iteration, if necessary. Let $\{\bar{\xi}_p\} = \{\bar{\xi}_{n+1}\}$

in Eq. (32). We then obtain the predictor step as

$$[M^e]\{\bar{\xi}_p\} = [M^e]\{\bar{\xi}_n\} - \Delta t[L^e]\{\bar{\xi}_n\} + \Delta t[R^e] + \frac{\Delta t}{Re}[K^e]\{\bar{\xi}_n\}$$

Putting $\{\bar{\xi}_n\} = 1/2(\{\bar{\xi}_p\} + \{\bar{\xi}_n\})$ in Eq. (32), we find

Fig. 6. Velocity profile (u) on the vertical centerline of a cubic cavity for $Re = 400$.

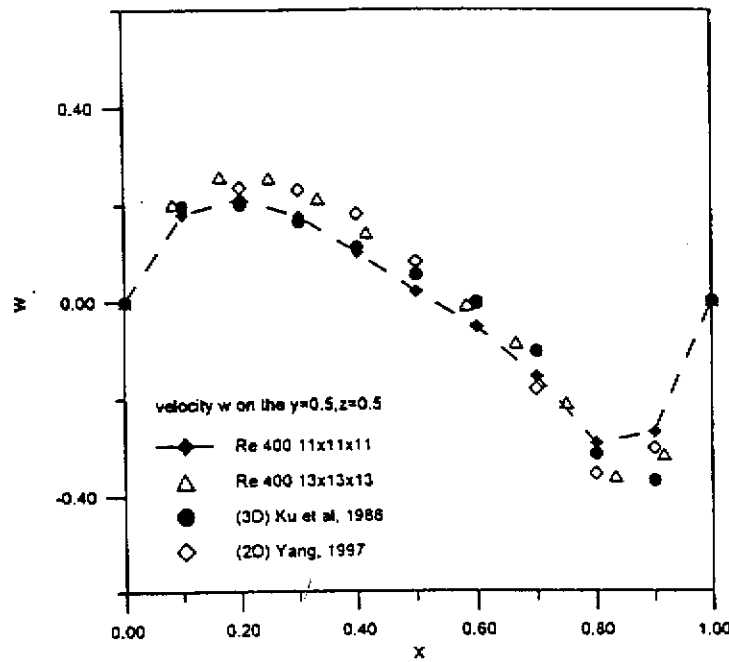


Fig. 7. Velocity profile (w) on the horizontal centerline of a cubic cavity for $Re = 400$.

the second-order RK method as

$$[M^e]\{\bar{\xi}_{n+1}\} = [M^e]\frac{\{\bar{\xi}_p\} + \{\bar{\xi}_n\}}{2} - \Delta t[L^e]\frac{\{\bar{\xi}_p\} + \{\bar{\xi}_n\}}{2} + \Delta t[R^e] + \Delta t[Q^e] - \frac{\Delta t}{Re}[K^e]\frac{\{\bar{\xi}_p\} + \{\bar{\xi}_n\}}{2} \quad (34)$$

In a similar way, other two vorticity transport equations can be solved in the 3D domain.

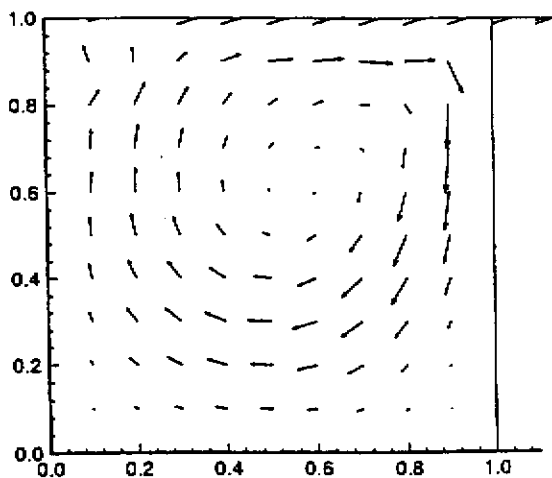


Fig. 8. Profile of the flow vectors in the $y = 1/2$ plane for $Re = 400$.

4. Solution procedure

As mentioned earlier, here an iterative scheme is used in the solution of the velocity–vorticity formulation of Navier–Stokes equations. In most of the incompressible viscous flow problems solved using Navier–Stokes equations, the most natural boundary condition arise when the velocity is prescribed all over the boundaries of the problem. The vorticity boundary conditions are seldom prescribed and hence should be determined from computation. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary condition which are used in the solution of the vorticity transport equations. The computational procedure adopted here includes the following iterative steps:

For the new time step $n = 1$:

1. Assume some initial values for vorticity distribution and derivatives, say zero.
2. Solution of the velocity Poisson equations using BEM:
 - Solve for the unknown boundary velocity or velocity flux values using Eqs. (11)–(13);
 - Calculate the velocity distribution and velocity derivatives at all nodal points using BEM;
 - Determine the new vorticity boundary values using Eq. (3).
3. Solution of the vorticity transport equations using FEM:
 - Solve for the unknown vorticity values throughout the domain using Eqs. (8)–(10);
 - Calculate the derivatives of the vorticity vectors to use in the velocity Poisson equation;

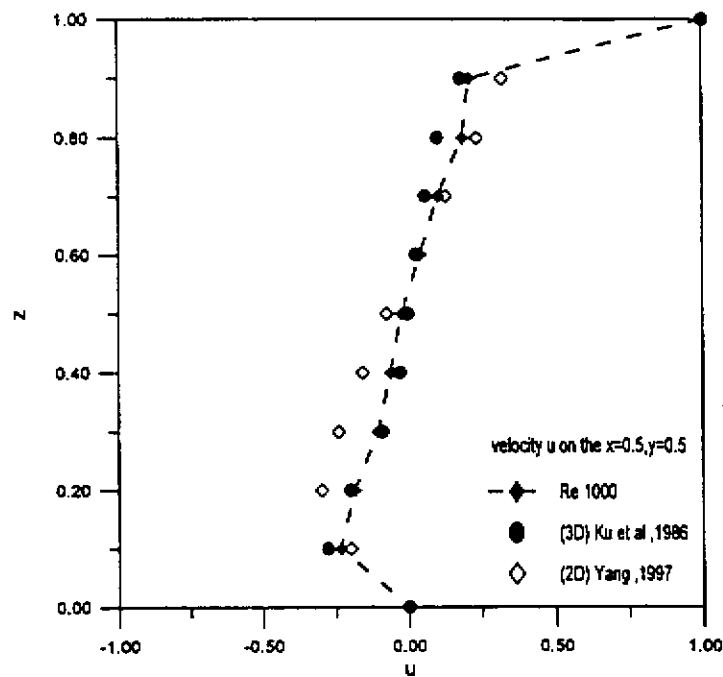


Fig. 9. Velocity profile (u) on the vertical centerline of a cubic cavity for $Re = 1000$.

- Relax the vorticity values using second-order RK method, Eq. (34).
4. Check for convergence of the velocity and vorticity components in the present iteration, for example

$$\frac{|\mu_n^{k+1} - \mu_n^k|}{|\mu_n^k|} \leq 0.001$$

If convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to Step 2.

5. In the successive time step, use the velocity and vorticity components from the previous time step as initial conditions and use the iterative procedure, Steps 2–4. The procedure is repeated until the prescribed time step is reached.

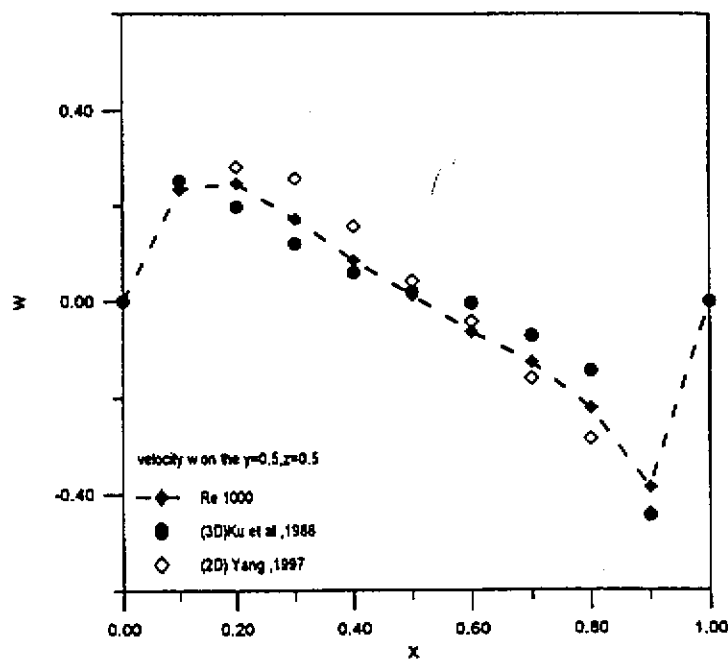


Fig. 10. Velocity profile (w) on the horizontal centerline of a cubic cavity for $Re = 1000$.

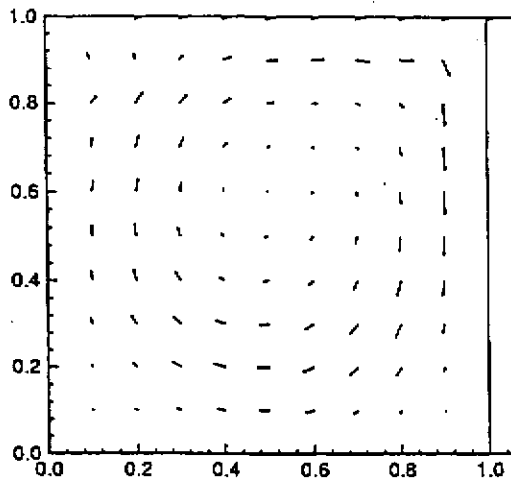


Fig. 11. Profile of the flow vectors in the $y = 1/2$ plane for $Re = 1000$.

5. Model results and discussion

The proposed BEM–FEM model has been applied on a test problem to verify the numerical procedure. The benchmark problem is the classical ‘driven flow in a cubic cavity’ for which many numerical model results are available in literature (see Fig. 1). Present model results are compared with the results of Goda [12] and Ku et al. [13] in three dimensions and with the results of Yang [14] in two dimensions.

The model problem consists of a cubic cavity with a moving top lid with constant velocity, totally filled with an incompressible viscous fluid. Fig. 1 shows the geometry and boundary conditions of the problem. Due to the computational limitations (we used an IBM AIX workstation with 128 MB RAM), the present analysis is limited to two sets of computational mesh points of $11 \times 11 \times 11$ and $13 \times 13 \times 13$ (on the boundary as well as internal domain).

Three analyses have been presented here, for Reynolds number: $Re = 100$, 400 and 1000. Although the computations were carried out with a fully implicit scheme in time, only steady state solutions are presented here. In all the cases, steady states are reached.

Fig. 2 shows the x -component velocity profiles (u) on the vertical centerline of a cavity for $Re = 100$. Fig. 3 shows the z -component velocity profile (w) on the horizontal centerline of the cavity for $Re = 100$. The results mostly agree with those by Goda [12] and Ku et al. [13] bearing in mind that the mesh density is coarse. We also give the 2D results obtained by Yang [14] (using a BEM scheme) for comparison. Fig. 4 shows the profile of flow vectors and Fig. 5 shows the vorticity profile (η) in the $y = 1/2$ plane for Reynolds number $Re = 100$. From Figs. 2 and 3, it can be seen that for both computational mesh grids, the results are almost same. As it is obvious, for the 2D comparison, the results vary slightly due to the 3D boundary effects.

Figs. 6–8 show, respectively, the x -component velocity

profile (u) on the vertical centerline, z -component velocity profile (w) on the horizontal centerline of the cavity and the profile of the flow in the $y = 1/2$ plane, for Reynolds number $Re = 400$. The present results mostly agree with those reported by Goda [12] and Ku et al. [13]. As the Reynolds number increases, the effect of the computational mesh is obvious. The finer mesh in the study ($13 \times 13 \times 13$) gives more agreeable results.

For a higher Reynolds number, $Re = 1000$, calculations are made for the finer computational mesh ($13 \times 13 \times 13$). Figs. 9–11 show, respectively, the x -component velocity profile (u) on the vertical centerline, the z -component velocity profile (w) on the horizontal centerline of the cavity and the profile of the flow in the $y = 1/2$ plane. Results of the analysis agree well with the results of Ku et al. [13] bearing in mind that the mesh density was only $13 \times 13 \times 13$, while in the test case there were $25 \times 13 \times 25$ nodes.

The merit of the present model is that, it provides the best way to treat the velocity–vorticity formulation for 3D flow by combining BEM and FEM. In general, the boundary conditions of vorticity are not known a priori, so that the solution of vorticity transport equation is rather difficult. However, the BEM solution of the velocity Poisson equation together with the no-slip boundary conditions will automatically render the necessary vorticity boundary conditions directly as the normal derivatives of velocity while solving the boundary integral equations. If numerical models like FDM and FEM are used in the solution of velocity Poisson equations, then the boundary vorticity values have to be separately determined from the velocity distribution which may reduce the accuracy in determining the vorticity boundary conditions for the solution of vorticity transport equations. As the vorticity transport equations include convective terms and time dependent terms, FEM solution is more suitable than the BEM. Hence the present model in which the velocity Poisson equations are solved using BEM and vorticity transport equations are solved using FEM and the iterative scheme combining both models provides the best way to treat the velocity–vorticity formulation for 3D incompressible flow problems. This study demonstrates that even with a very coarse mesh, the solutions are very stable and fairly accurate as shown in the case study with different Reynolds numbers.

6. Conclusions

A combined BEM–FEM model has been developed for solving the velocity–vorticity Navier–Stokes equations in three dimensions. The vorticity boundary conditions for the solution of vorticity transport equations are exactly obtained directly from the BEM solution of velocity Poisson equations. Here the results of medium Reynolds number up to 1000, in a typical cubic cavity flow are presented and compared with other numerical models. Despite the

relatively coarse mesh, the results show good convergence and generally in fairly close agreement with other model results using fine meshes. The computational results show that the combined BEM–FEM model presented here provides an efficient tool for the numerical investigation of 3D incompressible viscous fluid flow problems.

Acknowledgements

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SOLUTION OF STOKES FLOW PROBLEM USING DUAL RECIPROCITY BOUNDARY ELEMENT METHOD

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Key Words: velocity-vorticity formulation, Stokes flow, dual reciprocity boundary element method.

ABSTRACT

This paper describes a dual reciprocity boundary element model for the solution of incompressible viscous flows in slow motion, using velocity-vorticity variables. The method involves the solution of advection-diffusion type vorticity equations for vorticity whose solenoidal vorticity components are obtained by solving Poisson type equations involving the velocity and vorticity components. Both the Poisson type equations and the vorticity advection-diffusion type equations are solved using the dual reciprocity boundary element method (DRBEM). In DRBEM, all source terms, advective terms and time dependent terms are converted into boundary integrals and hence the computational domain of the problem reduces by one. Here the results of Stokes flow problems with very low Reynolds numbers in a typical square cavity are presented and compared with other model results. The DRBEM model has been found to be feasible and satisfactory.

I. INTRODUCTION

The incompressible viscous flows in slow motion, known as Stokes flows, have very important applications in many industries. Solutions of the fluid flow equations for Reynolds number $Re=0$ are of practical interest in the area of steady and unsteady slow motion (in reality for $Re \leq 1$) and in the final stage of decay of flows at initially larger Reynolds numbers. Stokes flow problems can be considered as a subset of Navier-Stokes flow problems, in which the non-linear convective terms are very small or neglected. For the solution of incompressible viscous flow problems, three formulations are well known, in terms of: primitive variables of pressure and velocity, velocity-stream function and velocity-vorticity. The

first two formulations have been thoroughly investigated by various researchers for two-dimensional and three-dimensional problems using various numerical methods like finite difference (FDM) (Anderson *et al.*, 1984), finite elements (FEM) (Gunzaburger, 1987) and boundary element methods (BEM) (Power and Wrobel, 1995). The third formulation in terms of velocity and vorticity also has been explained in the last decade, using various numerical schemes like FDM and FEM.

For the solution of Navier-Stokes flow problems using the velocity-vorticity formulation, the governing equations have been written as a system of advection-diffusion type and Poisson type equations for the components of the vorticity and velocity fields, respectively. The main advantage of this

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formulation includes the numerical separation of the kinematic and kinetic aspects of the fluid flow from the pressure computation, which is determined afterwards from the known velocity and vorticity fields.

Boundary Element Method (BEM) has been established as a powerful numerical tool in the solution of various fluid flow problems (Banerjee, 1994; Power and Wrobel, 1995). In BEM, the governing partial differential equations describing the problem domain are transformed into integral equations relating only to the boundary values. Thus BEM is a boundary-oriented method and hence the computational dimension of the problem is reduced by one, so that it is easier in discretization and data preparation for the problem considered. Moreover in BEM, the flux term is obtained directly, as the integral equation is a mix of the variable considered and its normal derivative. These advantages make BEM more suitable for the solution of incompressible viscous flow problems.

The major problems in using the general BEM techniques to solve the incompressible viscous flows are the difficulties in dealing with the convective and time dependent terms. Earlier, to solve any problem using BEM, a fundamental solution for the problem had to be available. The fundamental solution had to take into account all terms in the governing equations to avoid domain integration, otherwise internal cells had to be defined (Brebbia *et al.* 1984). Even though a fundamental solution is available for many problems, it does not ensure that one is available for any given case and it is inconvenient to alter a program by incorporating a new fundamental solution to study a slightly different problem. The use of cells to evaluate domain integrals implies internal discretization and hence BEM loses some of its attractions compared to other domain techniques like FDM and FEM. To avoid all these problems, it is desirable to have a boundary element technique which enables a boundary only solution, does not depend on obtaining a new fundamental solution for each case and can be applied using a similar approach in each case like FEM.

Dual reciprocity BEM (DRBEM) employs a fundamental solution corresponding to a simpler equation, and treats the remaining terms as well as other non-homogeneous terms in the original equation, through a procedure which involves a series expansion using global approximating functions and the applications of the reciprocity principle (Partridge *et al.*, 1992). The method is called dual reciprocity method because it utilizes twice times of the basic reciprocal theorem. The dual reciprocity BEM is essentially a generalized way of constructing particular solutions that can be used to solve non-linear and time-dependent problems as well as to

represent any internal source distribution. The method can be applied to define sources over the whole domain or only part of it. The dual reciprocity boundary element method was introduced by Nardini and Brebbia (1982) for elasto-dynamics problems and has been further extended for general engineering problems (Partridge *et al.*, 1992).

To solve Stokes flow problems, here the dual reciprocity boundary element method is used. For the solution of Navier-Stokes flow equations using DRBEM, the fundamental solution of the Laplace equation is proposed in the analysis. The time dependent term, convective terms and source terms in the governing equations will be approximated using the dual reciprocity method. The vorticity boundary conditions are exactly obtained by the DRBEM solution of the Poisson equation. An iterative scheme is used in the solution after numerical discretization using DRBEM.

The accuracy and feasibility of the DRBEM model has been demonstrated using the well-known model problem of flow in a driven square cavity. The cavity flow problem is of continuing interest because it offers a relatively simple model on which numerical techniques may be examined and verified with other numerical schemes. Using the DRBEM model, even for a coarse mesh, accurate results, comparable with other models using fine meshes, in the literature are obtained.

After presenting the governing equations, the numerical formulations using the DRBEM are briefly described. Then the solution procedures and numerical results for a two-dimensional driven cavity flow problem are provided followed by a few concluding remarks.

II. GOVERNING EQUATIONS

The governing equations for mass and linear momentum transport in a domain Ω with boundary Γ occupied by incompressible Newtonian fluid, can be written as (Liggett, 1994):

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{Re} \nabla^2 \bar{u} \quad (1)$$

$$\nabla \cdot \bar{u} = 0 \quad (2)$$

where $\bar{u}$ - is the velocity vector, p - is the pressure, Re - is the Reynolds number and t - is the time. Eqs. (1) and (2) represent the Navier-Stokes equation in the velocity-pressure formulation.

The vorticity vector $\bar{\omega}$ can be expressed as:

$$\bar{\omega} = \nabla \times \bar{u} \quad (3)$$

By taking the curl of both sides of Eq. (1) and

using Eqs. (2) and (3), one can obtain the vorticity transport equation as:

$$\frac{\partial \omega}{\partial t} + \bar{u} \cdot \nabla \omega = \omega \cdot \nabla \bar{u} + \frac{1}{\text{Re}} \nabla^2 \omega \quad (4)$$

By taking the curl of Eq. (3) and using Eq. (2) one gets,

$$\nabla^2 \bar{u} = -\nabla \times \omega \quad (5)$$

which is the vector form of Poisson's equation for $\bar{u}$. Eqs. (4) and (5) with $\bar{u}$ and ω as velocity and vorticity vectors are known as the velocity-vorticity formulation of the Navier-Stokes equations and can replace Eqs. (1) and (2) in which $\bar{u}$ and p are variables.

The Stokes flow problems are characterized by very small velocities (consequently very low Reynolds numbers), such that the nonlinear convective terms in the Navier-Stokes equations can be neglected. If, in addition, the flow is steady, the whole inertia force is everywhere small in magnitude compared with either pressure or viscous forces. The flow can then be approximated by the motion of a fluid with zero density (or infinite viscosity), generating the linear creeping flow equations (Currie, 1974):

$$-\nabla p + \frac{1}{\text{Re}} \nabla^2 \bar{u} = 0 \quad (6)$$

$$\nabla \cdot \bar{u} = 0 \quad (7)$$

The basic equations of Stokes flow in the velocity-vorticity formulation can be derived from the Navier-Stokes Eqs. (4) and (5) as:

$$\nabla^2 \omega = \frac{\partial \omega}{\partial t} \quad (8)$$

$$\nabla^2 \bar{u} = -\nabla \times \omega \quad (9)$$

In two dimensions, if (u, v) are the velocity vectors and $\omega = \omega \bar{e}_z$ is the associated vorticity vector, then the vorticity transport Eq. (4) can be written as:

$$\frac{\partial \omega}{\partial t} + \bar{u} \cdot \nabla \omega = \frac{1}{\text{Re}} \nabla^2 \omega \quad (10)$$

and Eq. (8) can be written as

$$\nabla^2 \omega = \frac{\partial \omega}{\partial t} \quad (11)$$

In steady state conditions, Eq. (11) can be written as:

$$\nabla^2 \omega = 0 \quad (12)$$

For Stokes flow, in two- dimensions, Eq. (9) can be

written as:

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (13)$$

$$\nabla^2 v = \frac{\partial \omega}{\partial x} \quad (14)$$

For Navier-Stokes equations, solution of the vorticity transport equation in ω (Eq. 10), in combination with the Poisson Eqs. (13) and (14), gives the velocity and vorticity distribution all over the domain at the concerned time step. For unsteady Stokes flow, solution of the vorticity transport Eq. (11), in combination with the Poisson Eqs. (13) and (14), gives the velocity and vorticity distributions all over the domain at the concerned time step. Similarly, in steady state conditions, solution of Eq. (12) in combination with the Poisson Eqs. (13) and (14), gives the velocity and vorticity distribution all over the domain.

A solution is sought in the domain Ω that satisfies the initial conditions,

$$\bar{u} = u_0; \quad \omega = \nabla \times u_0 \quad \text{at } t=0 \quad (15)$$

and the boundary conditions,

$$\bar{u} = u_f; \quad \omega = (\nabla \times u)|_\Gamma \quad \text{at } t=0 \quad (16)$$

on the boundary Γ of Ω .

III. NUMERICAL FORMULATION

As mentioned in section I, in the solution of the velocity-vorticity formulation of Stokes flow equations using the present model, the vorticity transport equation and Poisson type velocity equations are solved by DRBEM. In this section, the numerical formulation for DRBEM for Poisson type velocity equations and advection-diffusion or diffusion type vorticity equations are briefly described.

1. DRBEM Formulation for Velocity Poisson Equations

Consider the Poisson type velocity equation in u and ω , Eq. (13),

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} = b \quad (17)$$

with velocity boundary conditions as,

$$u = \bar{u} \quad \text{on } \Gamma_1; \quad \bar{q} = \frac{\partial \bar{u}}{\partial n} \quad \text{on } \Gamma_2 \quad (18)$$

where n is the unit outward normal vector. In the present model, an iterative algorithm is used such that the right hand side of Eq. (17) is known in the current iteration and time step from the previous step by

solving the vorticity transport Eq. (10) or (11).

Solution to Eq. (17) can be expressed as the sum of the solution of a homogeneous Laplace equation and a particular solution $\bar{u}$ as:

$$u = \bar{u} + \hat{u} \quad (19)$$

where $\bar{u}$ is the solution to the Laplace equation and $\hat{u}$ is a particular solution such that,

$$\nabla^2 \hat{u} = b \quad (20)$$

The dual reciprocity boundary element method (DRBEM) proposes the use of a series of particular solutions $\hat{u}_j$ instead of a single $\hat{u}$. The number of $\hat{u}_j$ used is equal to the total number of nodes in the problem. If there are N boundary nodes and L internal nodes, there will be $N+L$ values of $\hat{u}_j$.

The following approximation of b is then proposed,

$$b \approx \sum_{j=1}^{N+L} \alpha_j f_j \quad (21)$$

where the α_j are a set of initially unknown coefficients and the f_j are approximating functions. The particular solution $\hat{u}_j$ and the approximating function f_j are linked through the relation,

$$\nabla^2 \hat{u}_j = f_j \quad (22)$$

The expansion (21) may then be considered as valid over the whole problem domain as in the case of one large super-element. The functions f_j are geometrically dependent. Substituting (22) into (21) gives,

$$b = \sum_{j=1}^{N+L} \alpha_j (\nabla^2 \hat{u}_j) \quad (23)$$

Substituting (23) into (17) gives,

$$\nabla^2 u = \sum_{j=1}^{N+L} \alpha_j (\nabla^2 \hat{u}_j) \quad (24)$$

The source term b of Eq. (17) has been replaced in Eq. (24) by a summation of products of coefficients α_j and the Laplacian operating on the particular solution $\hat{u}_j$. The procedure for developing the boundary element method for the Laplace equation (Brebbia *et al.*, 1984) will now be applied. Eq. (24) can be multiplied by the fundamental solution u^* , for 2-D problems $u^* = -\ln(r)/2\pi$ and integrating over the domain producing,

$$\int_{\Omega} (\nabla^2 u) u^* d\Omega = \sum_{j=1}^{N+L} \alpha_j \int_{\Omega} (\nabla^2 \hat{u}_j) u^* d\Omega \quad (25)$$

where r is the distance from the collocation point (k)

to the other field points (i) given as,

$$r = \sqrt{(x_k - x_i)^2 + (y_k - y_i)^2}$$

Applying Green's second identity, (Brebbia *et al.*, 1984) produces the following integral equation for each source node i ,

$$\begin{aligned} C_i u_i + \int_{\Gamma} q^* u d\Gamma - \int_{\Gamma} u^* q d\Gamma \\ = \sum_{j=1}^{N+L} \alpha_j (C_j \hat{u}_{ij} + \int_{\Gamma} q^* \hat{u}_j d\Gamma - \int_{\Gamma} u^* \hat{q}_j d\Gamma) \end{aligned} \quad (26)$$

where C_i is the Green's constant which can be calculated by surrounding the boundary point i by a small circle of radius ε and taking each term in Eq. (26) in the limit as $\varepsilon \rightarrow 0$. Generally C_i can be represented as $\theta/2\pi$ where θ is the internal angle at point i in radians. The term $\hat{q}_j$ is defined as $\partial \hat{u}_j / \partial n$, q^* as $\partial u^* / \partial n$ where n is the unit outward normal to Γ .

Note that Eq. (26) involves no domain integrals. The source term b in Eq. (17) has been substituted for by equivalent boundary integrals. This was done by first approximating b using Eq. (23), and then expressing both right and left-hand sides of the resulting expression as boundary integrals using a weighted residual technique or Green's second identity. Now the discretized form of the boundary integral equation can be written for a source node i as:

$$\begin{aligned} C_i u_i + \sum_{k=1}^N \int_{\Gamma_k} q^* u d\Gamma - \sum_{k=1}^N \int_{\Gamma_k} u^* q d\Gamma \\ = \sum_{j=1}^{N+L} \alpha_j (C_j \hat{u}_{ij} + \sum_{k=1}^N \int_{\Gamma_k} q^* \hat{u}_j d\Gamma - \sum_{k=1}^N \int_{\Gamma_k} u^* \hat{q}_j d\Gamma) \end{aligned} \quad (27)$$

Here linear boundary elements are used for the boundary discretization. Details of linear elements and associated interpolation functions can be found in Brebbia *et al.* (1984) and are not repeated here. After introducing the interpolation functions and integrating over each boundary element, the above equation can be written in terms of nodal values as:

$$\begin{aligned} C_i u_i + \sum_{k=1}^N H_{ik} u_k - \sum_{k=1}^N G_{ik} q_k \\ = \sum_{j=1}^{N+L} \alpha_j (C_j \hat{u}_{ij} + \sum_{k=1}^N H_{jk} \hat{u}_{kj} - \sum_{k=1}^N G_{jk} \hat{q}_{kj}) \end{aligned} \quad (28)$$

where $H_{ik} = \int_{\Gamma_j} \phi_1 q^* d\Gamma$ and $G_{ik} = \int_{\Gamma_j} \phi_2 u^* d\Gamma$, in which

ϕ_1 and ϕ_2 are the interpolation functions (Brebbia *et al.* 1984). The index k is used for the boundary nodes

which are the field points. After application to all boundary nodes using a collocation technique, Eq. (28) can be expressed in matrix form as,

$$Hu - Gq = \sum_{j=1}^{N+L} \alpha_j (H\hat{u}_j - G\hat{q}_j) \quad (29)$$

Here the C_i terms have been incorporated onto the principal diagonal of H . If each of the vectors $\hat{u}_j$ and $\hat{q}_j$ is considered to be one column of the matrices $\hat{U}$ and $\hat{Q}$ respectively, then Eq. (29) can be written as:

$$Hu - Gq = (H\hat{U} - G\hat{Q})\alpha \quad (30)$$

Equation (30) is the basis for the application of the dual reciprocity boundary element method (DRBEM) and involves discretization of the boundary only. Internal nodes may be defined in the number and the location desired by the user. From Eq. (23),

$$b = \sum_{j=1}^{N+L} f_j \alpha_j \quad (31)$$

By taking the value of b at $(N+L)$ points, one can express (31) in a matrix form as:

$$b = F\alpha \quad (32)$$

where each column of F consists of vectors f_j containing the values of the function f_j at the $(N+L)$ collocation points. Therefore,

$$\alpha = F^{-1}b \quad (33)$$

Thus the right hand side vector of (32) is a known vector. Applying the boundary conditions to (30) gives a linear system of equations of the form:

$$Ax = y \quad (34)$$

where x contains the unknown boundary values of u and q . The Gauss elimination scheme is used to solve this system of equations to get the boundary unknowns. After finding the boundary unknowns, the function values at internal nodes can be found from,

$$u_i = - \sum_{k=1}^N H_{ik} u_k + \sum_{k=1}^N G_{ik} q_k + \sum_{j=1}^{N+L} \alpha_j (\hat{u}_{ij} + \sum_{k=1}^N H_{ik} \hat{u}_{kj} - \sum_{k=1}^N G_{ik} \hat{q}_{kj}) \quad (35)$$

The particular solution $\hat{u}$, its normal derivative and the corresponding approximating function f used in DRBEM analysis are limited by the formulation except that the resulting F matrix, should be non-singular. The generally used f function is:

$$f = 1 + r + r^2 + \dots + r^m \quad (36)$$

Correspondingly,

$$\hat{u} = \frac{r^2}{6} + \frac{r^3}{12} + \dots + \frac{r^{m+2}}{(m+2)^2 + (m+2)} \quad (37)$$

$$\hat{q} = (r_x \frac{\partial x}{\partial n} + r_y \frac{\partial y}{\partial n} + r_z \frac{\partial z}{\partial n}) \frac{1}{3} + \frac{r}{4} + \dots + \frac{r^m}{m+3} \quad (38)$$

Other than the boundary only solution, the main advantage of using DRBEM in the solution of the velocity Poisson equation is the exact determination of the vorticity boundary conditions. The vorticity boundary conditions, which are essential to solve the vorticity transport equation, are directly obtained as the velocity normal derivative from the solution of Eq. (26).

2. DRBEM Formulation for the Vorticity Transport Equation

Consider the advection-diffusion type vorticity transport equation,

$$\nabla^2 \omega = R_e \left(\frac{\partial \omega}{\partial t} + \bar{u} \cdot \nabla \omega \right) = R_e b(x, y, \omega, t) \quad (39)$$

The fundamental solution of the Laplace equation is used in the solution Eq. (39). Appropriate boundary conditions ω or $q(\partial \omega / \partial n)$ (Dirichlet condition or Neumann boundary condition) and initial conditions (prescribed ω) should be prescribed for the problem.

As in section III.1, using the dual reciprocity principle, the solution to Eq. (39) can be expressed as the sum of the solution of a homogeneous Laplace equation and a particular solution $\hat{\omega}$ as:

$$\omega = \bar{\omega} + \hat{\omega} \quad (40)$$

where $\bar{\omega}$ is the solution to the Laplace equation and $\hat{\omega}$ is a particular solution such that,

$$\nabla^2 \hat{\omega} = b \quad (41)$$

The dual reciprocity boundary element method (DRBEM) proposes the use of a series of particular solutions $\hat{\omega}_j$ instead of a single $\hat{\omega}$. The number of $\hat{\omega}_j$ used is equal to the total number of nodes in the problem. If there are N boundary nodes and L internal nodes, there will be $N+L$ values of $\hat{\omega}_j$.

The following approximation of b is then proposed,

$$b = \sum_{j=1}^{N+L} \alpha_j f_j \quad (42)$$

where the α_j are a set of initially unknown coefficients and the f_j are approximating functions. As explained in section III.1, we can finally write Eq. (39) as:

$$\nabla^2 \omega = R_e \sum_{j=1}^{N+L} \alpha_j (\nabla^2 \hat{\omega}_j) \quad (43)$$

The source term b of (39) has been replaced in Eq. (43) by a summation of products of coefficients α_j and the Laplacian operating on the particular solution $\hat{\omega}_j$.

Similar to the procedure in section III.1, using the 2D fundamental solution of the Laplace equation $(-\ln r/2\pi)$ and using the BEM procedure, the boundary integral equation is written as:

$$\begin{aligned} C_i \omega_i + \int_{\Gamma} q^* \omega d\Gamma - \int_{\Gamma} u^* q d\Gamma \\ = R_e \sum_{j=1}^{N+L} \alpha_j (C_i \hat{\omega}_{ij} + \int_{\Gamma} q^* \hat{\omega}_j d\Gamma - \int_{\Gamma} u^* \hat{q}_j d\Gamma) \end{aligned} \quad (44)$$

After the boundary discretization and integration as mentioned in section III.1, one can write the final system of equations in matrix form as:

$$H\omega - Gq = R_e(H\hat{\omega} - G\hat{Q})\alpha \quad (45)$$

In Eq. (42), the time dependent term and advective terms are approximated as:

$$b = \sum_{j=1}^{N+L} f_j(x, y, z) \alpha_j(t) \quad (46)$$

Here f_j are known functions of geometry and α_j are unknown functions of time. Then Eq. (46) can be written in matrix form as:

$$b = F\alpha \quad (47)$$

or

$$\alpha = F^{-1}b \quad (48)$$

Therefore, one can write Eq. (45) as,

$$H\omega - Gq = R_e(H\hat{\omega} - G\hat{Q})F^{-1}b \quad (49)$$

Putting,

$$S = (H\hat{\omega} - G\hat{Q})F^{-1} \quad (50)$$

Substituting for b , Eq. (50) can be written as,

$$H\omega - Gq = R_e[S(\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y})] \quad (51)$$

Setting,

$$\omega = F\beta \quad (52)$$

or

$$\beta = F^{-1}\omega \quad (53)$$

Differentiating (52) with respect to x and y ,

$$\begin{aligned} \frac{\partial \omega}{\partial x} &= \frac{\partial F}{\partial x} \beta \\ \frac{\partial \omega}{\partial y} &= \frac{\partial F}{\partial y} \beta \end{aligned} \quad (54)$$

Therefore,

$$\begin{aligned} \frac{\partial \omega}{\partial x} &= \frac{\partial F}{\partial x} F^{-1} \omega \\ \frac{\partial \omega}{\partial y} &= \frac{\partial F}{\partial y} F^{-1} \omega \end{aligned} \quad (55)$$

$$H\omega - Gq = R_e S[\frac{\partial \omega}{\partial t} + (u\frac{\partial F}{\partial x} + v\frac{\partial F}{\partial y})F^{-1}\omega] \quad (56)$$

Putting

$$\omega' = \frac{\partial \omega}{\partial t}; \quad E = u\frac{\partial F}{\partial x} + v\frac{\partial F}{\partial y} \quad (57)$$

One can write Eq. (56) as,

$$H\omega - Gq = R_e S[\omega' + EF^{-1}\omega] \quad (58)$$

Now substituting,

$$M = R_e S E F^{-1}; \quad N = -R_e S \quad (59)$$

The final equation system is written as:

$$N\omega' + (H - M)\omega = Gq \quad (60)$$

Using a two level time integration for ω and q and a difference scheme for the time derivative as,

$$\begin{aligned} \omega &= (1 - \theta_u)\omega^m + \theta_u\omega^{m+1} \\ q &= (1 - \theta_q)q^m + \theta_q q^{m+1} \\ \omega' &= \frac{1}{\Delta t}(\omega^{m+1} - \omega^m) \end{aligned} \quad (61)$$

where θ_u and θ_q are weighting factors which position the values of u and q , respectively, between time levels m and $m+1$. Substituting (61) into (60) gives:

$$\begin{aligned} &(\frac{N}{\Delta t} + \theta_u(H - M))\omega^{m+1} - \theta_q Gq^{m+1} \\ &= [\frac{N}{\Delta t} - (1 - \theta_u)(H - M)]\omega^m + (1 - \theta_q)Gq^m \end{aligned} \quad (62)$$

The right hand side of (62) is known at time

$(m+1)\Delta t$, since it involves values which have been specified as initial conditions or calculated previously. Upon imposing the boundary conditions at time $(m+1)\Delta t$, one can form a linear system of equations of the form,

$$A x = y \quad (63)$$

This linear system of equations is solved using the Gauss elimination scheme to find the unknown function values initially over the boundary and then at the internal nodes considered.

The approximating functions ' f ' given in section III.1 and corresponding to particular solutions and derivatives given in Eqs. (37) and (38) are used here also. As mentioned earlier, here an iterative scheme is used in the solution of Navier-Stokes equations or Stokes flows and the derivatives of the vorticity ω in x - and y - directions should be determined before the velocity Poisson equations are solved so that the right hand side of the Poisson equations are known in each iteration. Here a special DRBEM technique is used to determine the derivatives of ω . Once the vorticity values are known by solving the linear system of Eq. (63), then the derivatives of vorticity can be easily calculated from Eq. (55).

For unsteady Stokes flow problems, the vorticity diffusion Eq. (11) can be approximated using the DRBEM in a similar way and Eq. (62) can be expressed as:

$$\begin{aligned} & \left[\frac{N}{\Delta t} + \theta_u H \right] \omega^{m+1} - \theta_q G q^{m+1} \\ & = \left[\frac{N}{\Delta t} - (1 - \theta_u) H \right] \omega^m + (1 - \theta_q) G q^m \end{aligned} \quad (64)$$

As mentioned earlier, a linear system of equations can be formed as in Eq. (63), which is solved for the unknowns. All other procedures are the same as earlier.

IV. SOLUTION PROCEDURE

Here an iterative scheme is used in the solution of the velocity-vorticity formulation of Stokes flow equations. In most incompressible viscous flow problems, the most natural boundary condition arises when the velocity is prescribed all over the boundaries of the problem. Vorticity boundary conditions are seldom prescribed and hence should be determined from computation. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary conditions which are used in the solution of the vorticity transport equations. The solution procedure adopted here includes the following iterative steps:

For the time step $n=1$,

1. Assume some initial values for vorticity distribution and derivatives, say zero.
2. Solve the velocity Poisson Eqs. (13) and (14) using DRBEM
 - Get the unknown boundary velocity or velocity flux values
 - Calculate the velocity distribution and velocity derivatives at all nodal points
 - Determine the new vorticity boundary values using the definition of vorticity in Eq. (3)
3. Solve the vorticity transport Eq. (10)/(11) using DRBEM
 - Get the unknown vorticity values throughout the domain
 - Calculate the derivatives of the vorticity vectors using Eq. (55) to use in the velocity Poisson equation
 - Relax the vorticity values, if necessary
4. Check for the convergence of the velocity and vorticity components in the present iteration, for example,

$$\frac{|u_{k+1}^n - u_k^n|}{|u_k^n|} \leq 0.0001$$

If the convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to step 2.

5. For successive time steps, use the velocity and vorticity components from the previous time step as initial conditions and use the iterative procedure, steps 2 to 4. The procedure is repeated until the prescribed time step is reached.

V. RESULTS AND DISCUSSION

The proposed DRBEM model has been applied on a test problem to verify the accuracy and feasibility of the model. The test problem is the classical 'driven flow in a square cavity' for which many numerical model results are available in the literature (see Fig. 1). Present model results are compared with the results of a series solution, FEM and BEM models in two dimensions.

The model problem consists of a square cavity with a moving top lid with constant velocity, totally filled with an incompressible viscous fluid. Fig. 1 shows the geometry and boundary conditions of the problem. Reynolds number is so low that the induced motion can be described as Stokes flow. In all cases, the flow inside the cavity was initially at rest. No slip and impermeability conditions were imposed on all walls, with the velocity at the upper wall set equal to unity. Due to the computational limitations (an

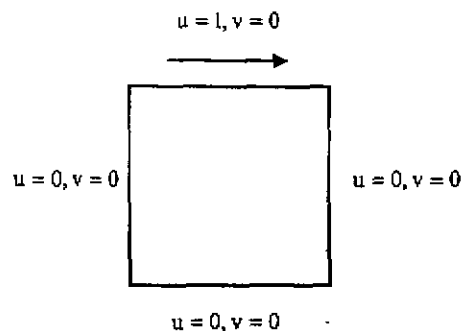
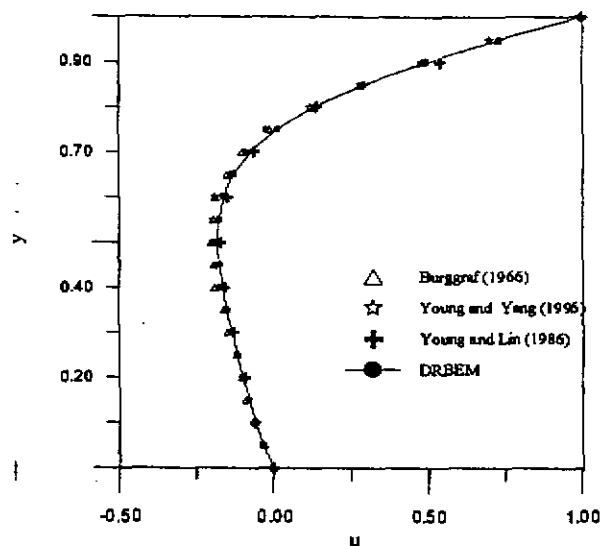
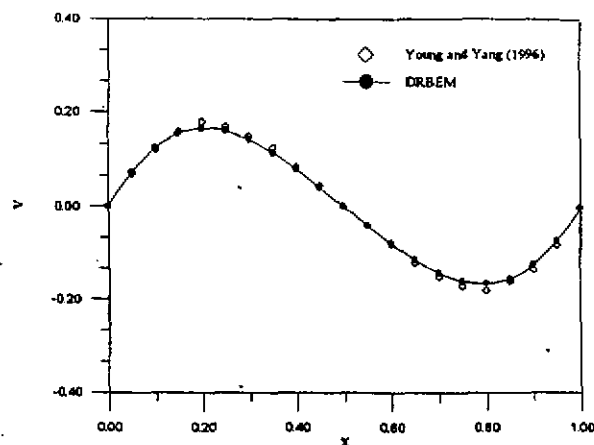
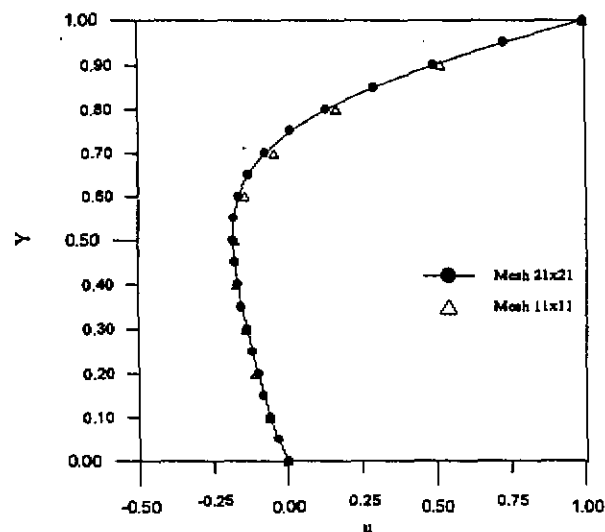


Fig. 1 Model problem with boundary conditions

Fig. 2 Velocity profile (u) on the centerline at $x=0.5$ of a square cavity for $Re=0$

IBM PC, Pentium II with 64 MB RAM, has been used), the present analysis is limited to a maximum of computational mesh points of 21×21 (on the boundary as well as the internal domain).

Two cases have been presented here, for steady state Stokes flow condition ($Re=0$) and very low Reynolds number ($Re=1$) Navier-Stokes equation problems. Fig. 2 shows the x -component velocity profile (u) on the vertical centerline of the cavity for steady state Stokes flow ($Re=0$) conditions for 21×21 mesh. The results are compared with a series solution (Burggraf, 1966), FEM solution (Young and Lin, 1986) and BEM solution (Young and Yang, 1996) and are in good agreement, bearing in mind that the mesh density is coarse. Fig. 3 shows the y -component velocity profile (v) on the horizontal centerline of the cavity for steady state Stokes flow ($Re=0$) conditions for 21×21 mesh. The results are also compared with the BEM solution of Young and Yang (1996) and is in good agreement.

Fig. 3 Velocity profile (v) on the centerline at $y=0.5$ of a square cavity for $Re=0$ Fig. 4 Velocity profile (u) on the centerline at $x=0.5$ of a square cavity for $Re=0$, Mesh convergence

As a convergence test for the grid, analysis has been done at $Re=0$ for the uniform meshes of 11×11 and 21×21 . Fig. 4 shows the x -component velocity profiles (u) on the vertical centerline with different meshes. The results seem to be varying slightly for both the meshes. The velocity vectors, u vs. v for $Re=1$, are shown in Fig. 5. The center of circulating gyre is estimated to be located around $x=0.5$ and $y=0.75$ which is the major circulation vortex. The distribution of vorticity ω , is shown in Fig. 6. The vorticity is symmetric along $x=0.5$. As can be visualized, two singular points near the two corners are very conspicuous, since there is velocity discontinuity occurring at the corner points.

A comparison of the x -component velocity profile (u) on the vertical centerline for $Re=0$ (steady state Stokes flow) and $Re=1$ (very low Reynolds

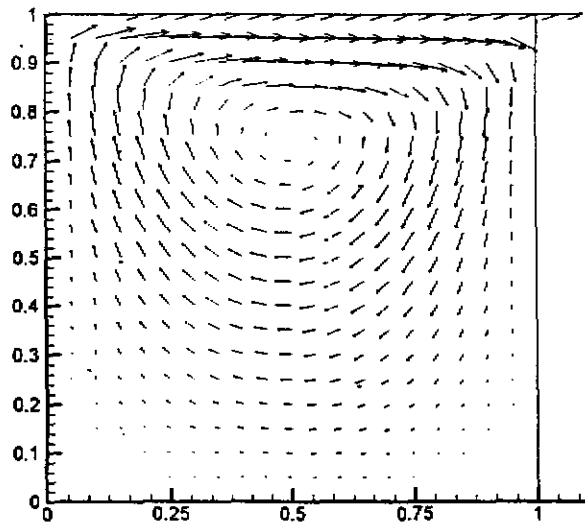


Fig. 5 Profile of the flow vector (u vs. v) in the square cavity for $Re=1$

number Stokes flow problem solved with Navier-Stokes equations) is shown in Fig. 7. As obvious from Fig. 7, there is an observable difference in the velocity profile for both Stokes flow regimes with $Re=0$ and $Re=1$. A comparison of the vorticity profiles for $Re=0$ and $Re=1$ also shows a difference, although the pattern is almost the same. The nonlinear convective effects have an obvious tendency to increase the vorticity and velocity intensities. Hence it can be concluded that when low Reynolds number Stokes flow is to be considered, for accurate solutions, Navier-Stokes equations should be employed.

The merit of the present model is that, it provides the best way to treat the velocity-vorticity formulation for two-dimensional Stokes flow by DRBEM without domain discretization. Hence the computational domain of the problem reduces by one, that is, the two-dimensional problem is solved in one dimension effectively. In general, the boundary conditions of vorticity are not known *a priori*, so that the solution of vorticity transport equation is rather difficult. However the DRBEM solution of the velocity Poisson equations will automatically render the necessary vorticity boundary condition. This study demonstrates that even with a relatively coarse mesh, the solutions are very stable and accurate.

VI. CONCLUDING REMARKS

A dual reciprocity boundary element method (DRBEM) model has been developed for solving the velocity-vorticity Navier-Stokes and Stokes flow equations. The vorticity boundary conditions for the solution of vorticity transport equations are exactly obtained directly from the DRBEM solution of velocity Poisson equations. The use of DRBEM enables

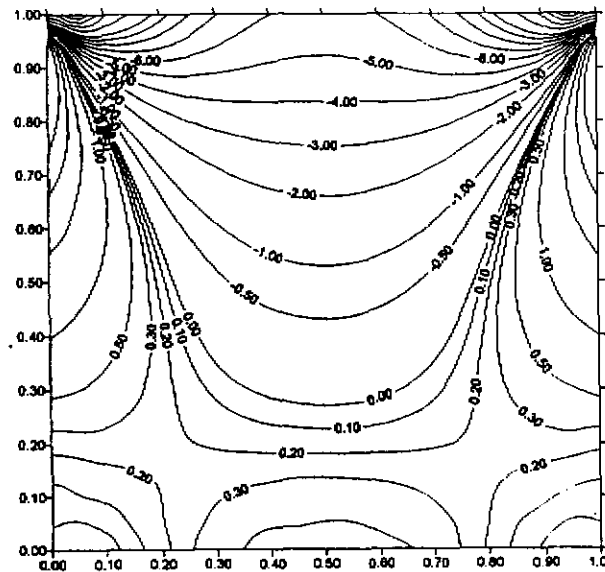


Fig. 6 Vorticity profile (ω) in the square cavity for $Re=1$

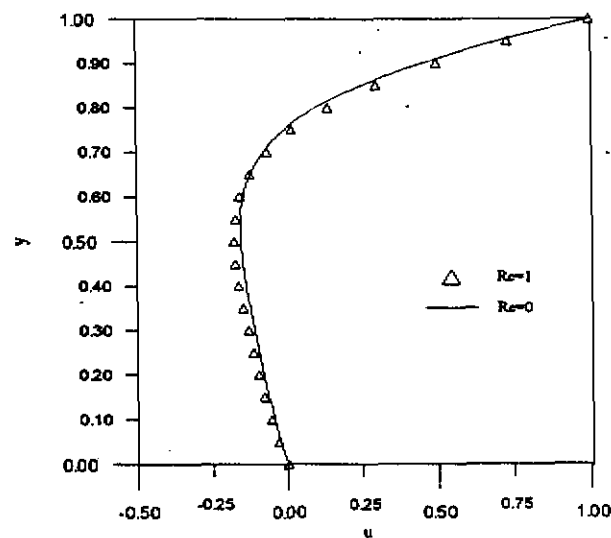


Fig. 7 Comparison of velocity profiles (u) on vertical centerline of a square cavity for $Re=0$ and $Re=1$

one to have a boundary only solution for the problem, and the computational dimensions of the problem are reduced by one. Here the results of low Reynolds number Stokes flow problems, in a typical square cavity flow are presented and compared with other numerical models. Computational results show that the DRBEM presented here provides a feasible tool for numerical investigation of incompressible viscous fluid flow in slow motion.

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NOMENCLATURE

f	approximating function
n	unit outward normal
p	pressure
Re	Reynolds number
t	time
$\vec{u}$	velocity vector
u, v	velocities in x -, y - directions
u^*	fundamental solution of Laplace equation

Greek symbol

α	a set of initially unknown coefficients
Ω	domain of the problem considered
Γ	boundary of the domain considered vorticity
$\vec{\omega}$	vorticity vector
ω	vorticity in two- dimensions

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利用雙倒易邊界元素法求解史托克斯流場

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摘 要

本文利用雙倒易邊界元素法，以速度及渦度為變數求解運動緩慢之史托克斯流場問題。利用速度-渦度法，速度場祇需求解卜松速度方程式，而渦度場則求解傳輸渦度方程式。這些方程式均利用雙倒易邊界元素法求解，以減少一個維度，本文發現雙倒易邊界元素法可以得到令人滿意的結果。

關鍵詞：速度-渦度法，史托克斯流場，雙倒易邊界元素法。

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TWO-DIMENSIONAL INCOMPRESSIBLE FLOWS BY VELOCITY-VORTICITY FORMULATION AND FINITE ELEMENT METHOD

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ABSTRACT

In this study, the motion of incompressible viscous fluid in a two-dimensional domain is solved by the finite element method using the velocity-vorticity formulation. To demonstrate the model feasibility, first of all the steady Stokes flow in a square cavity are computed. The results of square cavity flow are comparable with the numerical solutions of Burggraf (1966, FDM) [1]. Then the unsteady Navier-Stokes flow are computed and compared with other models [1-4]. The results reveal that finite element analysis is a very powerful approach in the realm of computational fluid mechanics.

Keywords : Velocity-vorticity formulation, Finite element method, Navier-Stokes equations.

1. INTRODUCTION

Finite element method (FEM) has been proved to be very convenient and most promising for obtaining spatial approximation to problems with complex geometries. Finite element theory provides an effective methodology for construction of discrete and/or semi-discrete approximations to various boundary value problems in computational mechanics, including the different forms of the Navier-Stokes equations in fluid mechanics. Three formulation are well known for the solutions of the incompressible Navier-Stokes equations, in terms of: primitive variables of pressure-velocity, velocity-stream function and velocity-vorticity. The first two formulations have been thoroughly investigated by various researchers for two dimensional and three dimensional problems using various numerical methods such as finite difference (FDM) [5], finite element (FEM) [6] and boundary element methods (BEM) [7]. The third formulation in terms of velocity and vorticity also has been explained in the last decade, mainly in two dimensions using various numerical schemes.

In the computational methodology of unsteady incompressible viscous fluid flows, the fractional step methods have been proven to be effective. However semi-implicit FEM methods have gained some advantages of stability and simplicity. Different time marching methods to solve the vorticity transport equation are another feature in this study. The

schemes include the explicit method, implicit method, and fully-implicit method. From the analysis of the results, the difference between these methods is that if we use explicit method it has the strict limitation of the timestep, Δt . On the other hand, if the implicit method is used, although the range of Δt is not restricted, it is suitable to use smaller value of Δt to ensure that at the high Reynolds number, each iterative steps can guarantee the convergence of the iterative solution.

2. GOVERNING EQUATIONS

The partial differential equation set governing viscous, laminar flow of an incompressible fluid is a subject class of the familiar nonlinear Navier-Stokes equations system. Let Ω be the fluid domain, which is surrounded by a piecewise smooth boundary Γ . By using the vector form, the corresponding basic equations of conservation of mass, and momentum are [8,9]

Continuity

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

Momentum

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \vec{u} \quad (2)$$

* Professor

where $\vec{u}$ is the velocity vector, p is the pressure, Re is the Reynolds number and t is the time. Equations (1) and (2) represent the Navier-Stokes equations in the pressure-velocity formulation.

The vorticity vector $\vec{\omega}$ can be expressed as:

$$\vec{\omega} = \nabla \times \vec{u} \quad (3)$$

By taking the curl of both sides of Eq. (2) and using Eqs. (1) and (3), we can obtain the vorticity transport equation as follows:

$$\frac{\partial \vec{\omega}}{\partial t} + \vec{u} \cdot \nabla \vec{\omega} = \vec{\omega} \cdot \nabla \vec{u} + \frac{1}{Re} \nabla^2 \vec{\omega} \quad (4)$$

By taking the curl of Eq. (3) and using Eq. (1) we get,

$$\nabla^2 \vec{u} = -\nabla \times \vec{\omega} \quad (5)$$

which is the vector form of Poisson equation for $\vec{u}$.

Equations (4) and (5) with $\vec{u} = (u, v, w)$ as velocity vector and $\vec{\omega} = (\omega_x, \omega_y, \omega_z)$ as vorticity vectors are known as Velocity-Vorticity formulation of the Navier-Stokes equations and can replace Eqs. (1) and (2) in which $\vec{u}$ and p are primitive variables.

The two-dimensional velocity-vorticity formulation for the incompressible flows can be derived from the Eqs. (4) and (5) as following:

$$\frac{\partial \omega}{\partial t} + u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} = \frac{1}{Re} \nabla^2 \omega \quad (6)$$

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (7)$$

$$\nabla^2 v = \frac{\partial \omega}{\partial x} \quad (8)$$

For the Navier-Stokes equations, the solution of vorticity transport equation in Eq. (6), in combination with the velocity Poisson Eqs. (7) and (8), gives the velocity and vorticity distributions all over the domain at the concerned time step.

We seek a solution in the domain Ω which satisfies the initial conditions,

$$u = u_0, v = v_0; \omega = \omega_0 \text{ at } t = 0 \quad (9)$$

and no-slip boundary conditions of velocity on the boundary Γ of Ω .

As far as vorticity boundary condition is concerned, it is not known *a priori*. From the Stokes theorem, the vorticity boundary conditions can be written as,

$$\omega = \frac{1}{\text{area}} \oint \vec{u} \cdot d\vec{s} \quad (10)$$

3. FINITE ELEMENT FORMULATION

The arbitrary element velocity and vorticity are approximated as (By using indicial notation and summation convention for repeated indices)

$$\omega_j = N_j \omega, \quad (11)$$

$$u_j = N_j u, \quad (12)$$

$$v_j = N_j v, \quad (13)$$

where N_j denotes the interpolation or shape function of vorticity and velocity. The weak formulations of Eq. (6), is obtained by using the standard Galerkin method

$$0 = \iint \left[N_i \left(\frac{\partial \omega}{\partial t} + u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} - \frac{1}{Re} \left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) \right) \right] d\Omega \quad (14)$$

and using a time integration for the time derivative of ω , Eq. (14) can be written as,

$$\begin{aligned} 0 = & \sum \iint N_i N_j \frac{d\omega_j}{dt} d\Omega \\ & + \sum \iint \left(N_k u_k N_i \frac{\partial N_j}{\partial x} + N_k v_k N_i \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \\ & - \sum_{\Gamma} \int q_n N_i d\Gamma \\ & + \frac{1}{Re} \sum \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \end{aligned} \quad (15)$$

$$\text{where } q_n = \frac{\partial \omega}{\partial x} n_x + \frac{\partial \omega}{\partial y} n_y,$$

For two dimensional flows, if $q_n = 0$ or ω is specified on the boundary, then the surface integration vanishes. Equation (15) can be written in the form,

$$\sum [M_{ij}^e] \{\dot{\omega}_j\} + [L_{ij}^e] \{\omega_j\} + \frac{1}{Re} [K_{ij}^e] \{\omega_j\} = \{0\} \quad (16)$$

where

$$M_{ij}^e = \iint N_i N_j d\Omega$$

$$L_{ij}^e = \iint \left(N_k u_k N_i \frac{\partial N_j}{\partial x} + N_k v_k N_i \frac{\partial N_j}{\partial y} \right) d\Omega$$

$$K_{ij}^e = \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega$$

$$\dot{\omega} = \frac{\omega^{n+1} - \omega^n}{\Delta t} \quad (17)$$

The fractional step methods have been proven to be effective, in the meantime semi-implicit FEM method has rendered some advantages of stability and simplicity.

So the Eq. (17) can be written

$$\begin{aligned} & \left\{ \frac{1}{\Delta t} [M_{ij}^{(e)}] + \theta \left[L_{ij}^{(e)} + \frac{1}{Re} K_{ij}^{(e)} \right] \right\} \{\omega_j\}^{n+1} \\ & = \left\{ \frac{1}{\Delta t} [M_{ij}^{(e)}] - (1-\theta) \left[L_{ij}^{(e)} + \frac{1}{Re} K_{ij}^{(e)} \right] \right\} \{\omega_j\}^n \end{aligned} \quad (18)$$

Equation (18) confirms that the needed additional data are integration time-step size Δt , integration factor θ , and the known data $\{\omega\}_j^n$ at any time t^n .

$\theta = 0$ means explicit method (always instable)

$\theta = 1$ means fully-implicit method

In this model, $\theta = 2/3$ is chosen.

Consider the Poisson type velocity equation in u and assuming that the vorticity and its derivatives are known, Eq. (7) can be written as follows:

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (19)$$

using the method of weighted residuals and Galerkin criterion, Eq. (19) can be written as,

$$0 = \iint N_i \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial \omega}{\partial y} \right) d\Omega \quad (20)$$

$$\Rightarrow 0 = \sum \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega - \sum \iint \left(N_i \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \quad (21)$$

$$\Rightarrow [K_y^{(e)}] \{u_j\} + [P_y^{(e)}] \{\omega_j\} = \{0\} \quad (22)$$

where

$$P_y^{(e)} = -\sum \iint \left(N_i \frac{\partial N_j}{\partial y} \right) d\Omega \quad (23)$$

Similar formulation is performed for the v component.

4. SOLUTION PROCEDURE

Here an iterative scheme is used in the solution of the velocity-vorticity formulation of the Navier-Stokes equations. In most of the incompressible viscous flow problems, the most natural boundary conditions arise when the velocity is prescribed all over the boundaries of the problem. The vorticity boundary conditions are originated from the Stokes theorem. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary conditions which are used in the solution of the vorticity transport equation. The solution procedures adopted here include the following iterative steps:

1. Initial condition: Let $\omega = 0$.
2. Solve the velocity Poisson Equation using FEM.
 - a. Calculate the velocity distribution and velocity derivatives at all nodal points.
 - b. Determine the new vorticity boundary values.
3. Solved the vorticity transport equation.
 - a. Get the unknown vorticity values through out the domain.

- b. Calculate the derivatives of the vorticity to be used in the velocity Poisson equations.

4. Check for the convergence of the velocity and vorticity components in the present iteration. If convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to step 2.
5. In the successive time step, we use the velocity and vorticity components from the previous time step as initial conditions and use the iterative procedures, steps 2 to 4. The procedures are repeated until the prescribed time step is reached.

5. NUMERICAL EXAMPLES

The aim of this paper is to compute a two-dimensional lid-driven cavity flow (see Fig. 1). The model problem consists of a square cavity of size 1: 1 (dimensionless) with a moving top lid with constant velocity of unity (dimensionless) in the x -direction, totally filled with an incompressible viscous fluid. Figure 1 shows the domain geometry and boundary conditions of the problem.

In the Navier-Stokes equations of system, the intensity of the nonlinearity and the convective effects, are known to be related with the magnitude of the Reynolds number. Therefore, the computational effort required for its numerical solution increases as the Reynolds number increases. An important consequence of this dependency is that the accuracy of the numerical solution, at different values of the Reynolds number, is strongly associated with the way in which the mesh discretisation is defined, requiring a higher density in the regions near the gradient contours, where the boundary layer is developed, as the Reynolds number increases.

For flows with high Reynolds numbers, the use of a coarse mesh often yields a convergent solution without physical meaning. By refining the computational mesh, it is possible to improve the solution of the flow phenomena, but at the expense of increasing the computational cost. In the present examples, a typical grid is shown in Fig. 2 for the fine mesh to solve the Navier-Stokes equations.

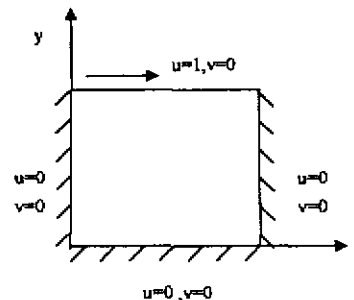


Fig. 1 Model problem with boundary conditions

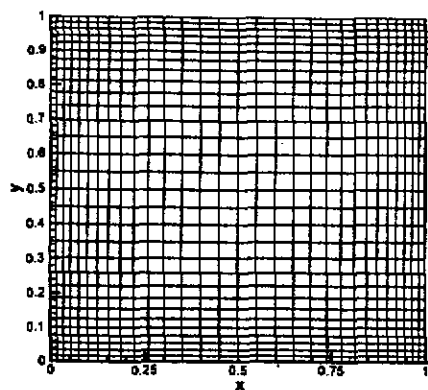


Fig. 2 Non-uniform mesh for cavity flow

The case presented here, is for steady state Stokes flow conditions. Figure 3 shows the velocity profiles for Stokes flow on vertical and horizontal centerlines. The results are compared with Burggraf (1966)[1] and Karageorghis and Fairweather (1989) [2]. The streamlines and velocity vectors are shown in Figs. 4 and 5, respectively, the distribution of vorticity contour is shown in Fig. 6. The symmetric properties of the physical features is similar to the circular cavity flow as obtained analytically by Hwu, *et al.* (1997)[10].

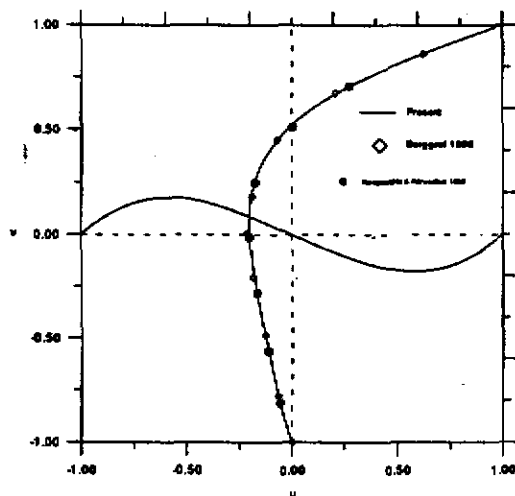


Fig. 3 Velocity profiles for Stokes flow

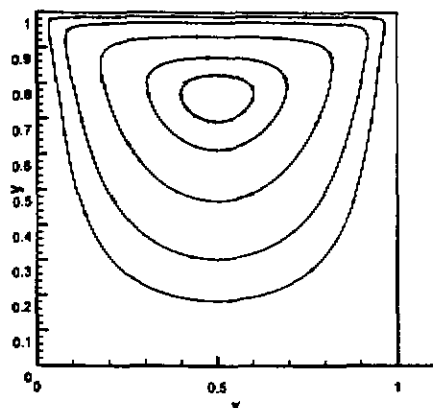


Fig. 4 Streamlines for Stokes flow

In Fig.7, we plot the velocity field, and the vertical and horizontal centre-line velocity profiles, respectively, obtained with the present approach without the use of the domain decomposition scheme for the case of $Re = 100$ and $Re = 400$. As can be observed, for this small values of the Reynolds number, the results based upon a velocity-vorticity formulation are in close agreement with the benchmark values obtained by Burggraf (1966) [1] and Ghia, *et al.* (1982)[3], using a finite difference multigrid numerical scheme. As pointed out previously, as the flow regions near the corners, the flow contains singularities associated with infinite values of the vorticity and surface traction. The distribution of vorticity contours for $Re = 100$ and $Re = 400$ are shown in Figures 8 and 9, respectively.

As Re is further increased, the inertia begins to play an important role. As a consequence, the vortex center has shifted downstream, vorticity distribution gets more complex, and corner eddies start to appear. As shown in Figs. 10 to 12 which illustrates the velocity profiles, velocity distribution and vorticity contours. As Re

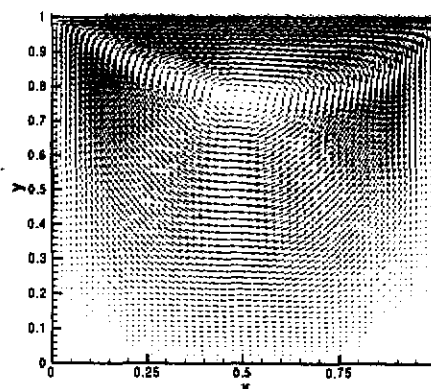


Fig. 5 Velocity distribution for Stokes flow

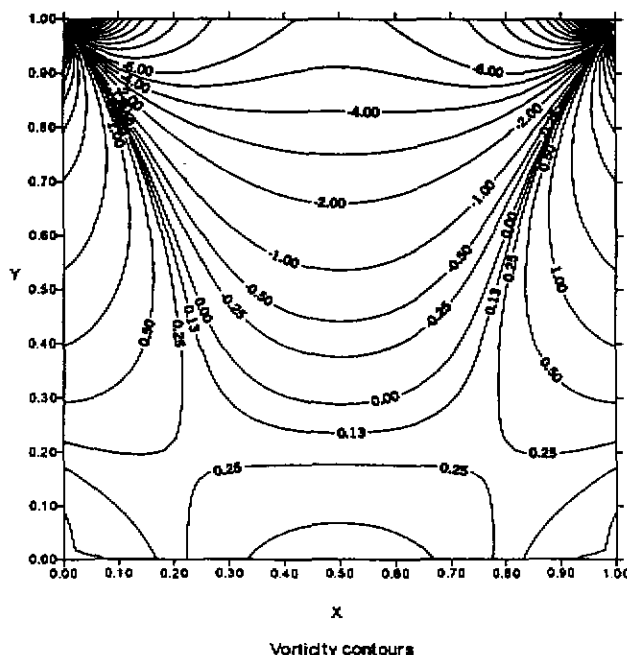


Fig. 6 Vorticity contours for Stokes flow

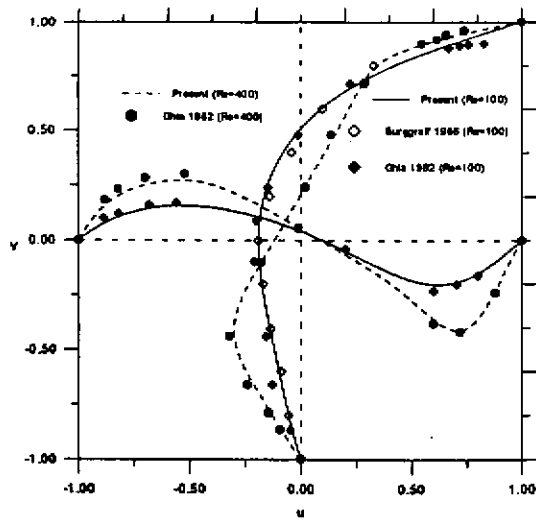


Fig. 7 Velocity profiles for $Re = 100$ and $Re = 400$ on vertical and horizontal centerlines

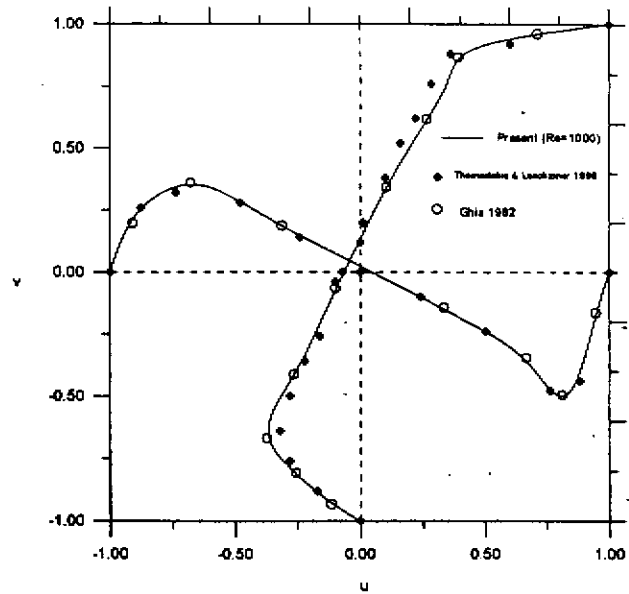


Fig. 10 Velocity profiles for $Re = 1000$ on vertical and horizontal centerlines

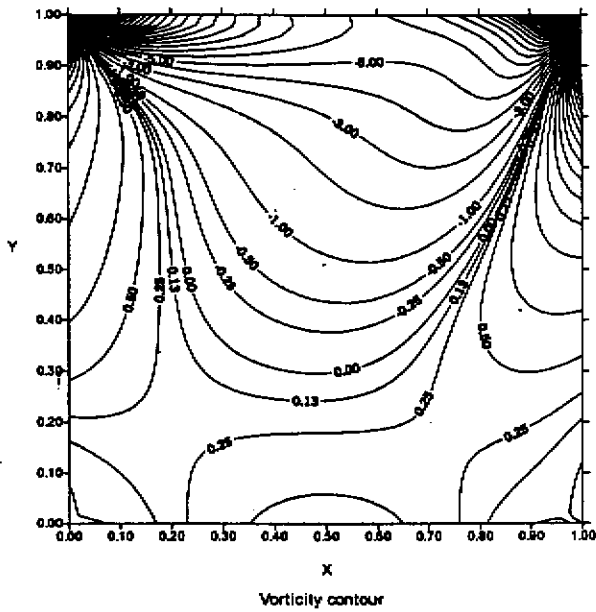


Fig. 8 Vorticity contours at $Re = 100$

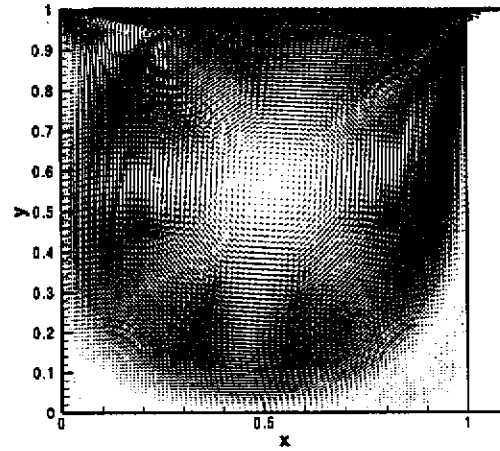


Fig. 11 Velocity distribution at $Re = 1000$

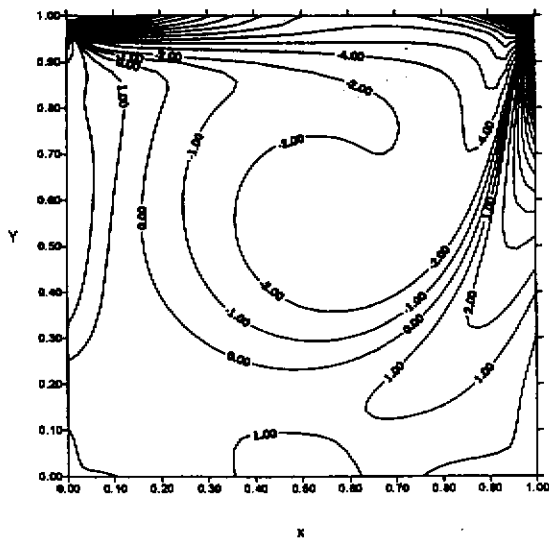


Fig. 9 Vorticity contours at $Re = 400$

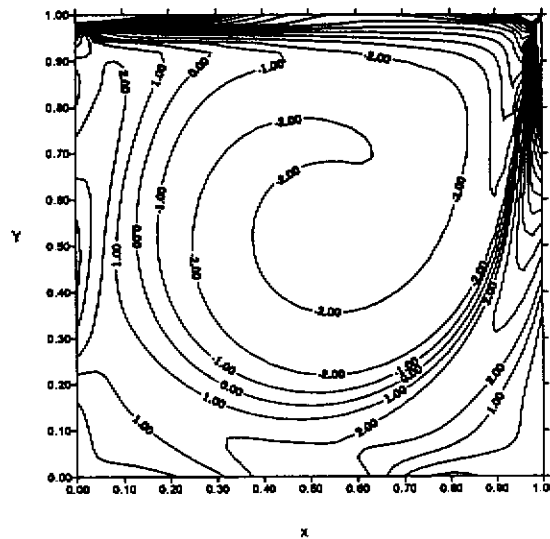


Fig. 12 Vorticity contours at $Re = 1000$

increases to 1000, the above-mentioned physical characteristics become more conspicuous. In particular, the vortex center first moves downstream, and finally moves back to the geometric center of the cavity. This illustrates the fact that viscous forces is confined only to the boundary layer, and most of the region away from the boundaries behaves like the core of a forced vortex, as mentioned by Burggraf (1966) [1].

The formation of corner eddies, as pointed out by Moffatt (1964) [11] is another very strange phenomenon in the square cavity simulation. It is seen that the nonlinearity (high Re) and corner separation are two major mechanisms to form the secondary currents. There appear a big lower right-hand secondary eddy and a small lower left-hand secondary eddy.

As Re increases further, the number of secondary eddies will increase. It is observed that as many as five secondary eddies will be formed in the upper left, lower right, and lower left corners when Re approaches 5000. This also indicates that the inertia force is another trigger factor in the formation of secondary

eddies. Figure 13 illustrates the transformation of vorticity in the cavity flow. Figures 14 and 15 show the distribution of streamlines and velocity of a recirculating flow at $Re = 5000$.

It is obvious that the influence of boundary layer for driven cavity is very significant when Re is increased to 20000. As a compromise between computing resource and accuracy, the 101×101 non-uniform mesh is used in this high Reynolds number. The Fig. 16 indicates that there are additional vortices in the lower right, lower left and upper left corners, although because of the contour intervals they do not show up clearly in the figure. The time evolution of vorticity at $Re = 20000$ will be shown in Figs. 17 and 18 at two fixed point $(x, y) = (0.93, 0.5)$ and $(x, y) = (0.065, 0.5)$ of the cavity. It should be noted that we would not get a steady solution for the driven cavity flow at higher Reynolds numbers, since at such a high Reynolds number, the flow may become transitional states, and chaotic or turbulent flows are the typical flow regimes at such a high Reynolds number.

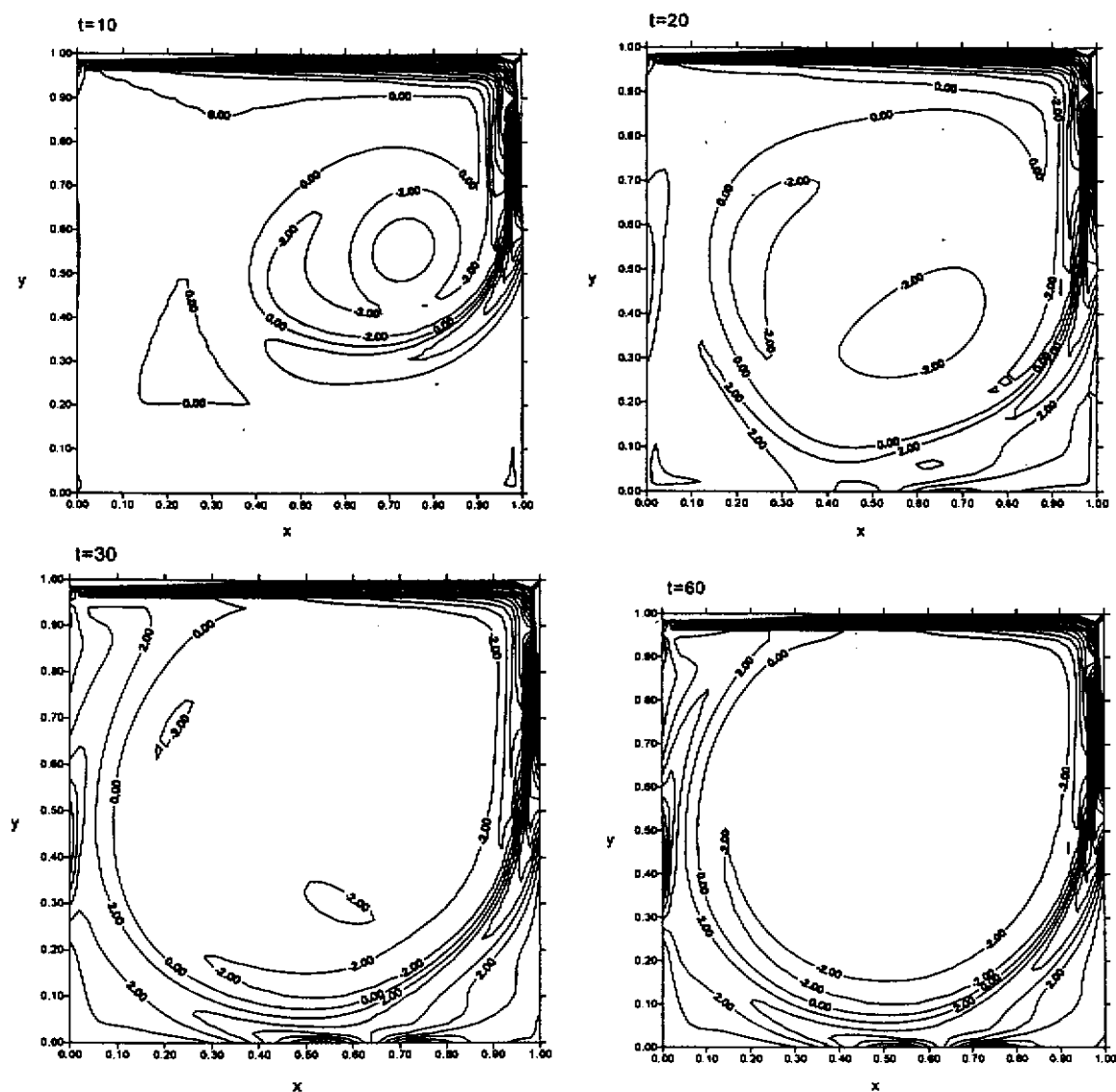


Fig. 13 Vorticity contours at $Re = 5000$

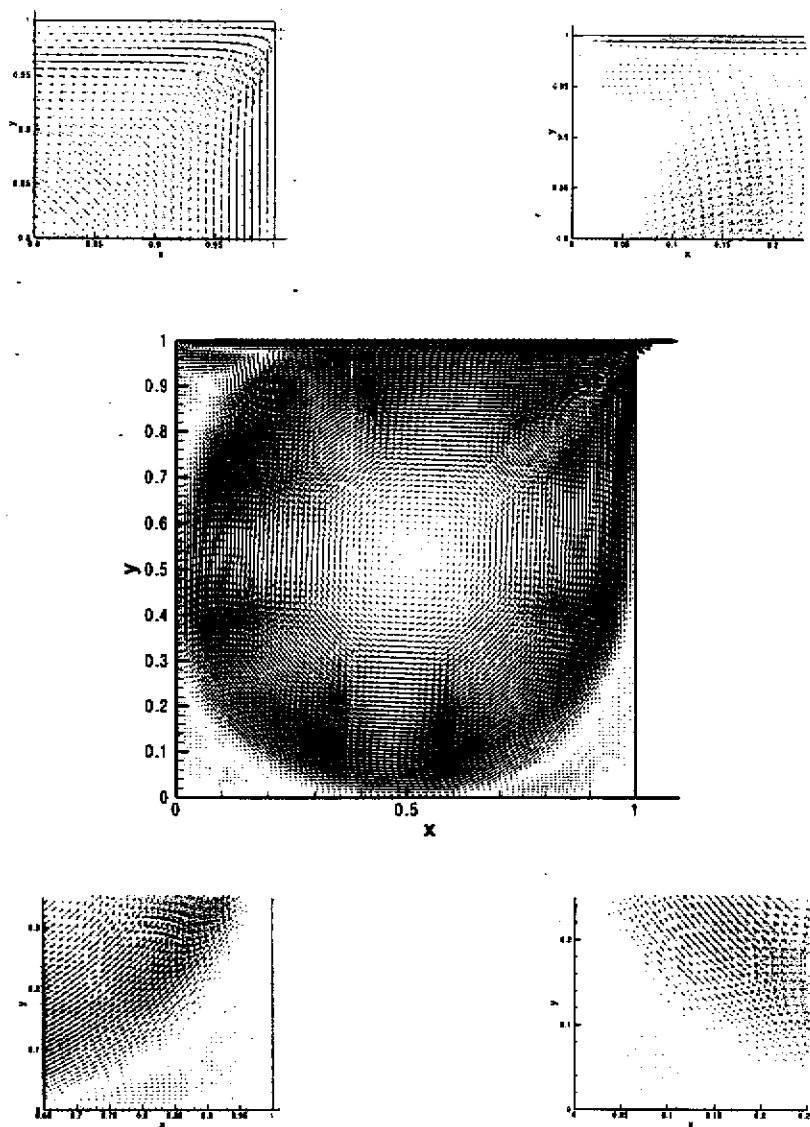


Fig. 14 Velocity distribution at $Re = 5000$

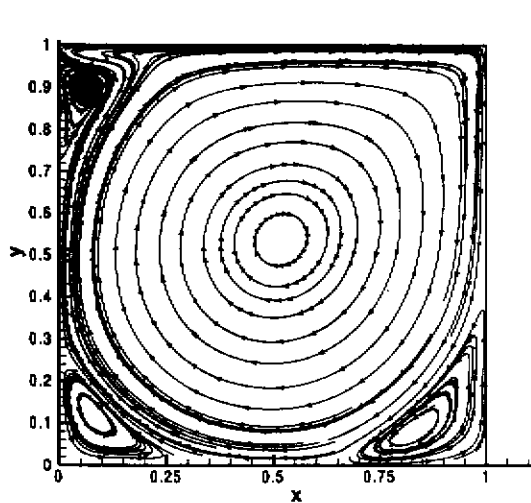


Fig. 15 Streamlines at $Re = 5000$

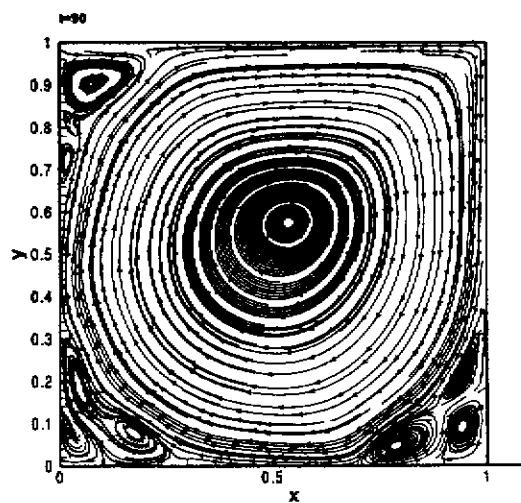


Fig. 16 Streamlines at $Re = 20000$

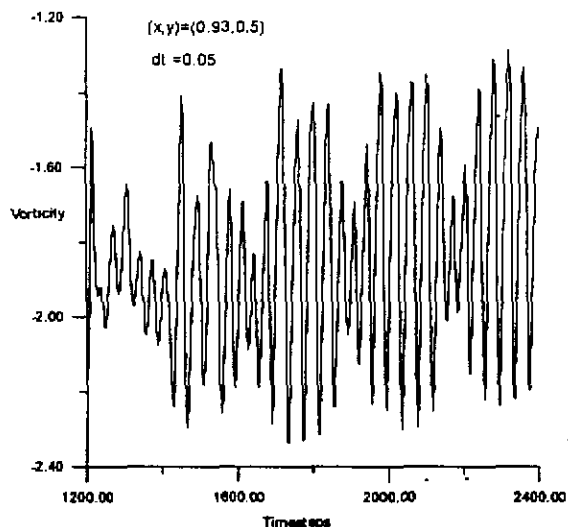


Fig. 17 The history of vorticity at $Re = 20000$

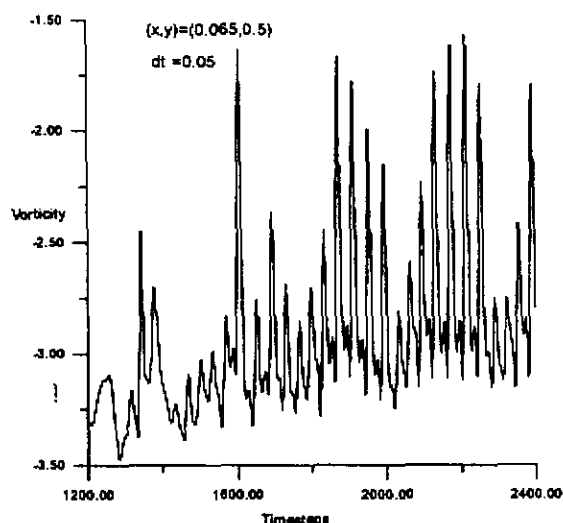


Fig. 18 The history of vorticity at $Re = 20000$

6. CONCLUDING REMARK

Finite element model has been developed for solving the velocity-vorticity Navier-Stokes equations in two-dimensions. Here the results of low Reynolds number to high Reynolds number problems, in a typical cavity flow are presented and compared with other numerical models. Computational results show that the Velocity-Vorticity formulation and FEM presented here provide an efficient method for numerical investigation of two-dimensional incompressible viscous fluid in motion.

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速度—渦度法應用於 自由液面流場之數值模擬

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速度-渦度法應用於 自由液面流場之數值模擬

羅德章* 楊德良**

摘 要

本文利用速度、渦度和自由液面的位置為主要的變數，對於具移動性邊界而控制方程式為 Navier-Stokes 方程式的流場，發展出一套垂直面二維的數值分析方法。在數值方法方面，本文採用有限元素法求解內部流場及配合穩定的有限差分法處理邊界條件，並將模式應用於孤立波過直立壁的最大溯升高度，水庫之壩樣現象。由這些結果顯示，有限元素法與有限差分法對於計算流體力學有著很好的解析。

一、前 言

在分析含自由液面而控制方程式為 Navier-Stokes 方程式之流場的數值模式，早期有 Halow 和 Welch(1965)⁽¹⁾以有限差分法所發展成功的 MAC (Marker and Cell)法，在這之後有 Vieceili(1969)⁽²⁾等學者研究 MAC 法。Chan and Street(1970)⁽³⁾修正了 MAC 方法並應用到研究孤立波在直立壁上溯升 (run up) 的情形，因此修正過的 MAC 方法稱之為 SUMMAC (Stanford University Modified MAC)。SUMMAC 與 MAC 的主要差別在於前者更準確地估算含有自由液面網格上的速度分量與自由液面上的壓力，從事這方面的研究學者如黃清哲等人^(4,5,6)。其次，有一些學者則採用 Lagrangian 的方法追蹤自由液面流體的質點，如 Bellet and Chenot(1993)等人⁽⁷⁾，採用 Lagrangian 觀點時，則格網隨其終點 (node) 上之流體速度移動，雖格網可隨著流場區域變動而移動，但不易控制而可能扭曲變形而造成數值發散。

此外，於 1960 年代中期起，有些學者則逐漸發展 ALE 法，以計算格網移動而處理各種計算區域不固定的問題。ALE 法首先於 1964 年由 Noh⁽⁸⁾所提出，其數值工具為有

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限差分，於有限元素法中首先應用 ALE 法者為 Donea(1977)⁽⁹⁾建立流體與結構物互制作用之模式。而 ALE 法在分析具自由液面而控制方程式為 Navier-Stokes 方程式的流場，則發端於 Hirt 等人(1974)⁽¹⁰⁾以有限差分法所發展的模式，此後有 Chan(1975)⁽¹¹⁾及 Pracht(1975)⁽¹²⁾等亦以有限差分法建立模式，然而有限差分法較不易處理不規則計算區域，所以，一些學者就利用容易處理不規則計算區域之有限元素法建立模式者，則始於 Hughes, Liu 及 Zimmermann(1981)⁽¹³⁾，此後有 Ramaswamy 及 Kawahara(1987)⁽¹⁴⁾與 Huerta 及 Liu(1988)⁽¹⁵⁾、Choi(1996)⁽¹⁶⁾等亦以有限元素法建立模式。林寬心(1992)⁽¹⁷⁾就是以有限元素法配合 ALE 法分析具自由水面移動邊界而控制方程式為 Navier-Stokes 方程式的流場之數值模擬。對於網格移動的問題，Thompson 等人(1982)⁽¹⁸⁾所提出的貼壁座標法 (boundary fitted coordinates method)，採用含自由液面的不固定流場區域轉換成固定而規則的計算區域，以利於數值計算，也是一種很好的方法。這方面的應用，譬如廖(1990)⁽¹⁹⁾研究含自由水面之強制渦流之有限差分法模式和 Young 及 Liu(1990)⁽²⁰⁾之有限元素法模式。張志華(1997)^(21,22,23)則利用此種座標系統進行孤立波與結構物互制的數值模擬。本文所採用的格網編制，亦是使用貼壁座標來進行網格的編制。就是說格網的邊界和流體的邊界是一樣的，網格的邊界是貼著自由液面的邊界與固體邊界而移動，此外，網格是單一格網系統（非交錯網格），就是將未知的變數放在同一個網格系統上。

然而以上的數值方法，有些是利用較簡單的勢能函數法、或者是應用渦度-流函數法、以及廣為使用的原始變數法 (u, v, p)，卻無人使用過速度-渦度法。今本文就是利用速度、渦度和自由液面位置之變數，以有限元素法配合 ALE 法求解流場內的速度場及渦度場並配合適當的有限差分處理邊界條件，來求解垂直二維具移動邊界的自由液面之流場。

二、流場控制方程式

本文依據流場方程式〔速度波松 (Poisson) 方程式、渦度傳輸方程式〕，利用速度-渦度函數建立一般化的流場方程式，並配合尤拉-拉格朗吉法 (Arbitrary Lagrangian Eulerian Method) 和適當的固定及自由液面邊界條件（運動邊界條件、動力邊界條件、連續方程式、渦度的邊界條件），求解完全非線性自由液面之流場。

1. 控制方程式於 ALE 法之座標系統

ALE 法的座標系統通稱為 Referential 座標系，有關 ALE 法的基本理論系統及其 Referential 座標系與傳統之 Eulerian、Lagrangian 座標系間的相互轉換關係式，可參考 Hughes

等 (1981) 或林 (1992) 之著作。

經由座標系統間之相互轉換關係式，通常表示於傳統 Eulerian 或 Lagrangian 座標系統下之渦度傳輸方程式與速度的波松方程式，可轉換於 Referential 座標系統下，其於垂直面二維時可寫成

$$\frac{\partial \omega}{\partial t} + (u - \hat{u}) \frac{\partial \omega}{\partial x} + (v - \hat{v}) \frac{\partial \omega}{\partial y} = \frac{1}{R_e} \nabla^2 \omega \quad (1)$$

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (2)$$

$$\nabla^2 v = \frac{\partial \omega}{\partial x} \quad (3)$$

其中 ω 、 u 、 v 分別為流體之渦度、水平速度及垂直速度。

$R_e = \frac{h\sqrt{gh}}{\nu}$ 表示流場的雷諾茲數 (h 為擾動前的水深， g 為重力加速度， ν 為流體的運動黏滯係數)

$\hat{u}$ 和 $\hat{v}$ 分別為水平與垂直格網速度而依定義為：

$$\hat{u} = \frac{\partial x}{\partial t} \quad (4)$$

$$\hat{v} = \frac{\partial y}{\partial t} \quad (5)$$

由於 Referential 座標系統本質上為一般化座標系統，而可相當於 Eulerian 或 Lagrangian 座標系統，此取決於格網速度：(1) 若格網速度為零，即格網固定，則相當於 Eulerian 座標系。(2) 若格網速度等於流速，及格網隨著結點上的流速移動，則相當於 Lagrangian 座標系。然而，為了避免傳統 Lagrangian 及 Eulerian 座標系之缺點，可依邊界移動而流場區域變動之情形而適當地計算及控制格網速度，以便能處理移動邊界又可避免格網扭曲而造成數值發散。

2. 初始條件 ($t=0$)

(1) 若給定初始孤立波流場

為了說明方便，今以一理論孤立波為入射條件，此孤立波之波高 (A_0)，波形 (ζ_f) 傳遞波速 (C)，由 Grimshaw(1971)⁽²⁴⁾ 勢能理論解 (Potential Flow)：

$$C = 1 + \frac{1}{2}A_0 - \frac{3}{20}A_0^2 + \frac{3}{56}A_0^3 \quad (6)$$

$$\zeta_f = A_0 \cdot \sec h^2 k \left[1 - \frac{3}{4}A_0 \cdot \tanh^2 k + A_0^2 \left(\frac{5}{8} \tanh^2 k - \frac{101}{80} \sec h^2 k \cdot \tanh^4 k \right) \right] \quad (7)$$

其中

$$k = \frac{\sqrt{3A_0}}{2} \left(1 - \frac{5}{8}A_0 + \frac{71}{128}A_0^2 \right) (x - x_0) \quad (8)$$

式中 x_0 為波峰的初始位置，選取位置以求解初始條件時，不受結構物或計算側邊界干擾為原則。

若觀察者以波速 C 跟著孤立波移動（移動座標系統），則自由液面為一流線，將波速乘上波形，即可得到自由液面的流函數：

$$\psi_f = C \cdot \zeta_f \quad (9)$$

上式配合底床與側向邊界條件，再去求解流函數方程式 ($\nabla^2 \psi = 0$)，就可得到流場的初始流函數值 (ψ)。配合流函數和速度的定義式，如下所示，即可求得流場得初始速度場：

$$u = \frac{\partial \psi}{\partial y} \quad (10)$$

$$v = -\frac{\partial \psi}{\partial x} \quad (11)$$

(2) 水庫之蕩漾情況說明

以長方形水庫之蕩漾為例，只給定初始水位函數值，其餘流場之速度場及渦度場皆為零。

3. 自由液面邊界條件

(1) 自由液面運動邊界條件(KFSBC)

自由液面流體粒子的法向速度與液面形狀變動的法向速度相等，亦即在表面上流體無法跳脫自由液面的行為，使自由液面之流體粒子永遠保持在此自由液面上滑動。自由液面高度 ζ 為含時間及空間的函數 $\zeta = \zeta(x, t)$ ，而其在 (x, y) 平面之函數關係可表示為 $y = \zeta(x, t)$ 以隱函數 $F = y - \zeta(x, t) = 0$ 表示，此邊界方程式可寫成 ALE 形式，即：

$$\frac{\partial \zeta}{\partial t} = v - (u - \hat{u}) \frac{\partial \zeta}{\partial x} \quad (12)$$

(2) 動力邊界條件 (DFSBC)

根據自由液面的動力關係式必須保持正向應力與表面張力平衡;而切線應力總和為零 (Wehausen and Laitone, 1960) ⁽²⁵⁾, 定義自由液面曲線座標系統由切線方向 (ξ) 與法線方向 (η) 所組成, 則沿著自由表面曲線座標的切向壓力變化關係為 (物理域與計算域之座標轉換之示意圖如圖 1 所示)

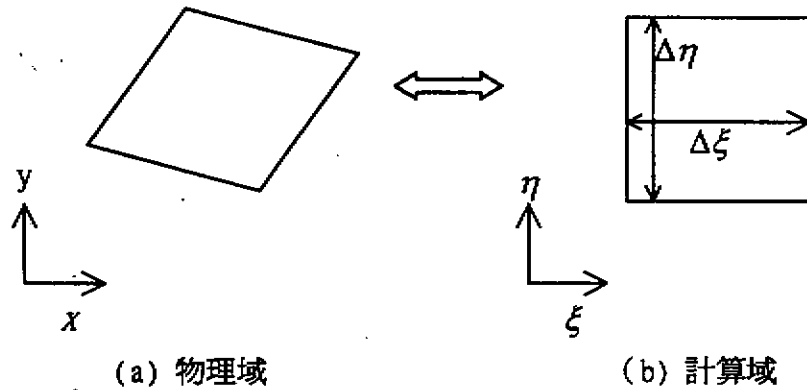


圖 1 物理域與計算域之座標轉換之示意圖

$$\begin{aligned} \frac{dP_w}{d\xi} &= \frac{\partial P_w}{\partial x} \cdot \frac{\partial x}{\partial \xi} + \frac{\partial P_w}{\partial y} \cdot \frac{\partial y}{\partial \xi} \\ &= \frac{dP_a}{d\xi} - \frac{1}{W_e} \left(\frac{dk}{d\xi} \right) \end{aligned} \quad (13)$$

其中 P_w 表示水粒子在自由表面之壓力; 接觸表面空氣壓力為 P_a ;

$W_e = Pgh^2/T$ 表示韋伯數, T = 表面張力係數; $k = \frac{\zeta_{xx}}{(1+\zeta_x^2)^{3/2}}$ 為表面曲率。

將 Navier-Stoke equations 無因次化, 並基於特性速度 $U = \sqrt{gh}$ (h 為擾動前的水深) 情況下可推導出:

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= -\frac{\partial P_w}{\partial x} + \frac{1}{R_e} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= -\frac{\partial P_w}{\partial y} - 1 + \frac{1}{R_e} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \end{aligned} \quad (14)$$

將 Navier-Stokes equations 代入(13)可得：

$$\begin{aligned} & \left[u_t + uu_x + vv_y - \frac{l}{R_e}(u_{xx} + v_{yy}) \right] \cdot x_\xi \\ & + \left[v_t + uv_x + vv_y + l - \frac{l}{R_e}(v_{xx} + v_{yy}) \right] \cdot y_\xi = -(P_a)_\xi + \frac{k_\xi}{W_e} \end{aligned} \quad (15)$$

因此，完整之自由液面正向動力邊界條件的曲線座標為，非穩態項、傳遞項、重力項、黏滯項、外力源項、及表面張力項之合併式，今將(15)式用 ALE 的座標系統來表示。

$$\begin{aligned} & u_t x_\xi + v_t y_\xi + [(u - \hat{u})u_\xi + (v - \hat{v})v_\xi] + \omega[(u - \hat{u})y_\xi - (v - \hat{v})x_\xi] + y_\xi \\ & + \frac{l}{R_e} \left[\left(\frac{x_\xi^2 + y_\xi^2}{J} \right) \omega_\eta - \left(\frac{x_\xi x_\eta + y_\xi y_\eta}{J} \right) \omega_\xi \right] = -(P_a)_\xi + \frac{k_\xi}{W_e} \end{aligned} \quad (16)$$

其中

$J = (x_\xi y_\eta - y_\xi x_\eta)$ = Jacobian，為 $x - y$ 座標系統與 $\xi - \eta$ 座標系統之轉化關係式。

上式的渦度 (ω) 若假設為已知，而方程式有速度 (u, v) 兩變數，所以必須使用連續方程式加以迭代，使速度 (u, v) 同時收斂後，才可進行下一步驟的計算。可將連續方程表示為：

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad \text{或} \quad \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 v}{\partial y^2} = 0 \quad (17)$$

若改寫成曲線座標形式可表示為：

$$(y_\eta u_\xi - y_\xi u_\eta) + (v_\eta x_\xi - v_\xi x_\eta) = 0 \quad (18)$$

4. 渦度傳輸方程式的渦度邊界條件

本文計算的格網系統為非交錯網格系統，亦即是單一格網系統。 u, v, ω 的變數皆在同一格網上。依據渦度及速度的關係式，邊界的渦度值給定由下式可得 (示意圖如圖 2)：

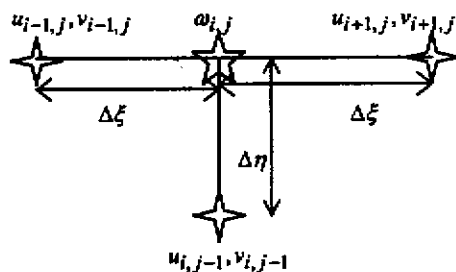


圖 2 渦度邊界條件差分示意圖

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \frac{[(y_{\eta} v_{\xi} - y_{\xi} v_{\eta}) - (u_{\eta} x_{\xi} - u_{\xi} x_{\eta})]}{J} \quad (19)$$

為了方便計算，可令 $\Delta\xi = \Delta\eta = 1$ 。

5. 固體邊界

在底床及固定邊界上，若有考慮流體黏滯性對流況的影響時必須設定為不可滑動條件 (non-slip condition)，若流體黏滯性可忽略時則可設定為滑動條件 (slip condition)。而不可滑動與可滑動邊界條件在底床與固體邊界皆須滿足無貫穿條件 (non-penetration)。

三、數值方法

本節將建立以有限元素法求解控制方程，亦即渦度傳輸方程式和波松方程式求解流場的渦度和速度的值。而對於渦度傳輸方程式並配合使用 ALE 格網移動的方法，必須計算格網移動的速度，這也是具移動邊界的流體動力學與固定邊界所不同的地方。本模式在求解渦度的邊界條件與自由液面位置和速度是使用有限差分來離散，差分離散式子的程式編寫較有限元素法簡單，但有一點須加以注意，由於計算的格網隨時間而變形，所以並非正交網格，故在計算時須經過座標轉換，轉換後的離散式子才可進行計算，而在處理動力邊界條件時須加入連續方程式加以迭代直到自由液面上的節點速度都收斂為止。

1. 有限元素法離散渦度傳輸方程式

本數值模式在求解渦度傳輸方程式是以有限元素法離散，所使用的格網元素是線性三角元素。

由權重殘值法 (Method of Weighted Residuals) 中的葛樂金準則 (Galerkin Criterion)，可將 (1) 式變為

$$0 = \iint N_i \left[\left(\frac{\partial \omega}{\partial t} + (u - \hat{u}) \frac{\partial \omega}{\partial x} + (v - \hat{v}) \frac{\partial \omega}{\partial y} \right) - \frac{1}{R_e} \left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) \right] d\Omega \quad (20)$$

令 $\omega = \omega(x, y, t) = \sum N_j \omega_j$, $u = \sum N_k u_k$, $v = \sum N_k v_k$ ，則 (20) 式可變為：

$$\begin{aligned}
0 = & \sum \iint N_i N_j \frac{\partial \omega_j}{\partial t} d\Omega + \sum \iint \left(N_k (u_k - \hat{u}_k) N_i \frac{\partial N_j}{\partial x} + N_k (v_k - \hat{v}_k) N_i \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \\
& - \sum_{i \in \Gamma} \int \frac{\partial \omega}{\partial n} N_i d\Gamma + \frac{1}{R_e} \sum \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega
\end{aligned} \tag{21}$$

將 (21) 式寫成矩陣方程式

$$\sum [M^{(e)}] \left\{ \frac{\partial \omega}{\partial t} \right\} + \sum [L^{(e)}] \{\omega\} + \frac{1}{R_e} \sum [K^{(e)}] \{\omega\} = 0 \tag{22}$$

其中

$$M_{ij}^{(e)} = \iint N_i N_j d\Omega \tag{23}$$

$$L_{ij}^{(e)} = \iint \left(N_k (u_k - \hat{u}_k) N_i \frac{\partial N_j}{\partial x} + N_k (v_k - \hat{v}_k) N_i \frac{\partial N_j}{\partial y} \right) d\Omega \tag{24}$$

$$K_{ij}^{(e)} = \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega \tag{25}$$

$$\frac{\partial \omega}{\partial t} = \frac{\omega^{n+1} - \omega^n}{\Delta t} \tag{26}$$

其中

ω^n 為 ω 在時間 $t = n$ 之節點值；

ω^{n+1} 為 ω 在時間 $t = n+1$ 之節點值；

Δt 為在時間 $t = n$ 至 $t = n+1$ 之時間差。

所以 (22) 式可變為：

$$\begin{aligned}
& \left\{ \frac{1}{\Delta t} [M_{ij}^{(e)}] + \theta \left[L_{ij}^{(e)} + \frac{1}{R_e} K_{ij}^{(e)} \right] \right\} \{\omega_j\}^{n+1} \\
& = \left\{ \frac{1}{\Delta t} [M_{ij}^{(e)}] - (1-\theta) \left[L_{ij}^{(e)} + \frac{1}{R_e} K_{ij}^{(e)} \right] \right\} \{\omega_j\}^n
\end{aligned} \tag{27}$$

θ 表示為隱示因子 (implicit factor)；

$\theta = 0$ 表示為顯示法 (explicit method)；

$\theta = 1$ 表示為完全隱示法 (fully-implicit method)。

顯示法在數值計算時較快速，但其系統常發生不穩定的現象。而隱示法卻有數值穩定的優

點，所以本模式在計算(27)式時皆採用隱示法($\theta = \frac{2}{3}$)。

2. 有限元素法離散速度的波松方程式

由權重殘值法 (Method of Weighted Residuals) 中的葛樂金準則 (Galerkin Criterion) 可將 (2), (3) 式變為：

$$0 = \iint N_i \left(\nabla^2 u + \frac{\partial \omega}{\partial y} \right) d\Omega = \iint N_i \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial \omega}{\partial y} \right) d\Omega \quad (28)$$

$$0 = \iint N_i \left(\nabla^2 v - \frac{\partial \omega}{\partial x} \right) d\Omega = \iint N_i \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} - \frac{\partial \omega}{\partial x} \right) d\Omega \quad (29)$$

其中

$N_i = N_i(x, y)$ 為形狀函數；

Ω 為離散化後各小元素的區域。

令各元素中 $u = \sum N_j u_j$ ， u_j 為元素上節點的速度(u)值，將(28)式做分部積分，則可得(30)式：

$$\sum \left[\iint \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} d\Omega \right] \cdot u_j = \sum \left[\iint N_i \frac{\partial N_j}{\partial y} d\Omega \right] \cdot \omega_j \quad (30)$$

寫成矩陣方程式可得(31)式：

$$\sum [K_{ij}] \{u_j\} = \sum [f_j] \quad (31)$$

其中

$$K_{ij} = \iint \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} d\Omega \quad (32)$$

$$f_j = \left[\iint N_i \frac{\partial N_j}{\partial y} d\Omega \right] \cdot \omega_j \quad (33)$$

同理，可將(29)式依上述方法離散。

3. 自由液面邊界條件之有限差分離散方程式

(1) 自由液面動力邊界條件(DFSBC) 之有限差分之離散

本文處理自由液面動力邊界條件之方式採用二階段求解，由非穩態項、傳遞項、重力項、

黏滯項所組合之自由液面動力邊界條件 (DFSBC) 並忽略大氣壓力及表面張力之影響為：

$$u_i x_\xi + v_i y_\xi + [(u - \hat{u})u_\xi + (v - \hat{v})v_\xi] + \omega[(u - \hat{u})y_\xi - (v - \hat{v})x_\xi] + y_\xi + \frac{1}{R_e} \left[\left(\frac{x_\xi^2 + y_\xi^2}{J} \right) \omega_\eta - \left(\frac{x_\xi x_\eta + y_\xi y_\eta}{J} \right) \omega_\xi \right] = 0 \quad (34)$$

在經過數值上的測試，對 ξ 方向採用二階差分（中央差分）， t 與 η 採用一階差分（後項差分）結果最好。如下說明：

$$\frac{\partial f^n}{\partial \xi} = \frac{[f_{i+1,j} - f_{i-1,j}]}{2\Delta\xi}, \quad \frac{\partial f^n}{\partial \eta} = \frac{[f_{i,j} - f_{i,j-1}]}{\Delta\eta}, \quad \frac{\partial f}{\partial t} = \frac{f_{i,j}^{n+1} - f_{i,j}^n}{\Delta t} \quad (35)$$

為了方便計算，可令 $\Delta\xi = \Delta\eta = 1$ ， Δt 表示時間的前後時距。

上式在解得水平速度(u)後再利用連續方程式(18)式可解得垂直速度(v)，將所求得的垂直速度值代入(34)式進行迭代直到兩者都收斂。

(2) 自由液面運動邊界條件(KFSBC) 之有限差分之離散

自由液面的運動邊界條件可寫成：

$$\zeta_i^{n+1} = \Delta t \cdot \left[v_i - (u_i - \hat{u}_i) \left(\frac{\zeta_{i+1} - \zeta_{i-1}}{2\Delta x} \right) \right]^n + \zeta_i^n \quad (36)$$

4. 格網速度

由 (4) 和 (5) 式可知水平與垂直格網速度：

$$\hat{u} = \frac{\partial x}{\partial t} = \frac{x^{n+1} - x^n}{\Delta t} \quad (37)$$

計算水平格網速度時，可經由第 $n+1$ 時段的水體在 X 軸方向的位置減去第 n 時段的水體在 X 軸方向的位置，然後在除以前後時刻差，此為水平的格網速度。若所求解的流場其左右邊界皆無改變，則此時流場的水平格網速度為零。

$$\hat{v} = \frac{\partial y}{\partial t} = \frac{y^{n+1} - y^n}{\Delta t} \quad (38)$$

計算垂直格網速度時，由自由液面的運動邊界條件可求出自由液面的位置，然後再分配流場內部結點的位置變化，而第 $n+1$ 時刻和第 n 時刻垂直位置的差值除以前後時刻的時間差，亦即垂直格網的移動速度。

四、結果與討論

1. 孤立波碰撞垂直壁之反射-黏性與無黏性之比較

今討論一孤立波碰撞垂直壁之反射現象，並分別用加入黏性效應與不加入黏性效應之比較，藉以說明流體黏滯性在流場往往是不容忽略的(流場的初始條件示意圖如圖 3 所示)。首先的數值模擬條件如下，渠道長 20，右邊設一直立反射牆，起始流體深 1，波高 0.2，流場計算的網格數目為 100×20 ，每個時刻流場水平與垂直速度、渦度及自由流液面的位置皆須滿足 $|u_{k+1}^n - u_k^n| \leq 10^{-5}$, $|v_{k+1}^n - v_k^n| \leq 10^{-5}$, $|\omega_{k+1}^n - \omega_k^n| \leq 10^{-5}$, $|\zeta_{k+1}^n - \zeta_k^n| \leq 10^{-5}$ ，才可進行下一

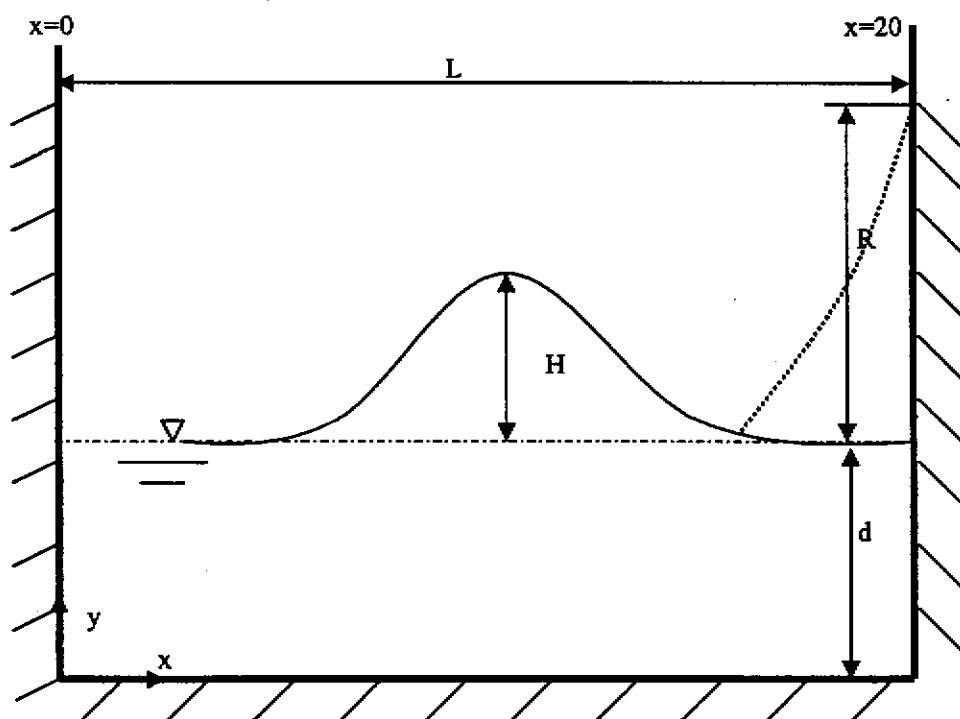


圖 3 孤立波遇直立牆的流場各參數說明圖

時刻的計算。考慮黏滯性的雷諾茲數為 1,000 與 50,000，另一為不考慮黏滯性的勢能流場，數值模擬時間為 25。考慮黏滯性的邊界條件流體必須滿足無穿越左右兩端固體邊界的條件 ($u=0$)，在底床邊界條件為無滑動邊界條件 ($u=v=0$)，不考慮黏滯性的流場左右兩端邊界 ($u=0$) 及底床邊界 ($v=0$)，不管無黏性或是黏性流體必定要滿足自由液面的運動與動力邊界條件。

勢能流場由於無摩擦損失，所以其波形皆保持原波形及波高向前傳遞。當 $t=10$ 時，流場的動能此時大都轉化成重力位能，所以此時的溯升較高，大約為 2 倍的入射波高，而其速度場幾乎皆為零。在與 Byatt and Smith(1971)⁽²⁶⁾之理論比較，發現其間的相關性很高。Byatt and Smith(1988)⁽²⁷⁾所推導一入射孤立波遇直立壁最大溯升高度的三階解為：

$$\frac{R_{\max}}{d} = 2\frac{H}{d} + \frac{1}{2}\left(\frac{H}{d}\right)^2 + o\left(\frac{H}{d}\right)^3 \quad (39)$$

其中 $R_{\max}$ 為最大溯升高度；

d 為靜止水深；

H 為初始波高。

本節把初始波高 ($H=0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5$) 與最大溯升高度 (R) 繪於 Y 軸，如圖 4 所示，而數值模擬出的結果顯示，當 R_e 為 50,000 時，此時的黏滯性類似於水（甚小），在此種型態流場黏滯效應對溯升高度影響甚小，所以不論是速度-渦度模式或者勢能函數法，其結果皆很接近。並與前人的理論近似解、實驗值(Maxworthy, 1967)⁽²⁸⁾與數值計算結果(Sung et al., 1999)⁽²⁹⁾做一比較，發現相關性很好，代表本模式無論在黏性（速度-渦度法）或者是無黏性的模式在求解自由液面流場的問題，也有很好的解析。

圖 5(a) 及 5(b) 為孤立波隨時間的波形變化，由圖形中很顯然的看出：(a) 由於勢能流況沒有受到流體黏滯性的影響，使得無黏性的流體波速傳遞得較快。(b) 雷諾茲數為 50,000 的流況，流體的黏滯效應很小且孤立波在撞到光滑直立壁時流體與固體邊界的作用時間太快，以致於波形與無黏性流場甚為接近。(c) 雷諾茲數為 1,000 的流體，其黏滯性所扮演的角色相當重要，所以當波浪在傳遞的過程時，必會受到黏滯性的牽制，使得其最大溯升小於勢能流場。考慮黏性效應的最大溯升約為 0.3。而不考慮黏性效應的最大溯升約為 0.41，約等於兩倍的入射波高。

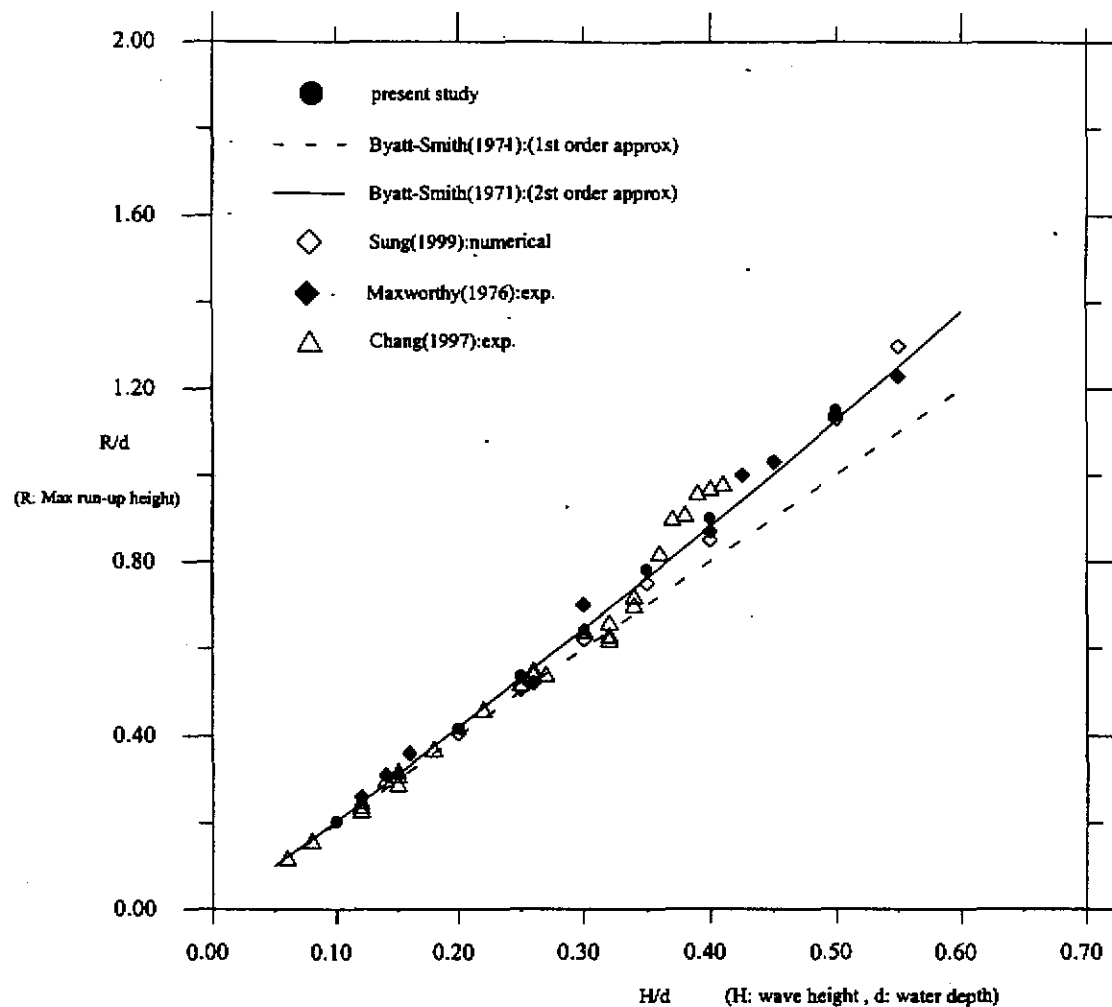


圖 4 單一孤立波碰撞直立牆之溯升最大高度

對於雷諾茲數為 1,000 的等渦度分佈圖亦是本節所要觀察的。孤立波在遇直立壁反射後，形成反向的波浪，並與壁面發生了渦流的交互作用。當時間 $t=5$ 時流場的等渦度值如圖 6 所示，渦度存在於底床和孤立波的表面，而此時的渦度場和初始的渦度場並不一樣，這是由於底床的無滑動邊界條件和流體黏滯性效應的影響，因而造成渦度的變形與擴散。 $t=10$ 時孤立波碰到直立牆而往上爬升，此時波浪並還沒有反射回來，其渦度場是延續 $t=5$ 時的渦度場型態下往前傳遞。當 $t=15$ 時，雖遇直立壁反射，由於直立壁的邊緣為黏滯無滑溜效應，亦產生微弱渦流於壁上。

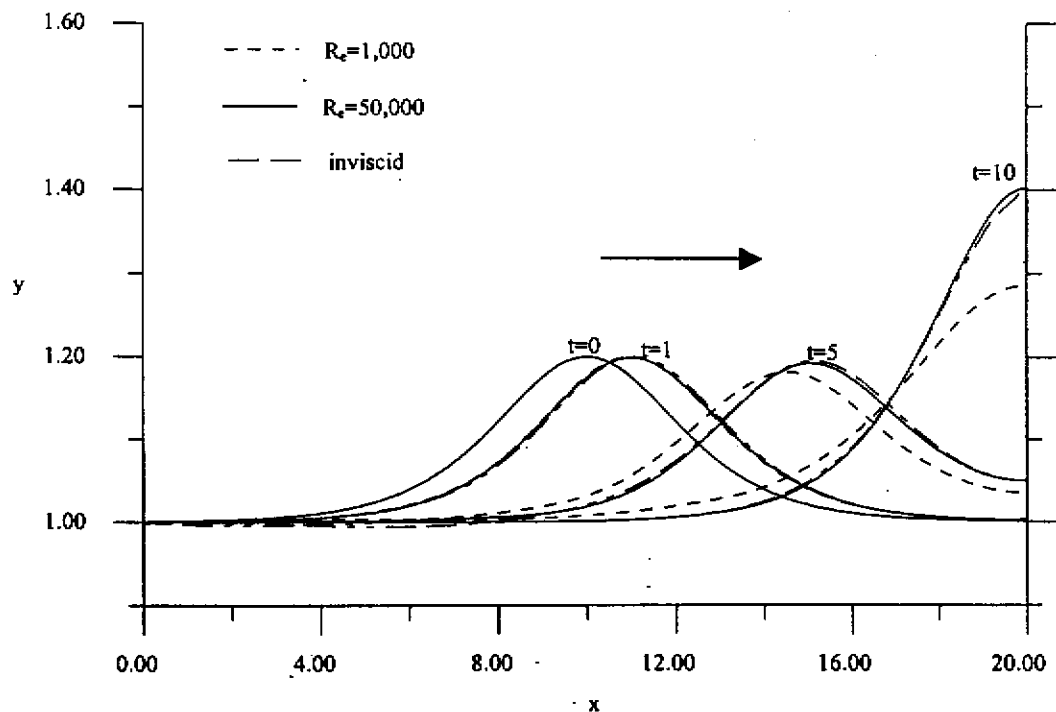


圖 5(a) 孤立波碰撞垂直壁之波高變化圖(黏性與無黏性之比較)

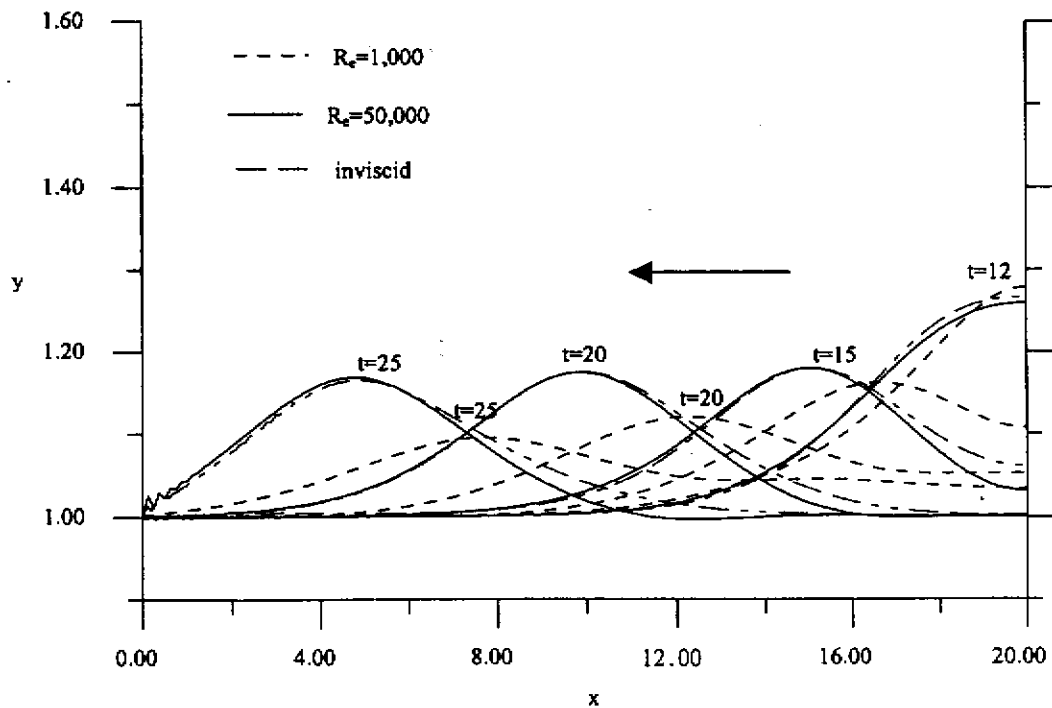


圖 5(b) 孤立波碰撞垂直壁之波高變化圖(黏性與無黏性之比較)

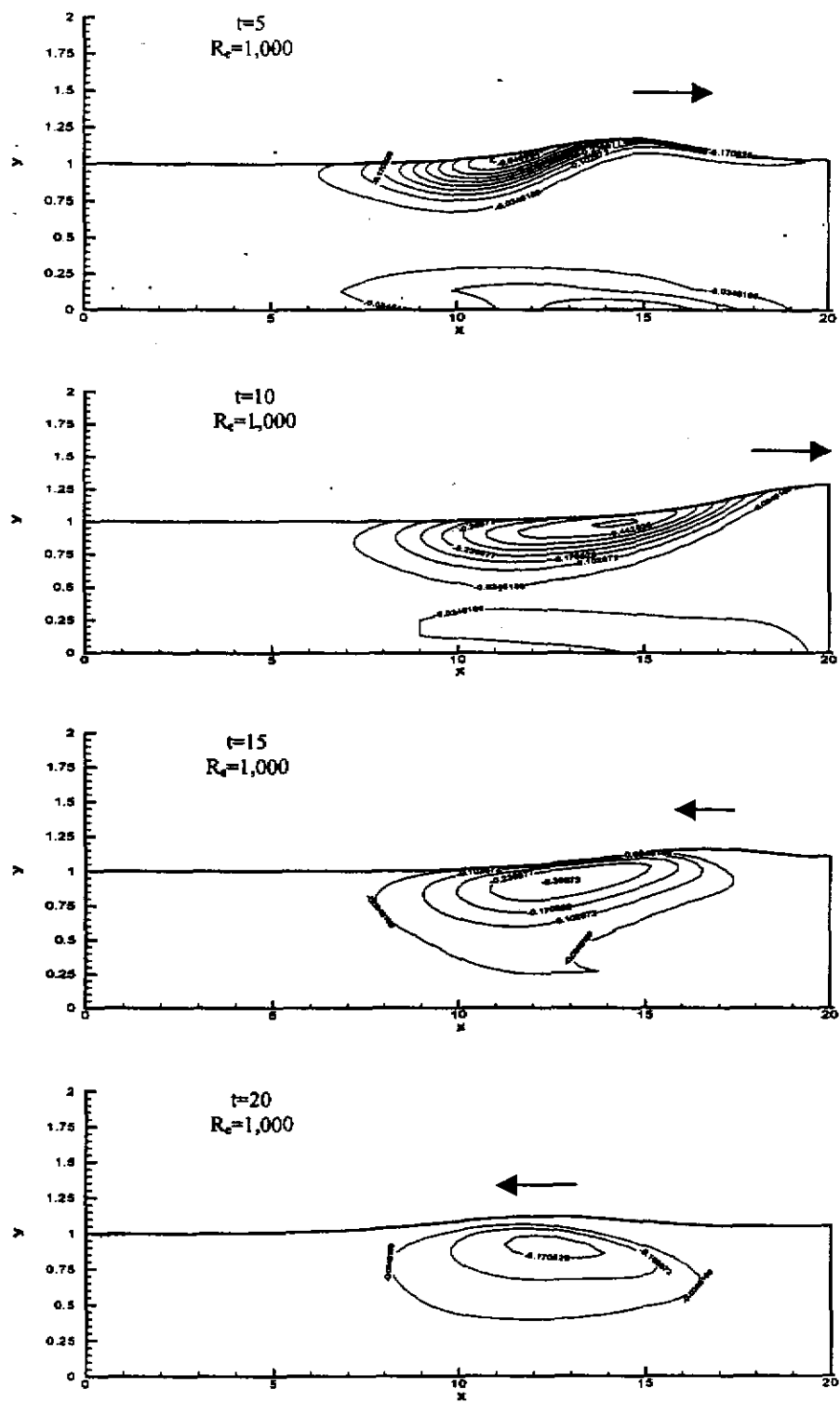


圖 6 孤立波碰撞直立壁的流場渦度變化圖($R_e=1,000$)

2. 長方形水庫之盪漾現象

盪漾 (seiche) 現象常發生在水庫、湖泊及海灣。於一長方形水庫，本文討論其發生單結駐立波 (uninode standing wave) 型態的盪漾。如圖 7 為起始的計算邊界條件，假設水庫長 $L=98\text{ m}$ ，平均水深 $d=5\text{ m}$ ，左右兩端為固定壁 (設定為光滑的直立壁)，底床為水平底面。而流場的初始條件為一振幅為 A 的餘弦函數： $y_s = A \cos(\frac{\pi x}{L}) + d$ ，速度 u 與 v 皆為零。上述之所以要用有因次的物理量是因為要和林寬心(1992)⁽¹⁷⁾的博士論文做比較，但由於本文的控制方程式為無因次的物理量，所以在利用電腦所執行的無因次模式其輸出格式要經過有因次與無因次之間的轉換，而有因次與無因次的轉換關係如下所述 (如表 1 的轉換關係之物理量)：

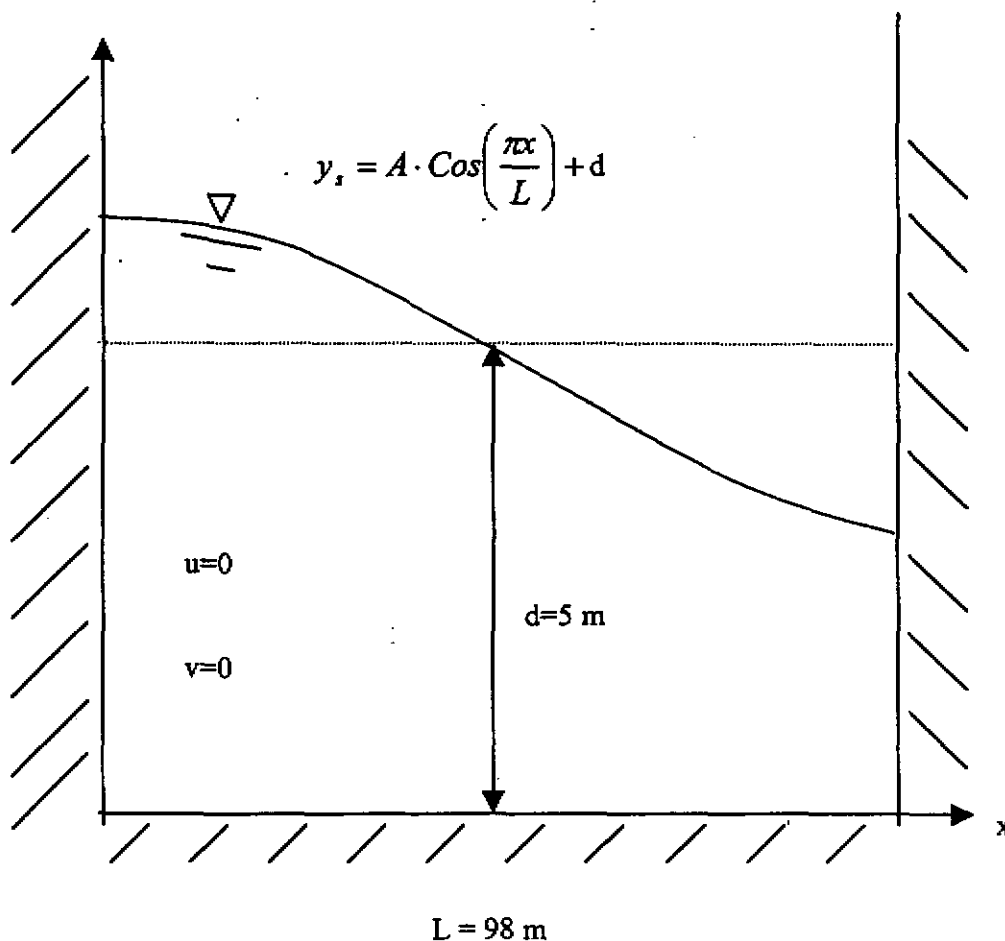


圖 7 長方形水庫盪漾現象之計算區域及初始條件

$$\text{特徵時間 } t^* = \frac{d}{\sqrt{gd}} = \frac{t'}{t} \Rightarrow t = \frac{t'}{\left(\frac{d}{\sqrt{gd}}\right)}, \text{ 若 } d=5\text{m}, g=9.8\text{m/s}^2$$

$$\Rightarrow t = \frac{t'}{\left(\frac{5}{\sqrt{9.8 \times 5}}\right)} = \frac{t'}{0.71428} = 1.4t' \quad \text{或} \quad t' = 0.71428t \quad (40)$$

$$\text{特徵長度 } H^* = \frac{d}{h} \quad (41)$$

$$\text{特徵速度 } u^* = \sqrt{gd} = \frac{u'}{u}, \quad v^* = \sqrt{gd} = \frac{v'}{v} \quad (42)$$

其中 d 為實際水深 (單位 m), h 為無因次化後的靜止水深;

t' 為實際時間 (單位 sec), t 為無因次時間;

u' 與 v' 為實際流場的水平與垂直速度 (單位 m/s);

u 與 v 為無因次化的水平與垂直速度。

表 1 無因次與有因次的轉換關係之物理量

	長度	時間	週期 (T)	速度 (u)	速度 (v)
無因次物理量	1	1	39.2	1	1
有因次物理量	5 (m)	0.71428 (sec)	28 (sec)	7 (m/sec)	7 (m/sec)

(1) 線性解析解

在進行數值分析前, 先了解水庫蕩漾的線性解析解, 以奠定以後數值結果討論的基礎。在忽略流體的黏滯性及非線性效應 (由 DFSBC 可知非線性項為:

$$(u - \hat{u})u_x + (v - \hat{v})u_y + (u - \hat{u})v_x + (v - \hat{v})v_y, \text{ KFSBC 的非線性項為: } (u - \hat{u})\frac{\partial \zeta}{\partial x},$$

可求得線性解析解為:

$$y_s = d + A \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi C_0 t}{L}\right) \quad (43)$$

$$u' = \frac{AC_0}{d} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi C_0 t}{L}\right) \quad (44)$$

$$v' = -\frac{AC_0 \pi y}{dL} \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi C_0 t}{L}\right) \quad (45)$$

此流場之重力長波波速 $C_0 = \sqrt{gd} = 7$ m/sec，其半波長即為水庫長度 L ，則流場蕩漾來回一次之週期為 $2L/C_0 = 28$ sec。若流場為無因次則水庫長為 19.6、水深為 1、波速為 1，所以一個週期的蕩漾為 39.2。如圖 8 表示左壁、中央、右壁之水面變化歷程。在左右壁處水面呈餘弦週期運動，中央處為節點故水面保持不變，這是因為忽略非線性效應使其波形不變，故蕩漾永遠保持相同的振幅及波形運動。值得注意的是線性的解僅是用在振幅很小 ($A \leq 0.1$ m) 的情況（微小振幅波），所以若流場的初始振幅較大時，線性解析解就不能描繪真實的流場，必須經過數值解加以模擬。

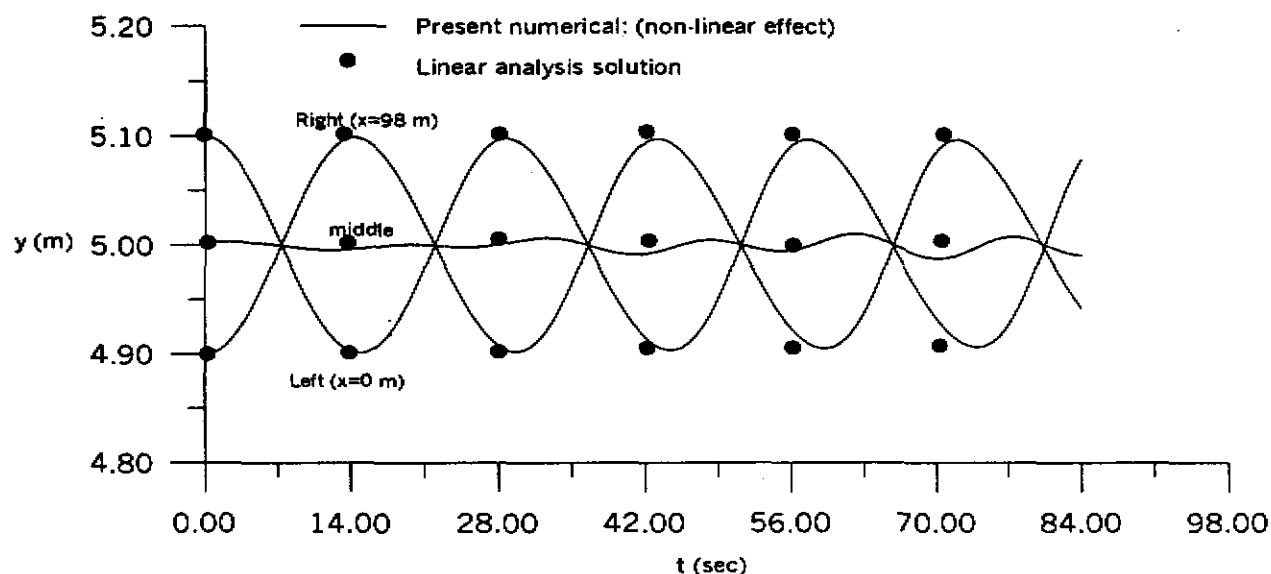


圖 8 長方形水庫蕩漾， $A=0.1$ m，非線性數值解與線性解析解之比較，水面波動歷程

(2) 非線性數值解

上述蕩漾現象之線性解析解，忽略非線性效應，並不符合實際情況（除了微小振幅波以外）。而且當流場的初始振幅愈大時，其非線性效應愈明顯（因為波狀變得十分的陡又大，不像小波小振幅之線性化）。本文的數值模式利用完整的運動、動力邊界條件，並配合格網移動，可計算波面有大振幅的流場分析。

值得一提的是，本節所模擬的流況皆採用無因次化的方程式，故需加以注意所計算出的流場速度、波高都需轉成有因次化的流況，以利觀察比較。下列分別就 a. 速度場及 b. 水面波動歷程加以討論。

a. 速度場

當振幅為 2 m 時，此時流況的非線性效應很大，速度在半週期 ($t=14$ sec) 及一週期 (28 sec) 的時候，流場的速度場並非如同線性解的速度場（速度皆為零），至一週期 28sec 時，於流場中央靠左的位置似乎形成一水面高度突升之向右運動之湧波 (surge)，如圖 9 所示，在網格移動方面，如圖 10 所示為格網移動隨時間變化的歷程。

b. 水面波動歷程

如圖 11 為振幅為 1 m 的水面波動，而圖 12 為振幅為 2 m 的水面蕩漾情況。因初始振幅較大，在經過一個週期後，其非線性效應相互牽制影響而使得水面波形改變較快且雜亂無章，水面波動在此高度非線性效應的影響下產生了不規則波了。當初始振幅為 0.5 m 的表面波動歷程圖，如圖 13 所示。本文的 $R_e=50,000$ 與無黏性比較時，其波形趨勢一致，尤其是在第一個週期前，但在隨著流場在較長時間流體黏滯性發生了作用致兩者會有較大的差別。而本文的黏性流場 ($R_e=50,000$ ，近似水波) 在與林寬心 (Lin, 1992)⁽¹⁷⁾ 比較時其趨勢相近，但和線性的解析解相比，發覺有相當的落差。

五、結論與建議

1. 結論

- (1) 由數值模擬結果顯示，收斂條件對結果影響大，基本上，收斂條件愈嚴格則結果愈接近解析解，但所需迭代的步數就愈多。格網大小對數值結果有很大的影響，基本上，格網愈細則數值結果愈精準，相對的運算時間也就較費時。所以，本文若用適當的非均勻格網切割，一來可節省相當多的時間，二來也可提高運算的精度，對於細部的流況有著更好的解析。

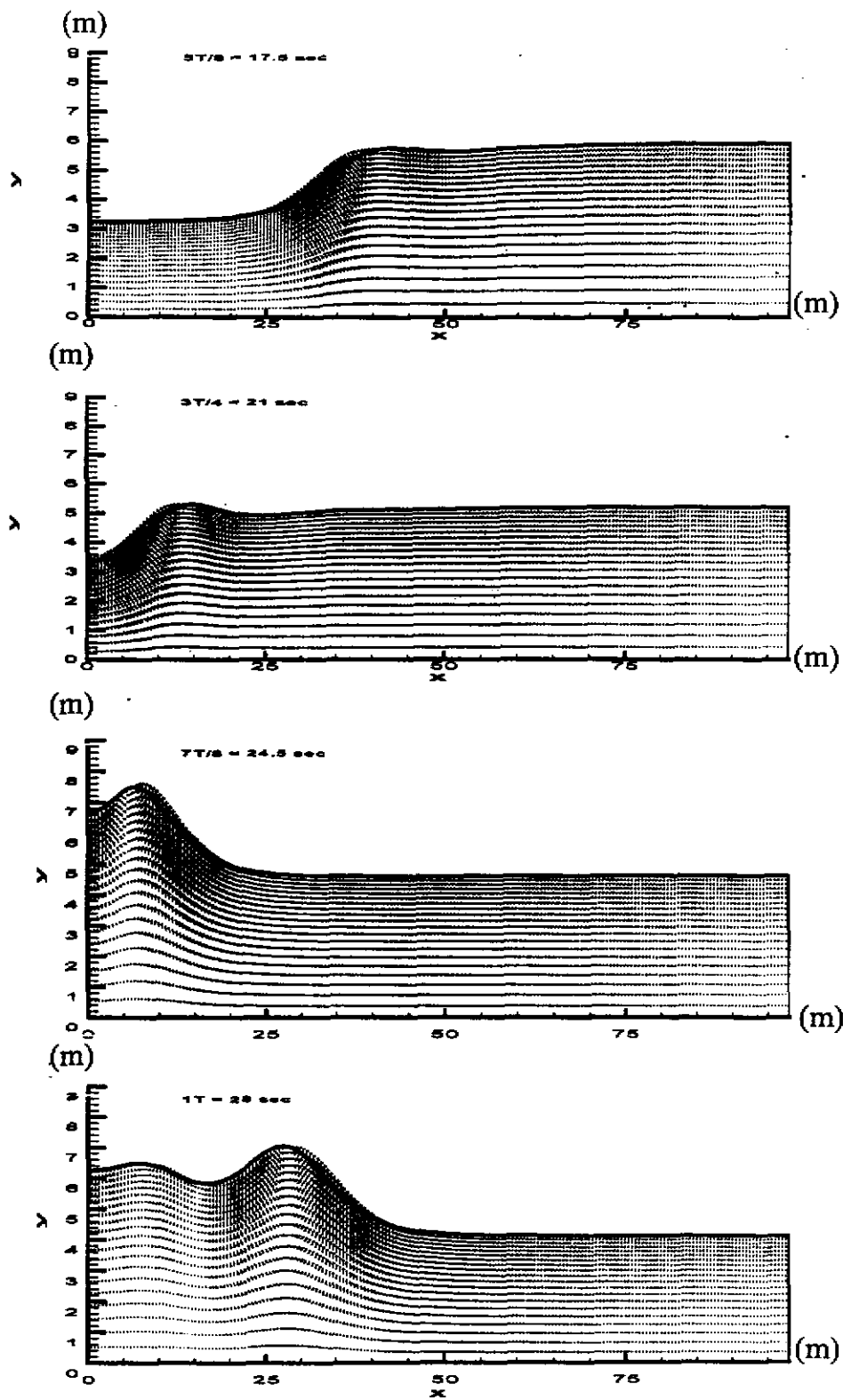


圖 9 長方形水庫蕩漾現象， $A=2.0$ m，非線性數值解，流速場之歷程

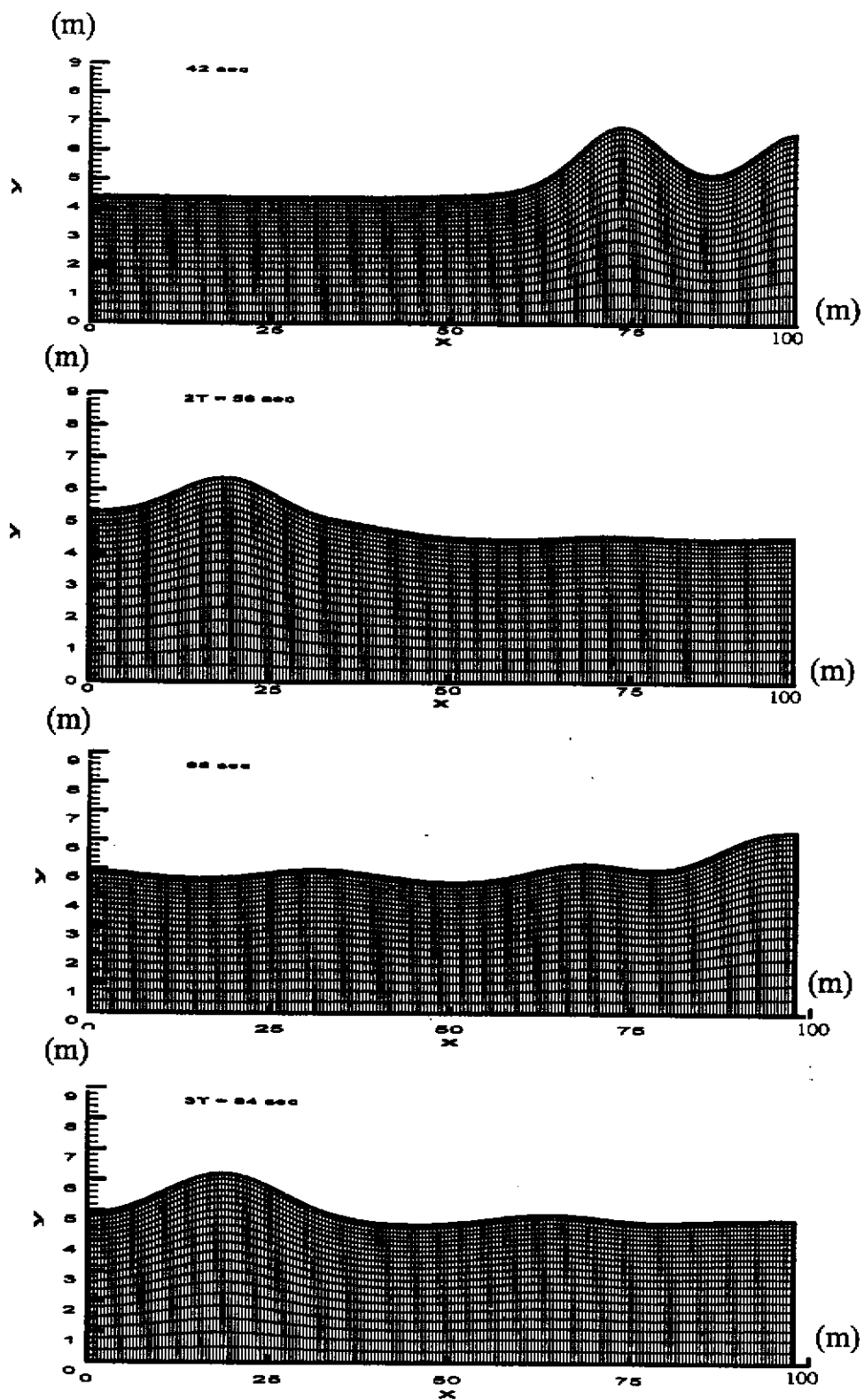


圖 10 長方形水庫蕩漾現象， $A=2.0$ m，非線性數值解，格網變化之歷程

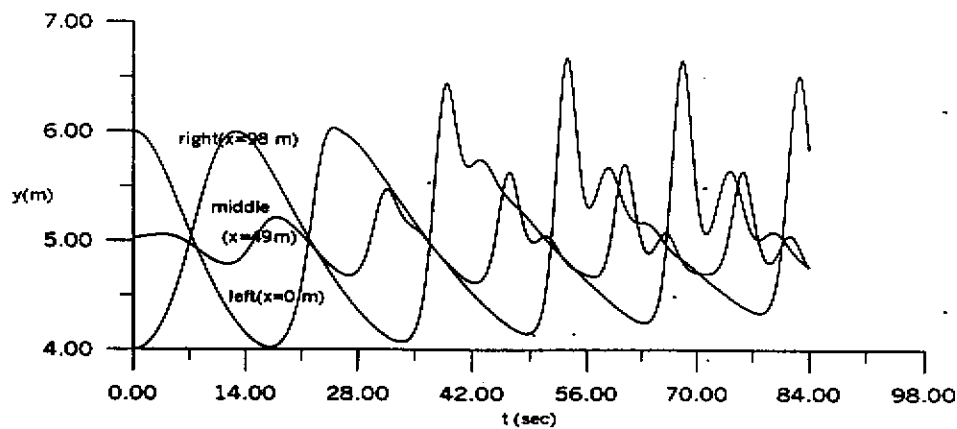


圖 11 長方形水庫蕩漾現象， $A=1.0$ m，非線性數值解，水面波動之歷程

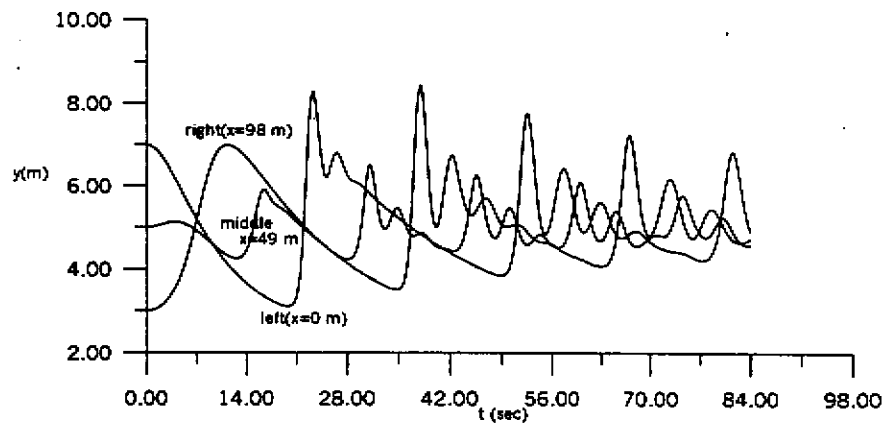


圖 12 長方形水庫蕩漾現象， $A=2.0$ m，非線性數值解，水面波動之歷程

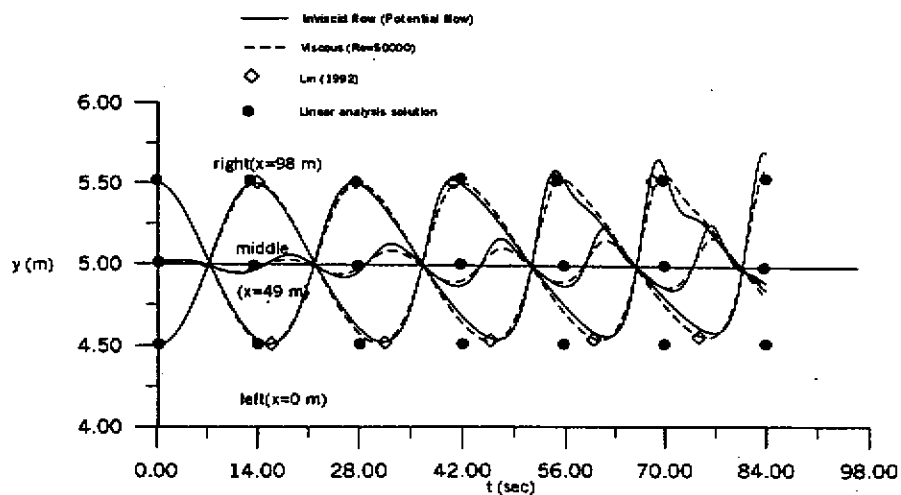


圖 13 長方形水庫蕩漾， $A=0.5$ m，非線性數值解，水面波動歷程
(黏性流場與無黏性流場之比較)

- (2) 由孤立波之黏性減衰及碰撞直立壁之反射，可說明黏性對於波之流場所造成的影響是不容忽略的，但在高雷諾茲數下的流況，流體黏滯性甚小，則其結果類似於勢能流場；但若流體的黏滯性較大時，則數值結果顯示，波高會隨著時間而有黏性減衰的情況，且其波速與波形相位圖皆較勢能流場慢。
- (3) 長方形水庫蕩漾的非線性數值解，當流場初始的振幅小時，流場以週期 28 sec 來回蕩漾，其解接近線性解析解。當流場的初始振幅加大時，非線性效應導致數值解偏離線性解析解且流場會產生湧波。在比較黏性與無黏性效應下，兩者的水面波動歷程在第一個週期相似，但流場在長時間流體黏滯效應的作用下，兩者的水面波動歷程相互偏離，初始振幅愈大愈是明顯。
- (4) 本文在求解自由液面之流場，利用兩種模式，一為勢能函數法（無黏性流場，只求解流場的速度及自由液面的位置），另一為速度-渦度法的模式（黏性流場，求解流場的速度、渦度及自由液面的位置），兩種模式的優缺點與限制分述如下：
 勢能函數法：此法的優點是較為簡單，只需求解拉普拉斯方程式，並配合自由液面的運動及動力邊界條件，所以較為簡單且求解快速。其缺點是無法求解黏性流場，遇到固體邊界不可滑動的邊界條件或底床的邊界層效應之影響則此法就不適用。
 速度-渦度法：此法的優點是無論黏性與無黏性流場皆可適用，若考慮黏性效應則利用完整的速度-渦度法去解之，但相對的程式的編寫也較複雜，解問題所需消耗的時間當然較勢能流場來的多。
- (5) 本文建立的速度-渦度法求解垂直二維自由液面之流場，較傳統的原始變速法及渦度-流函數法，具有下列幾種優勢：（i）速度-渦度模式以流場的速度分佈圖即可知道流動的方向與大小，在觀察渦度的分佈，速度-渦度法將更敏感表現流場的對流、擴散以及漩渦流散（Vortex Shedding）的過程；（ii）速度-渦度法是以 Navier-Stokes 方程式直接計算紊流（Turbulence）問題時，較能展現其物理的特性。因為在物理上，微小速度的變化和漩渦（eddy）的生成和消失有著密切的關係。由速度來直接計算渦度，更容易表現渦流在流場的作用程度；（iii）所得解必滿足質量守恆關係，但不需要直接求解連續方程；（iv）對於垂直二維的 Navier-Stokes 方程式需求解水平方向與垂直方向的動量方程式，而本模式只需求解渦度傳輸方程式，特別是避免壓力項之困擾；（v）速度-渦度法計算時收斂性強，所以可大大的節省計算時所需的時間，而且可由二維推廣至三維的計算而且此點也較渦度-流函數法僅能計算二維流場的問題，顯而易見的速度-渦度法優於渦度-流函數法。

2. 建議

- (1) 研究所建立的垂直二維的自由液面流場模式，在電腦容量容許下，則可考慮將其推展至三維情況，以擴大其應用範圍。
- (2) 有限元素法雖具有求解不規則區域的優點，但其在求解矩陣方程組時，常常需要費較長的時間，所以，可考慮發展平行計算或者利用特殊求解矩陣的技巧以節省運算時間。
- (3) 未來可加以探討黏性流體與結構物間的互制作用，並模擬各種不同結構物的長寬比例、以及各種不同福祿數下的明渠流況，以了解水流經潛堤所引起的渦流 (Vortex Shedding) 效應及渦流可能使結構物和基礎底床承受不均勻負荷而可能導致其變形、沖蝕、翻轉甚至嚴重破壞，以提供日後在水利工程設計的一些參考。
- (4) 目前發展的數值模式尚未能發展到能應用於碎波的計算情況，日後可配合 Lagrangian 質點法模擬碎波現象，而能使模式對非線性效應之分析，更具有完整性及潛力。

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Chapter ??

FINITE ELEMENT ANALYSIS OF STRATIFIED LAKE HYDRODYNAMICS

Der-Liang Frank Young¹

ABSTRACT

The detailed formulation of laterally averaged two-dimensional stratified lake modeling with free surfaces by the finite element analysis is given in this chapter. The Galerkin finite element method with arbitrary Lagrangian-Eulerian (ALE) computing mesh enables us to treat the Navier-Stokes equations of stratified flows with free surfaces under the assumptions of fluid incompressibility, hydrostatic pressure distribution, and the Boussinesq approximation. The model is first tested for the laboratory data of the gravitational underflows of the Generalized Reservoir Hydrodynamics (GRH) flume model taking at the Waterways Experiment Station, U.S. Army Corps of Engineers. After the successful verification with the laboratory scale, the model is then applied to simulate the field scale of two-year annual cycles of the stratified man-made lake of the Te-Chi reservoir located at central Taiwan.

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1. INTRODUCTION

A lake can be considered as an open system with an upper free surface boundary exposed to the atmosphere and a solid boundary, called the basin, made of minerals. Various geological processes such as weathering, mass wasting, erosion and deposition by streams are responsible for the existence of these basins of natural lakes. Artificial lakes are also created for storing water obtained from rain and other natural streams. The stream-eroded valleys serve as basins for most of the reservoirs that are built behind dams. Apart from serving as reservoirs for storing water, lakes and lake sediments provide useful information about environmental changes. The analysis of fossil pollen provides information about the changes that have taken place in the nearby vegetation. The changes in the shoreline elevations can be used along with the pollen records to study the recent changes in the environment. The variations in lake levels also serve as an indication on the amount of rainfall or evaporation. Some geologists have discovered that lakebeds are a common source of petroleum. Hence the study of old lake deposits has become a major research activity.

Lakes serve as a major source of water supply for human activities. The demand for water is continuously increasing with growing population and civilization. In recent years there is much concern about the quality of lake water, since the lake water is contaminated due to different kinds of interactions of a lake with its surroundings. These interactions vary widely as listed below:

- (i) Lake water absorbs heat from solar radiation and also from power plant cooling water while released to the lake; it also loses heat to the atmosphere.
- (ii) Lake receives water as inflow from streams and also in the form of precipitation; water leaves the lake as outflow for various purposes.
- (iii) Lake receives contaminated water and liquids in varying densities.
- (iv) Wind blowing over the lake surface changes the wave pattern of water surface and thus the surface roughness thereby increases the momentum and energy transfer.
- (v) Lake interacts with the ground water table; this may affect the mass and momentum balances of the lake.

Many of these interactions result in coupled activities, affecting the balances of mass, momentum, heat and concentration of water in the lake. Furthermore, the flows associated with lakes are always turbulent and the turbulence varies with time and space at different scales. In order to have control over the quality of lake water, knowledge about the dynamics of lake water is essential. The study of variation of velocity, temperature and concentration of lake water due to various kinds of interactions of a lake with its surroundings is called

'lake hydrodynamics', also called the 'physical limnology'.

2. MASS, MOMENTUM, HEAT AND CONCENTRATION TRANSPORTS IN LAKES

One important characteristic of a lake is its density stratification (Harleman, 1961, and Yih, 1980). The density stratification in lakes takes place both by means of thermal effects as well as by the inflow of liquids with varying densities. The thermal stratification in a lake is formed primarily by solar radiation. The heat transfer mechanism at the water surface together with solar radiation plays a major role in deciding the surface water temperature (Verevochkin and Startsev, 2000). Consequently, the temperature of water in a lake varies seasonally. In spring the water temperature increases due to heating of surface water by growing solar energy. The resulting thermal stratification becomes strong in the late summer. The various thermal regimes developed inside a lake due to thermal stratification are shown in Fig.1. The warm upper layer is called the 'epilimnion' and the cold lower layer is referred to as the 'hypolimnion'. The region of the

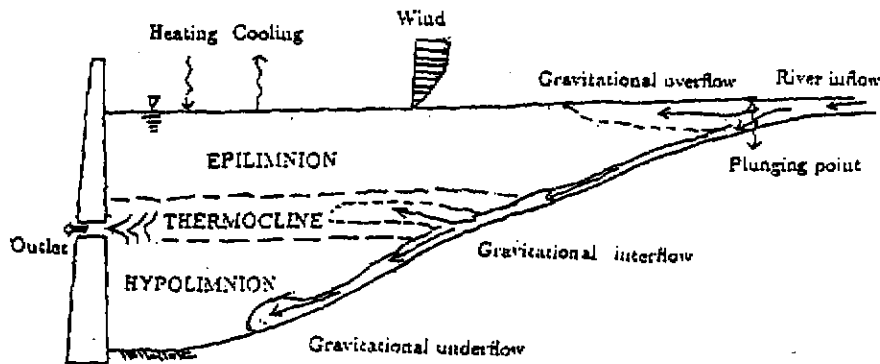


Fig. 1. Schematic diagram of a stratified lake or reservoir showing the transport processes of mass, momentum, heat, and sediment.

largest temperature gradient is often denoted as the 'metalimnion'. When the continuous stratification is idealized by a two-layer model with a light upper layer and a heavier lower layer, the plane of separation is called the 'thermocline'. This is usually taken to be the position of the strongest vertical temperature gradient. The stability of thermal stratification is characterized by the Richardson number, defined as

$$Ri = - \frac{\left(\frac{g}{\rho} \right) \frac{\partial \rho}{\partial z}}{\left(\frac{\partial u}{\partial z} \right)^2}$$

The stability of thermal stratification increases when Ri increases.

Apart from thermal effects the density of the incoming flow into the lake also affects the stratification. The inflow of liquids with varying densities results in different types of flow within the lake. When the density of the incoming flow is lower than that of the water in the lake, a layer of flow will move along the free surface. This type of flow is called 'overflow'. When the density of the incoming flow is greater than that of the water in the lake, then a layer of flow will move along the reservoir bed and this flow is called 'underflow'. When the density of water in a lake is not homogeneous due to thermal stratification, the incoming flow will move towards an intermediate layer and this is called 'interflow'. When a flow with sediment reaches the backwater zone of a reservoir, the suspended sediments start to deposit at the bottom of the lake. When the sediment-laden flow plunges beneath the free surface under certain circumstances, the layer of underflow formed is called 'turbidity current' (Lee and Yu, 1997). The nature of density current also depends on whether the flow is steady or unsteady and continuous or instantaneous.

Thermal stratification plays a vital role in water quality modeling. When thermal stratification exists for a longer period, the water in the hypolimnion layer is cut off from contact with the atmosphere with respect to oxygen supply and this will have an adverse effect on the quality of water. A lake can be destratified by artificial means to overcome this problem. However, sometimes nature also helps us to weaken the stratification by turbulent mixing. The flow into a lake is always turbulent. When such flow enters the lake, there will be turbulent exchange of momentum across the interface of the density current. The low momentum liquid easily enters into the density current by interfacial mixing. The interfacial mixing is an important process for destratification to maintain water quality. This depends on the shear stress and hydrostatic pressure gradient at the interface. Hence knowledge about density stratification is essential for water quality modeling. The study of lake hydrodynamics mainly concentrates on the determination of various types of density currents developed for the imposed conditions on a lake.

3. MATHEMATICAL MODELING OF LAKE HYDRODYNAMICS

The hydrodynamics of lakes has been studied by collecting field data and by conducting experiments on laboratory scale models. Since the hydrodynamic processes are in general transient, coupled and non-linear in nature, pure

experimental approach will demand enormous amount of tests. The physics of the phenomena can be well understood by representing the various physical processes and interactions by suitable mathematical model and making use of the field data (Hutter, 1984, Hutter, 1987, and Mortimer, 1974). A mathematical model can be built to represent various interactions such as (i) heating of water in lake due to solar radiation, (ii) heat exchange at the air-water interface, (iii) vertical mixing of water due to wind action, (iv) convective water movement due to density currents, (v) turbulent nature of flow within the lake and (vi) interaction of lake bottom with the ground water movement. Developing a mathematical model including all the above effects is very complex and difficult. Moreover, the study of lake hydrodynamics may vary depending upon the applications. Hence a suitable mathematical model for lake hydrodynamics is problem dependent.

In all the mathematical models it is assumed that the principles of conservations of mass, momentum, energy and concentration provide the basic equations for describing the hydrodynamics of lakes. With respect to the size of the lakes studied, in general, the Coriolis parameter is neglected in the study of lake hydrodynamics except for the Great Lakes. Most numerical models assume hydrostatic approximation (due to small value of depth to length ratio, i.e. $H/L \ll 1$), Boussinesq approximation and incompressible flows. The hydrostatic approximation implies that any change of pressure due to the movement of air-water interface, is transmitted through the entire water column instantly. The Boussinesq approximation (Gray and Girgini, 1976) treats density as constant throughout the governing equations except those associated with gravitational terms (Turner, 1973). With the above approximations, the variation of density is only explicitly included in a limited way. The additional influences of density gradients will appear in the turbulent mixing coefficients (Cheng, 1977). With the above assumptions a mathematical model can be developed to study the hydrodynamic behavior of a lake. Depending upon the topography, meteorological conditions and the nature of inflow and outflow into a lake, the hydrodynamic model may be used to focus on specific phenomenon such as thermal stratification, density circulation, wind-induced circulation etc. With an aim to make the reader appreciate the on-going research in various fields of lake hydrodynamics, an overview of some important literatures are highlighted in the following sections.

3.1 Thermal stratification

The water temperature in a lake is affected by the phenomenon of stratification. The development of thermocline and erosion of thermocline have been studied using mathematical models (see Csanady, 1975, Graf and Mortimer, 1979,

o Hutchinson, 1957, Kawahara, 1977, Spalding and Svensson, 1977, and Street et al., 1977). Herleman (1982) gives a review of vertical temperature structure of lakes using different models such as diffusion models and mixed-layer models. The thermal stratification can be studied using simple models like cavity flow models (Young et al., 1976a and 1976b). Sundermann (1978) discusses circulation in lakes using barotropic one-layer model, barotropic Ekman type model and baroclinic multi-layer model. Three-dimensional transient models also have been used to study lake hydrodynamics (Bauer, 1978, and Wittmiss, 1978).

3.2 Density-driven circulation

Mass, in the form of suspended sediments, algae or nutrients such as phosphorus, is distributed in lake water by the action of hydrothermal processes. They also undergo biogeological transformations simultaneously. Density currents may be created either by dense or lighter inflows into stratified or unstratified lakes and reservoirs (Alavian et al., 1992). Turbidity currents are generated by sediment-laden flow into the reservoir (Lee and Yu, 1997). The contaminant dispersion in lakes (Salmon et al., 1980) also creates density currents giving rise to different flow regimes such as plunging flow, underflow and interflow (Chung and Gu, 1998). The migration of plunge point in reservoir affects the hydraulic characteristic of the reservoir.

3.3 Wind-driven circulation

The wind-driven circulation in lakes has been studied using different types of numerical models (Cheng, 1977). Commonly used models include layered models, Ekman type models and three-dimensional models. Wind acting on the surface of a stratified lake gives rise to large changes in the distribution of pressure. These pressure changes cause circulation gyre and modify the position of the interface. The shear stress exerted by the earth on the atmosphere slows down the air currents. In response to this resistance, the water surface generates a drift current and a wave pattern (Simpson, 1995, and Stoker, 1957) as a result of boundary layer effects. The drift velocity profile and wave pattern evolve with space and time (Cheng, 1977, Hansen, 1975, Hansen, 1978, Plate and Wengefeld, 1978, and Ramming, 1978) and this causes changes in the airflow pattern. Due to the drift current, a "slip" condition prevails at the lower boundary of the airflow. Finally the shear stress is altered resulting from the above phenomena. Another effect due to wind is the deepening of upper layer caused by the entrainment of water from the lower denser layer (Hansen, 1975). The earth rotation also affects the changes that

are taking place in a stratified lake in addition to wind effects (Mortimer, 1984).

3.4 Interaction between lake and ground water systems

Surface water bodies such as lakes, ponds, streams etc. are all integral parts of groundwater flow systems. The interaction of a surface water body such as a lake with ground water flow systems, affect the distribution pattern of hydraulic head, specific discharge and stream lines. This interaction depends on the positions of the lake with respect to groundwater flow system, geologic characteristic of their beds and their climatic settings (Winter, 1999). Kacimov (2000) developed an analytical model for a regional 3-D groundwater flow interacting with a lake. He found that any lake can change its regime from gaining to losing or flow-through, depending on the varying incident ground water flow velocity, evaporation-precipitation-runoff rates in the lake, lake sizes, thickness of silt layer at the bottom of the lake and other hydrological characteristics. The information on gaining or losing of lakes is important for water budget calculation. Water quality also can be assessed by this information because it is affected by the contaminants present in the ground water flow systems.

3.5 Water quality

Lake is a major source of fresh water supply. The quality of lake water is affected by the biological and biochemical reactions taking place within the water body. In addition, inflow water also carries a number of contaminants. The mixing of these contaminants with the lake water causes degrade of water. The degree of degrade depends upon how well these contaminants are mixed with the water. The hydrodynamic transport mechanisms such as convection and advection and thermal stratification influence the mixing of these contaminants. Furthermore, these mixing take place in different time scales. A numerical model developed by Imberger et al. (1978) incorporated all the dominant physical processes taking place at different time scales. Imberger and Patterson (1981) used a one-dimensional model for daily prediction of salinity and temperature for small lakes. The hydrodynamic processes within a lake are also influenced by the thermal stratification. Markofsky (1978) suggested that a coupled thermal stratification-water quality model has to be used in order to correctly predict the quality of water.

3.6 Numerical methods

The governing equations used to study the lake hydrodynamics are transient, coupled and non-linear and hence they are solved only by numerical methods. Finite difference method (FDM) has been widely used to solve such complex equations. In the case of FDM, the governing equations are reduced to difference equations using Taylor's series expansion. Hence the governing equations are modified by representing the differential terms in terms of finite values of the variables at fixed nodes. The approximation can be made either by using forward difference, backward difference or central difference schemes. The difference equations are obtained for all nodes in a computational domain, resulting in a number of simultaneous algebraic equations.

In the case of finite element method (FEM), an approximate solution for the nodal variables of the finite element is assumed. In addition, the piecewise variation of the given variables between the nodes is represented by means of a function called the shape function. When the approximate solution is substituted into the governing equation, a residue is obtained in the case of weighted residual method. The residue is minimized with the help of a weighting function. The shape function itself is taken as the weighting function in the case of Galerkin's weighted residual method. The residue is minimized in the entire computational domain. This procedure also results in a number of simultaneous nodal equations.

It is very difficult to represent irregular geometries by FDM. This is a major disadvantage of these models (Bauer, 1978). As it is well known, the boundaries of the basins of lakes or reservoirs are highly irregular in geometry. The problem of representing irregular geometry is overcome by FEM. Thacker (1977) proposed an irregular grid FDM by combining the advantage of a smooth geometrical representation using FEM and the advantage of fast execution using FDM.

3.7 Application of finite element method for lake hydrodynamic model studies

With the advancement of high-speed computers, FEM has become the most powerful method to treat irregular boundaries. FEM provides the user with flexibilities with respect to the computational effort and accuracy by appropriate discretization of the computational domain. In addition the spatial variations of physical properties can easily be taken into account by FEM. Moreover, isoparametric elements can be used to effectively map curvilinear boundaries. This is another attractive feature of FEM compared to other numerical methods. Since the boundary of a lake is of irregular geometry, FEM is found to be an efficient numerical tool to handle such situations. FEM has been used successfully by a number of researchers to solve the governing equations of lake hydrodynamics.

Detailed study on the application of finite element method for lake hydrodynamics using different types of models may be found in the literature (Gallagher et al., 1973, Gallagher and Chan, 1973, Young, 1980, Young et al., 1976(a) & 1976(b), and Young and Liggett, 1977).

4. DERIVATION OF GOVERNING EQUATIONS

The governing equations for lake hydrodynamics are obtained by applying the conservation laws of mass, momentum, energy and species concentration to an elemental control volume. These equations differ from the general conservation equations in certain aspects: the general conservation equations are derived based on the assumption that the control volume is uniform. In the case of lakes, the width varies both in vertical and in longitudinal directions. In order to make the reader appreciate the application of conservation laws to a real system such as a lake, the important steps in the derivation are discussed in the following section. The coordinate system used to represent different dimensions of the lake is shown in Fig. 2a.

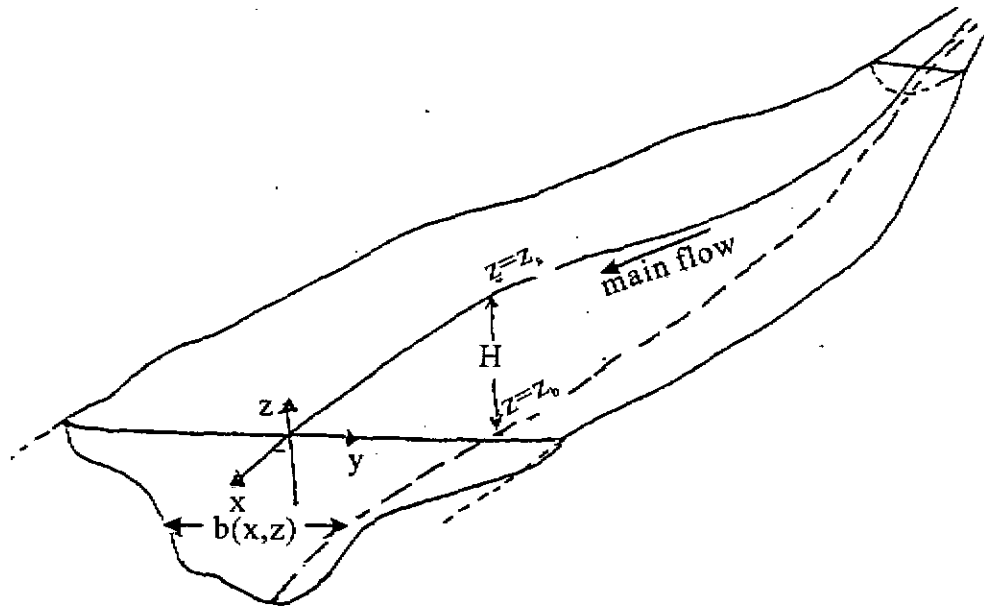


Fig. 2a. The coordinate system and geometry layout of a stratified lake or reservoir with free surface and moving bed.

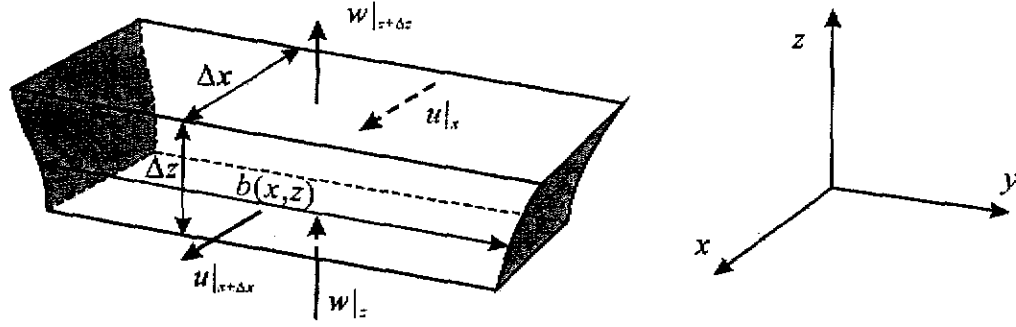


Fig. 2b. Elemental control volume.

4.1 Assumptions

The following assumptions are made in the derivation of conservation equations.

- (i) The fluid is incompressible.
- (ii) Boussinesq approximation applies.
- (iii) The flow in the lake satisfies hydrostatic approximation.
- (iv) Surfaces perpendicular to the y-direction are impermeable for any mode of transport (laterally averaged).

4.2 Continuity equation

The continuity equation is derived based on the conservation of mass principle applied to a small elemental control volume as shown in Fig.2b.

We know from the conservation of mass principle,

$$\left(\begin{array}{c} \text{rate of mass} \\ \text{increase in the} \\ \text{elemental volume} \end{array} \right) = \left(\begin{array}{c} \text{rate of mass} \\ \text{entering the} \\ \text{elemental volume} \end{array} \right) - \left(\begin{array}{c} \text{rate of mass} \\ \text{leaving the} \\ \text{elemental volume} \end{array} \right) +$$

$$\left(\begin{array}{c} \text{rate of mass} \\ \text{addition by} \\ \text{lateral flows} \end{array} \right)$$

x-direction:

Rate of mass flow into the elemental volume is given by

$$(\rho u)|_x b(x, z) \Delta z = (\rho u b)|_x \Delta z$$

Rate of mass flow out of the elemental volume is given by

$$(\rho u) \Big|_{x+\Delta x} b(x, z) \Delta z = (\rho u b) \Big|_{x+\Delta x} \Delta z$$

z-direction:

Rate of mass flow into the elemental volume is given by

$$(\rho w) \Big|_z b(x, z) \Delta x = (\rho w b) \Big|_z \Delta x$$

Rate of mass flow out of the elemental volume is given by

$$(\rho w) \Big|_{z+\Delta z} b(x, z) \Delta x = (\rho w b) \Big|_{z+\Delta z} \Delta x$$

Rate of mass increase in the elemental volume is given by

$$\left(\frac{\partial \rho}{\partial t} \right) b(x, z) \Delta x \Delta z$$

Rate of mass addition to the elemental volume due to lateral flow is

$$\rho q_i \Delta x \Delta z$$

Hence the application of mass conservation principle gives

$$(\rho u b) \Big|_x \Delta z - (\rho u b) \Big|_{x+\Delta x} \Delta z + (\rho w b) \Big|_z \Delta x - (\rho w b) \Big|_{z+\Delta z} \Delta x + \rho q_i \Delta x \Delta z = \left(\frac{\partial \rho}{\partial t} \right) b(x, z) \Delta x \Delta z$$

Dividing throughout by $\Delta x \Delta z$ and applying the principle of differential equation we get

$$-\frac{\partial}{\partial x}(\rho u b) - \frac{\partial}{\partial z}(\rho w b) + \rho q_i = b(x, z) \frac{\partial \rho}{\partial t}$$

Since the fluid density is assumed to be constant except when associated with a gravitational term, the term on the right hand side of the above equation becomes zero. The final form of the continuity equation can be written as follows:

$$\frac{\partial(u b)}{\partial x} + \frac{\partial(w b)}{\partial z} = q_i \quad (1)$$

4.3 Momentum equation

The momentum equation is also derived based on the principle used in any fluid mechanics texts. The only difference in the present formulation is the variation of lateral width of the lake $b(x, z)$. Since this term is used frequently in the derivations, henceforth only 'b' will be used in place of ' $b(x, z)$ '. Only the x-momentum equation is derived. The z-momentum equation is represented by the hydrostatic equation and the gravity term. The shear stress on the x-z plane is neglected.

x-momentum equation:

From Newton's second law of motion we can write the force balance for the elemental control volume shown in Fig.2b as follows:

$$\left(\begin{array}{c} \text{rate of momentum} \\ \text{increase within} \\ \text{the elemental volume} \end{array} \right) + \left(\begin{array}{c} \text{net efflux of} \\ \text{momentum out of} \\ \text{the elemental volume} \end{array} \right) -$$

$$\left(\begin{array}{c} \text{rate of momentum} \\ \text{entering the elemental volume} \\ \text{due to lateral flow velocity} \end{array} \right) = \left(\begin{array}{c} \text{rate of external} \\ \text{forces acting on} \\ \text{the elemental volume} \end{array} \right)$$

Net efflux of momentum of the elemental volume = rate of momentum leaving the elemental volume – rate of momentum entering the elemental volume

Rate of accumulation of momentum within the elemental volume is given by

$$\frac{\partial(\rho ub)}{\partial t} \Delta x \Delta z = b \rho \frac{\partial u}{\partial t}$$

Rate at which x-momentum enters the element at $x = (\rho uub) \Big|_x \Delta z$

Rate at which x-momentum leaves the element at $x + \Delta x = (\rho uub) \Big|_{x+\Delta x} \Delta z$

Rate at which x-component of momentum enters the element at $z = (\rho uwb) \Big|_z \Delta x$

Rate at which x-component of momentum leaves the element at

$z + \Delta z = (\rho uwb) \Big|_{z+\Delta z} \Delta x$

After dividing by $\Delta x \Delta z$, the net efflux of momentum from the elemental volume in the x-direction can be written as follows:

$$\frac{\partial(\rho ubu)}{\partial x} + \frac{\partial(\rho ubw)}{\partial z} = \rho u \frac{\partial(ub)}{\partial x} + \rho ub \frac{\partial(u)}{\partial x} + \rho u \frac{\partial(wb)}{\partial z} + \rho wb \frac{\partial(u)}{\partial z}$$

Since the density is constant, the above equation can be rewritten as

$$\rho u \left[\frac{\partial(ub)}{\partial x} + \frac{\partial(wb)}{\partial z} \right] + \rho b \left[u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} \right] = \rho u q_x + \rho b \left[u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} \right]$$

Because the total external forces acting on the element is the sum of forces due to liquid pressure and due to shear stresses, we next derive all external forces as follows:

Forces due to liquid pressure:

The net pressure force acting on the element in the x-directions is

$$(bp|_x - bp|_{x+\Delta x})\Delta z$$

After dividing by $\Delta x \Delta z$ we get the differential form of the equation as

$$-\frac{\partial(bp)}{\partial x}$$

Forces due to shear stresses:

The forces due to the shear stresses in the x-direction are:

$$\left(\tau_{xx}b|_{x+\Delta x} - \tau_{xx}b|_x\right)\Delta z + \left(\tau_{zx}b|_{z+\Delta z} - \tau_{zx}b|_z\right)\Delta x$$

After dividing by $\Delta x \Delta z$ we get the final form of the equation as

$$\frac{\partial(b\tau_{xx})}{\partial x} + \frac{\partial(b\tau_{zx})}{\partial z}$$

For turbulent flow the shear stresses can be written in terms of eddy viscosities and velocity gradients as

$$\tau_{xx} = \rho K_x^M \left(\frac{\partial u}{\partial x} \right) \text{ and } \tau_{zx} = \rho K_z^M \left(\frac{\partial u}{\partial z} \right)$$

where K_x^M, K_z^M - longitudinal and vertical eddy viscosities respectively.

The final form of the equation for forces due to shear stresses is written as

$$\frac{\partial}{\partial x} \left(\rho b K_x^M \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial z} \left(\rho b K_z^M \frac{\partial u}{\partial z} \right)$$

Now we derive the inertial terms as follows.

Rate of momentum entering into the elemental volume due to the lateral flow:

Rate of x-component of momentum entering at $x = \rho u b|_x \Delta z u_i$

Rate of x-component of momentum leaving the elemental volume at

$x + \Delta x = \rho u b|_{x+\Delta x} \Delta z u_i$

Rate of x-component of momentum entering the elemental volume at $z = \rho u b|_z \Delta x u_i$

Rate of x-component of momentum leaving the elemental volume at

$z + \Delta z = \rho u b|_{z+\Delta z} \Delta x u_i$

where u_i is the lateral inflow velocity component parallel to the longitudinal direction.

Following similar steps used in the derivation of x-momentum equation, the differential form of the rate of change of momentum due to lateral flow velocity is

given by

$$\left[\frac{\partial}{\partial x}(ub) + \frac{\partial}{\partial z}(wb) \right] \rho u_i = \rho u_i q_i$$

By substituting various force terms in the momentum conservation equation, we get finally

$$\rho b \frac{\partial u}{\partial t} + \rho b \left(u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} \right) + \rho u q_i - \rho u_i q_i = -\frac{\partial(bp)}{\partial x} + \frac{\partial}{\partial x} \left(\rho b K_x^M \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial z} \left(\rho b K_z^M \frac{\partial u}{\partial z} \right)$$

Dividing the above equation throughout by ρb the final form of the x-momentum equation is obtained as follows:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho b} \frac{\partial(bp)}{\partial x} + \frac{1}{b} \frac{\partial}{\partial x} \left(b K_x^M \frac{\partial u}{\partial x} \right) + \frac{1}{b} \frac{\partial}{\partial z} \left(b K_z^M \frac{\partial u}{\partial z} \right) + \frac{q_i}{b} (u_i - u) \quad (2)$$

4.4 Energy equation

The energy equation is derived based on the conservation of energy principle as postulated by the First law of Thermodynamics. The First law for an open system like the one shown in Fig.2b states that

$$\frac{d E_{cv}}{dt} = \frac{d Q_{cv}}{dt} - \frac{d W_{cv}}{dt} + \dot{m} e_{out} - \dot{m} e_{in}$$

which means that

$$\left(\begin{array}{c} \text{rate of storage of} \\ \text{internal energy in} \\ \text{the elemental volume} \end{array} \right) = \left(\begin{array}{c} \text{rate of heat} \\ \text{transfer into the} \\ \text{elemental volume} \end{array} \right) - \left(\begin{array}{c} \text{rate of work} \\ \text{done within} \\ \text{the elemental volume} \end{array} \right) + \left(\begin{array}{c} \text{net efflux of} \\ \text{energy from the} \\ \text{elemental volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of energy} \\ \text{input due to} \\ \text{lateral flow} \end{array} \right)$$

$$\text{Rate of internal energy storage within the elemental volume} = \frac{\partial}{\partial t} (\rho e) b \Delta x \Delta z$$

Total internal energy leaving the elemental volume is given by

$$(\rho e u b) \Big|_{x+\Delta x} \Delta z + (\rho e w b) \Big|_{z+\Delta z} \Delta x$$

Total internal energy entering the elemental volume is given by

$$(\rho e u b) \Big|_x \Delta z + (\rho e w b) \Big|_z \Delta x$$

Hence the net efflux of energy leaving the elemental volume is obtained by dividing the differences of the above two expressions by $\Delta x \Delta z$. The final equation

obtained is

$$\begin{aligned}\frac{\partial}{\partial x}(\rho e u b) + \frac{\partial}{\partial z}(\rho e w b) &= \rho e \left[\frac{\partial}{\partial x}(u b) + \frac{\partial}{\partial z}(w b) \right] + \rho b \left[u \frac{\partial e}{\partial x} + w \frac{\partial e}{\partial z} \right] \\ &= \rho e q_t + \rho b \left[u \frac{\partial e}{\partial x} + w \frac{\partial e}{\partial z} \right]\end{aligned}$$

(where equation (1) is used.)

The net rate of heat flux entering the control volume is given by

$$q b|_{x+\Delta x} \Delta z - q b|_x \Delta z + q b|_{z+\Delta z} \Delta x - q b|_z \Delta x$$

After dividing by $\Delta x \Delta z$ the differential form of the above expression is

$$\frac{\partial}{\partial x}(q_x b) + \frac{\partial}{\partial z}(q_z b)$$

where $q_x = k_x \frac{\partial T}{\partial x}$ and $q_z = k_z \frac{\partial T}{\partial z}$ and k_x, k_z are the thermal conductivities in the x

and z directions respectively.

The energy input to the elemental control volume due to the lateral flow is

$$(\rho u b|_{x+\Delta x} - \rho u b|_x) \Delta z e_t + (\rho w b|_{z+\Delta z} - \rho w b|_z) \Delta x e_t$$

where e_t is energy per unit mass due to the lateral flow.

After dividing by $\Delta x \Delta z$, the differential form of the above expression is

$$\rho e_t \left[\frac{\partial}{\partial x}(u b) + \frac{\partial}{\partial z}(w b) \right] = \rho e_t q_t$$

The internal energy for an incompressible fluid is given by $e = CT$, where C = specific heat capacity and T = temperature.

By substituting the respective expressions in the energy balance equation we get

$$\rho b C \frac{\partial T}{\partial t} + \rho b C \left[u \frac{\partial T}{\partial x} + w \frac{\partial T}{\partial z} \right] + \rho C T q_t = \frac{\partial}{\partial x} \left(b k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial z} \left(b k_z \frac{\partial T}{\partial z} \right) + \rho C T_t q_t$$

By dividing the above equation throughout by $b \rho C$, we get

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + w \frac{\partial T}{\partial z} = \frac{1}{b} \frac{\partial}{\partial x} \left(b \frac{k_x}{\rho C} \frac{\partial T}{\partial x} \right) + \frac{1}{b} \frac{\partial}{\partial z} \left(b \frac{k_z}{\rho C} \frac{\partial T}{\partial z} \right) + \frac{q_t}{b} (T_t - T)$$

For turbulent flows, the thermal diffusivity terms are replaced by means of eddy diffusivity coefficients. That is

$$\frac{k_x}{\rho C} = K_x^H, \frac{k_z}{\rho C} = K_z^H \text{ where } K_x^H, K_z^H = \text{longitudinal and vertical eddy diffusivity}$$

coefficients respectively. After substituting these coefficients, the final form of the energy equation is reduced to the following form

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + w \frac{\partial T}{\partial z} = \frac{1}{b} \frac{\partial}{\partial x} \left(b K_x^H \frac{\partial T}{\partial x} \right) + \frac{1}{b} \frac{\partial}{\partial z} \left(b K_z^H \frac{\partial T}{\partial z} \right) + \frac{q_i}{b} (T_i - T) \quad (3)$$

4.5 Sediment transport equation

Applying the principle of conservation of mass principle to sediment transport through the elemental control volume, we get

$$\begin{aligned} \left(\begin{array}{c} \text{rate of storage of} \\ \text{sediment in the} \\ \text{elemental volume} \end{array} \right) &= \left(\begin{array}{c} \text{rate of sediment} \\ \text{entering the} \\ \text{elemental volume} \end{array} \right) - \left(\begin{array}{c} \text{rate of sediment} \\ \text{leaving the} \\ \text{elemental volume} \end{array} \right) \\ &+ \left(\begin{array}{c} \text{diffusive flux of} \\ \text{sediment entering into} \\ \text{the elemental volume} \end{array} \right) + \left(\begin{array}{c} \text{rate of sediment} \\ \text{input due to} \\ \text{lateral flow} \end{array} \right) \end{aligned}$$

$$\text{Rate of storage of sediment in the elemental volume} = \left(\frac{\partial C}{\partial t} \right) b \Delta x \Delta z$$

The net efflux of sediment from the elemental volume is given by

$$\left(ucb \Big|_{x+\Delta x} \Delta z - ucb \Big|_x \Delta z \right) + \left(wcb \Big|_{z+\Delta z} \Delta x - wcb \Big|_z \Delta x \right)$$

After dividing by $\Delta x \Delta z$ we get the differential form of the above equation as

$$\begin{aligned} \frac{\partial}{\partial x} (uCb) + \frac{\partial}{\partial z} (wCb) &= \left[ub \frac{\partial C}{\partial x} + wb \frac{\partial C}{\partial z} \right] + C \left[\frac{\partial}{\partial x} (ub) + \frac{\partial}{\partial z} (wb) \right] \\ &= b \left(u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} \right) + Cq_i \end{aligned}$$

(where equation (1) is used.)

Net rate of diffusive sediment transport into the elemental volume is given by

$$\dot{m}b \Big|_{x+\Delta x} \Delta z - \dot{m}b \Big|_x \Delta z + \dot{m}b \Big|_{z+\Delta z} \Delta x - \dot{m}b \Big|_z \Delta x$$

After dividing the above by $\Delta x \Delta z$, we get the differential form of the equation as

$$\frac{\partial}{\partial x} \left(\dot{m}_x b \right) + \frac{\partial}{\partial z} \left(\dot{m}_z b \right)$$

Applying the Fick's law of diffusion, the above equation can be rewritten as

$$\frac{\partial}{\partial x} \left(b D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial z} \left(b D_z \frac{\partial C}{\partial z} \right)$$

where the mass flux $\dot{m}_x = D \frac{\partial C}{\partial x}$ and $\dot{m}_z = D \frac{\partial C}{\partial z}$.

It can be shown that the sediment inflow due to lateral flow is given by the following expression using the similar steps for the derivation of lateral energy flow in the energy equation.

$C_i \left[\frac{\partial}{\partial x}(ub) + \frac{\partial}{\partial z}(wb) \right] = C_i q_i$, where C_i = the concentration of the sediment due to the lateral flow.

After substituting the respective expressions in the sediment conservation equation, we get the following expression

$$b \frac{\partial C}{\partial t} + b \left(u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} \right) + C q_i - C_i q_i = \frac{\partial}{\partial x} \left(b D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial z} \left(b D_z \frac{\partial C}{\partial z} \right)$$

For turbulent flow, the diffusion coefficients are replaced by turbulent eddy diffusion coefficients as was done in the derivation of the momentum and energy equations. With this substitution and dividing the above equation throughout by 'b', the final form of the sediment transport equation is obtained as

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} = \frac{1}{b} \frac{\partial}{\partial x} \left(b K_x^C \frac{\partial C}{\partial x} \right) + \frac{1}{b} \frac{\partial}{\partial z} \left(b K_z^C \frac{\partial C}{\partial z} \right) + \frac{q_i}{b} (C_i - C) \quad (4)$$

where t = time ; x = longitudinal Cartesian coordinate; z = vertical Cartesian coordinate; u = longitudinal flow velocity; w = vertical flow velocity; u_i = lateral inflow velocity component which is parallel to the longitudinal direction; p = pressure; b = lateral width; g = gravitational acceleration; ρ = ambient fluid density; T = ambient temperature; C = concentration of suspended sediment; q_i = lateral inflow per unit area; T_i = lateral inflow temperature; C_i = lateral inflow concentration of suspended sediment; K_x^M, K_z^M = longitudinal and vertical eddy viscosity, respectively; K_x^H, K_z^H = longitudinal and vertical eddy diffusivity for heat transport, respectively; K_x^C, K_z^C = longitudinal and vertical eddy diffusivity for sediment transport, respectively.

5. FINITE ELEMENT FORMULATION

The mass, momentum, energy and sediment transport equations can be solved using Galerkin's weighted residual method which is widely used for field problems. Considering a triangular element, any field variable can be written in terms of its nodal values and the respective shape functions as follows:

$$\phi = N_i \phi_i + N_j \phi_j + N_k \phi_k$$

The above expression represents the form of solution assumed for the variable. When this solution is substituted into the differential equation, a residue will be obtained because the assumed solution is not the exact solution. The principle of

weighted residual method is that the given differential field equation multiplied by a weighting function will be integrated (in the case of Galerkin's method, the shape function itself is the weighting function) throughout the computational domain in order to make the residue minimum. The resultant integrated equations will yield a number of simultaneous algebraic equations. The simultaneous equations may be linear or non-linear depending upon the type of governing equations. Details about the application of FEM for the solution of the governing equations pertaining to lake hydrodynamics are discussed by Gallagher et al. (1973), Gallagher and Chan (1973), King (1982, 1982a & 1982b), Lin (1992), Lin and Young (1995), Young (1980 & 1999), Young et al. (1976a & 1976b), Young and Liggett (1977), and Young and Lin (1993). Standard textbooks on finite element method by Gallagher (1975), Segerlind (1984) or Zinkiewicz (1983 & 1977) can also be referred.

6. AN EXAMPLE PROBLEM

The governing equations developed for the study of lake hydrodynamics will be applied to a specific problem in order to understand the physics of the phenomenon. Details about the application of the mathematical model are discussed in the following sections.

6.1 Numerical scheme for moving boundary problems

Simulation of free surface flows is an interesting and challenging subject in the realm of computational hydraulics. The boundary conditions on the free surface or moving surface are not known *a priori* and hence it is difficult to numerically model such flow situations using conventional numerical schemes. In general, there are three approaches to deal with the dynamics of free surface or moving boundary flow problems, namely the Lagrangian, Eulerian, and Arbitrary Lagrangian-Eulerian (ALE) methods (Young and Lin, 1993).

In the purely Eulerian description (Harlow and Welch, 1965) the mesh is fixed in space, and is very difficult to treat the free surfaces or moving boundaries with such fixed mesh. On the other hand, a purely Lagrangian coordinate system follows the movement of the fluid particle and hence it is better off to deal with the free surface flows by a moving mesh. However, the mesh can get distorted very easily and hence this scheme is not convenient to model the free surface problems. On the contrast, Arbitrary Lagrangian-Eulerian (ALE) is based on the arbitrary movement of the reference frame, which is continuously rezoned in order to allow a precise description of the moving interfaces. Noh (1964) and Hirt et al. (1974) developed

the ALE scheme for FDM and later Donea et al. (1975 & 1982) and Hughes et al. (1981) developed it for FEM.

6.2 Justification for two-dimensional model

y The lake or reservoir hydrodynamics has to be analyzed using three-dimensional models in order to obtain realistic predictions for the natural environments. Further the numerical predictions have to be obtained over a period of a year or more. But the cost of three-dimensional computation is too expensive to be used for multiple year computations. Therefore, to simplify the problem, some appropriate assumptions are employed. For lakes or reservoirs with the characteristics of relatively narrow width and long reach, a laterally averaged two-dimensional model in the longitudinal-vertical profile is a good choice (Street, et al., 1977, Edinger and Buchak, 1979, Buchak and Edinger, 1982, King, 1985a, Karpik and Raithby, 1990). Because the most important features of the stratified lakes or reservoirs, such as the circulation gyres, density currents, as well as the thermal structures like thermocline process, will be retained in the longitudinal-vertical plane (Young et al., 1976a & 1976b, and Meyer, 1986). Other depth-averaged horizontal two-dimensional model can be applied to the shallow homogenous lakes or reservoirs. The laterally averaged two dimensional, longitudinal-vertical model will automatically rule out the consideration of the Coriolis forces for large lakes or reservoirs, since the Coriolis forces are relevant only in three dimensional modeling (Pedlosky, 1982). Furthermore, since there is no vortex stretching in two-dimensional flows, there is no need to include the Coriolis force effect into the governing equations.

6.3 Turbulence closure model

It is visualized that flows occurring in lakes or reservoirs are highly turbulent. One of the most difficulties in modeling the stratified lakes or reservoirs is the choice of turbulence closure model. There are different types of turbulence closure models such as the Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) or higher order turbulence closure models, such as the $k - \varepsilon$ models (Rodi, 1980) available in literature, for developing flows and thermal structures and its associated transport processes. However, for the sake of economical computations and practical engineering applications, in this example, the semi-empirical

formulation of turbulence closure models will be used. By the consideration of the influence of stability parameter, such as of the Richardson number, Munk and Anderson (1948) and Mamayev (1957) were able to propose their semi-empirical formulae of the vertical turbulent mixing for stratified flows.

6.4 Modified governing equations for moving boundary problem

The governing equations for the study of stratified lakes or reservoirs are the conservation laws of the fluid mass, linear momentum, and transport processes of heat and suspended sediment derived in section 4 and the equation of state, to link the constitutive relationship between density, temperature and sediment concentration. The equations become complete with the introduction of turbulence closure model. The continuity equation remains unaltered. Since the numerical model has to take care of the moving boundaries, mesh velocities in x and z directions are introduced in the convective terms of the momentum, energy and sediment transport equations from the ALE considerations. Due to the settling velocity of the sediments, the vertical velocity term in the convective part of the sediment transport equation will have an additional velocity term. With these modifications, the governing equations developed in section 4 are modified as follows (Lin, 1992):

a) Continuity equation (local)

$$\frac{\partial}{\partial x}(ub) + \frac{\partial}{\partial z}(wb) = q_i \quad (1)$$

b) Longitudinal momentum equation

$$\begin{aligned} \frac{\partial u}{\partial t} + (u - \tilde{u})\frac{\partial u}{\partial x} + (w - \tilde{w})\frac{\partial u}{\partial z} = & -\frac{1}{b} \frac{1}{\rho} \frac{\partial (bp)}{\partial x} \\ & + \frac{1}{b} \frac{\partial}{\partial x} (bK_x^M \frac{\partial u}{\partial x}) + \frac{1}{b} \frac{\partial}{\partial z} (bK_z^M \frac{\partial u}{\partial z}) + \frac{q_i(u_i - u)}{b} \end{aligned} \quad (2a)$$

c) Vertical momentum equation

$$0 = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g \quad (2b)$$

d) Heat transport equation

$$\begin{aligned} \frac{\partial T}{\partial t} + (u - \tilde{u})\frac{\partial T}{\partial x} + (w - \tilde{w})\frac{\partial T}{\partial z} = & \frac{1}{b} \frac{\partial}{\partial x} (bK_x^H \frac{\partial T}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z} (bK_z^H \frac{\partial T}{\partial z}) + \frac{q_i(T_i - T)}{b} \end{aligned} \quad (3a)$$

e) Suspended sediment transport equation

$$\begin{aligned} \frac{\partial C}{\partial t} + (u - \tilde{u}) \frac{\partial C}{\partial x} + (w - w_s - \tilde{w}) \frac{\partial C}{\partial z} = & \frac{1}{b} \frac{\partial}{\partial x} (b K_x^C \frac{\partial C}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z} (b K_z^C \frac{\partial C}{\partial z}) + \frac{q_i (C_i - C)}{b} \end{aligned} \quad (4a)$$

f) Equation of state for water to determine density in terms of temperature

$$\rho_w = 999.841 + 6.59585 \cdot 10^{-2} T - 8.45123 \cdot 10^{-3} T^2 + 5.29157 \cdot 10^{-5} T^3 \quad (5)$$

Ambient fluid density

$$\rho = (1 - C) \rho_w + C \rho_c \quad (6)$$

g) Turbulence closure model (Munk and Anderson, 1948)

$$K_z^M = K_0^M (1 + 10 R_t)^{-0.5} \quad (7a)$$

$$K_z^H = K_0^H (1 + 3.33 R_t)^{-1.5} \quad (7b)$$

$$K_z^C = K_z^H \quad (7c)$$

$$R_t = \frac{-g \frac{\partial \rho}{\partial z}}{\rho \left(\frac{\partial u}{\partial x} \right)^2} \quad (7d)$$

h) Mesh velocity

$$\tilde{u} = \frac{dx}{dt} \quad (8a)$$

$$\tilde{w} = \frac{dz}{dt} \quad (8b)$$

6.4.1 Velocity Boundary conditions

The above governing equations need appropriate initial and boundary conditions for obtaining the numerical solutions. For the lake hydrodynamic simulation, the initial conditions (IC) are unavailable in general. A more practical and feasible way is to execute a start-up run from any accepted initial conditions, generally from a motionless and homogeneous case or even from a potential flow condition. The associated boundary conditions (BC) are listed as follows:

1. The kinematic free surface BC

$$\frac{\partial z_\infty}{\partial t} + (u_\infty - \tilde{u}_\infty) \frac{\partial z_\infty}{\partial x} - w_\infty = 0 \quad (9)$$

2. The dynamic free surface BC

$$\tau_{\infty} = \mathfrak{I} \rho_a U_{10} |U_{10}| \quad (10)$$

3. At the bottom of lake or reservoir

$$\frac{\partial z_0}{\partial t} - \tilde{u}_0 \frac{\partial z_0}{\partial x} = 0 \quad (11)$$

4. At the solid boundaries (no-slip BC)

$$u = u_f, \quad w = w_f \quad (12)$$

where τ_{∞} = wind shear stress on the free surface; ρ_a = air density; ρ_w = pure water density; ρ_c = sediment density; $\mathfrak{I}$ = an empirical constant = 0.0026 in this study; U_{10} = wind speed at 10 m above the water surface; K_0^M, K_0^H = eddy viscosity and diffusivity for homogeneous lake and they are calculated using empirical relations, as functions of velocity of water within the eddies, the sizes of the eddies, wind shear and size of lakes; $\tilde{u}, \tilde{w}$ = mesh velocity in the ALE system for x and z direction respectively; w_s = settling velocity of suspended sediment; u_f, w_f = the specified boundary velocity in x and z direction respectively, such as the inflow/outflow velocity; the subscript '0' stands for the physical properties associated with the bottom of the lake and the subscript ' ∞ ' stands for the physical

properties with respect to the free surface. $Ri = -g \frac{\partial \rho}{\partial z} \left[\rho \left(\frac{\partial u}{\partial z} \right)^2 \right]^{-1}$ is the

Richardson number for the consideration of density stratification, $Ri=0$ in a homogeneous environment.

6.4.2 Temperature and sediment boundary conditions

As far as the boundary conditions of temperature and sediment concentration are concerned, the most commonly used boundary conditions are, the Dirichlet BC of specified temperature or concentration, or the Neumann BC of specified heat flux or flux of sediment concentration. On the free surfaces, the heat transfer on the air-water interface is specified by the Newton's law of cooling which represents the net heat flux between the water surface and atmosphere, as

$$q_{\infty} = h(T_e - T_{\infty}) \quad (13)$$

where q_{∞} = heat flux on the free surface; T_e = the equilibrium temperature; T_{∞} = surface water temperature; h = convective heat transfer coefficient.

6.4.3 Calculation of equilibrium temperature

The equilibrium temperature, T_e , is a calculated, hypothetical surface water temperature obtained by assuming a balance between the incoming and outgoing heat flux across the air-water interface. Under normal conditions at which the surface water temperature is higher than the equilibrium temperature, the lake or reservoir dissipates excess heat into the atmosphere and acts as a cooling body of water. However, during calm and hot summer days when the equilibrium temperature is higher than the surface temperature, the lake or reservoir gains heat from the atmosphere. Initially, the water at the surface of the lake will warm up and eventually the thermal stratification is formed in due course.

The heat transfer coefficient h depends on the thermo-physical properties of water at the surface of a lake. Since the properties of water will vary with temperature, h is evaluated by two different empirical formulae, one proposed by Rimsha and Dochenko (1958) for surface water temperature below 41° F (5 ° C) and the other proposed by and Brady et al. (1969), for surface water temperature above 41° F (5° C) and they are as given below:

The formula proposed by Rimsha and Dochenko (1958), applicable for $T_\infty < 41^\circ \text{F}$ (5°C):

$$h = 2.32 + \{1.56[8.0 + 0.35(T_\infty - T_a)] + 6.08U_2\}[\beta + 0.61] \quad (14a)$$

where

$$\beta = 0.612 - 0.0204T_m + 0.00049T_m^2 \text{ and } T_m = (T_a + T_\infty)/2$$

In the above, T_a is the air temperature and U_2 is the wind speed at 2 meter above the water surface. The formula proposed by Brady et al. (1969), applicable for $T_\infty \geq 41^\circ \text{F}$ (5°C):

$$h = 15.7 + (\beta + 0.26)(70 + 0.7U_2^2) \quad (14b)$$

where

$$\beta = 0.255 - 0.085T_m + 0.000204T_m^2$$

The equilibrium temperature, T_e , can be obtained using the following expressing.

$$T_e = T_a + \frac{I}{h} \quad (14c)$$

where I = Solar radiation and T_d = dew point temperature.

6.4.4 Hydrostatic pressure distribution

The assumption of hydrostatic pressure distribution enables us to integrate the vertical momentum equation (2b) to get the pressure field as:

$$p(x, z, t) = p_{\infty}(x, t) + \rho g(z_{\infty} - z) + \hat{p}(x, z, t) \quad (15)$$

$$\hat{p} = \int_{z_0}^{\infty} [\rho(x, z, t) - \rho_r] g dz$$

where p_{∞} = pressure on the water surface and is included for the consideration of the pressure depression on the water surface; ρ_r = the reference fluid density; $\hat{p}$ = perturbed pressure due to the density stratification and becomes equal to zero in a homogeneous environment. It is also related to the index for the measure of the potential energy associated with the stability of density stratification. The first two terms on the right hand side of equation (15) are called the barotropic or external pressure, which is governed by the atmospheric pressure and the positions of free surface and fluid. On the other hand, the integral term is named the baroclinic or internal pressure, which is dependent upon the internal density distribution by stratification.

Substituting the pressure gradient of $\partial p / \partial x$ from equation (15) into the horizontal momentum equation (2a), we get

$$\begin{aligned} \frac{\partial u}{\partial t} + (u - \tilde{u}) \frac{\partial u}{\partial x} + (w - \tilde{w}) \frac{\partial u}{\partial z} = & -g \left(\frac{\partial H}{\partial x} + S_0 \right) - \frac{1}{b\rho} \frac{\partial(b p_{\infty})}{\partial x} - \frac{1}{b\rho} \frac{\partial(b \hat{p}_{\infty})}{\partial x} + \frac{1}{b} \frac{\partial}{\partial x} (b K_x^M \frac{\partial u}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z} (b K_z^M \frac{\partial u}{\partial z}) + \frac{q_i (u_i - u)}{b} \end{aligned} \quad (16)$$

where $H = z_{\infty} - z_0$ = total water depth; $S_0 = \partial z_0 / \partial x$ = bottom slope.

6.4.5 Relation between water depth equation and continuity equation

In order to link the calculation of the water depth H and also to filter out the instability caused by the gravity wave on the water surface, the local continuity equation (1) together with the kinematic BC on the free surface of equation (9) and lake bottom of equation (11), are used to yield the following water depth equation.

$$\frac{\partial H}{\partial t} + \left(\frac{\overline{ub}}{b_{\infty}} - \tilde{\tilde{u}} \right) \frac{\partial H}{\partial x} + \frac{H}{b_{\infty}} \frac{\partial(\overline{ub})}{\partial x} = \frac{q_i}{b_{\infty}} \quad (17)$$

in which, $\overline{ub} = \frac{1}{H} \int_{z_0}^{\infty} ub dz$ and $\tilde{\tilde{u}} = \frac{1}{H} \int_{z_0}^{\infty} \tilde{u} dz$, where b_{∞} = surface width; $\overline{ub}$ = average lateral velocity flux; $\tilde{\tilde{u}}$ = average mesh velocity. It is noted that equation

(17) is a one-dimensional equation in x , since the z direction has already been integrated from the lake bottom to the surface.

Finally, to assure a better imposition of boundary condition for the vertical velocity, w , we have to differentiate the local continuity equation (1) with respect to z and get the following differentiated form for the continuity equation (King, 1985a):

$$\frac{\partial^2(ub)}{\partial x \partial z} + \frac{\partial^2(wb)}{\partial z^2} = \frac{\partial q_t}{\partial z} \quad (18)$$

In summary, equations (15), (16), (17), (18), (3a), (4a), (5) and (6) are the final governing equations to be solved for the unknown variables u , w , H or z_∞ , ρ , T , C , and p .

6.5 Numerical scheme

The Arbitrary Lagrangian-Eulerian (ALE) finite element method (FEM) is employed to discretize the space domain for obtaining the solution of the nonlinear partial differential governing equations (15-18) and (3a-6). To avoid the time step constraint of numerical instability, or the so-called Courant-Friedrichs-Levy (CFL) condition, an implicit finite difference method (FDM) is used for the time and finite element method (FEM) is used for the space domain, for solving the one-dimensional water depth equation (17). On the other hand, to achieve the most economic computation, other governing equations used to solve the longitudinal velocity, temperature, and sediment concentration equations (16), (3a) and (4a) are all discretized by the explicit finite difference scheme in time domain and by finite element scheme in space domain. The existence of free surface not only gives complicated boundary condition, but also restricts the severe time step used for the numerical computation. By this implicitness in one dimension and explicitness in two dimensions, we have circumvented the difficulty of the excessive computation. The advantage of this modeling strategy will become more obvious when a three dimensional modeling is undertaken.

To further increase the accuracy, consistency and stability of the numerical solutions, the concept of the so-called artificial balancing tensor diffusivity (BTD) is introduced in this study (Dukowica and Ramshaw, 1979). The objective of introducing the BTD model is to overcome the negative numerical damping caused by the advection dominated flows when the Gelerkin FEM is adopted (Gresho et al., 1984). As mentioned before, the variations of lake or reservoir storage and the corresponding fluctuation of free surface as well as the deposition/erosion of the

lake or reservoir bottom, are easily taken care by the ALE moving boundary technique.

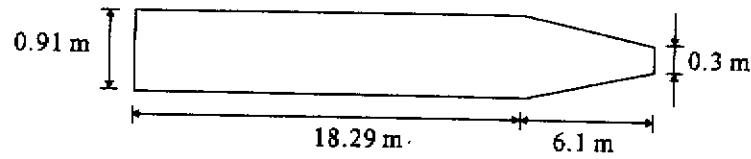
In the computational aspects of hydrodynamic processes of stratified lakes or reservoirs, in order to avoid the numerical instability caused by the internal gravity wave, the procedures used by Sun (1980) are adopted in the present study. Namely, the temperature and sediment concentrations are computed first, after that, velocity field and water depth or free surface are obtained. It is worthwhile to observe that the matrix equations for T , C , and u are all time-invariant as far as the matrix inversion is concerned. In addition, they all have the same property of symmetric matrix equation solver, except the calculation of water depth, H , which is nonlinear and needs Newton-Raphson iteration technique. All other variables are uncoupled and can be calculated in a similar way.

The final governing equations after time discretization are solved using Galerkin's weighted residual method of FEM. The resultant simultaneous algebraic equations are solved using available standard routines to obtain the variations of temperature, velocities, concentration, density and free surface, in space and time.

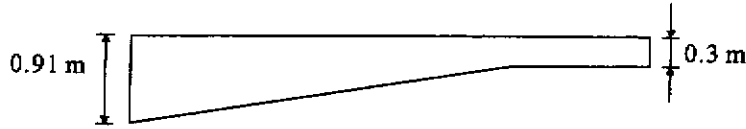
6.6 Model verification

The mathematical model developed has to be verified for accuracy so that it can be employed for hydrodynamic analysis of real lakes. The U.S. Army Corps of Engineers has carried out a number of experiments on the Generalized Reservoir Hydrodynamics flume, which is designed to test the behaviors of reservoir hydrodynamics for gravitational underflow. The reservoir data generated in this flume have been used to verify a number of models (Johnson, 1980 & 1981, King, 1982, and Karpik and Raithby, 1990). Hence the two-dimensional model developed in the present work is used to simulate the Generalized Reservoir Hydrodynamics flume experiments for the verification of the model.

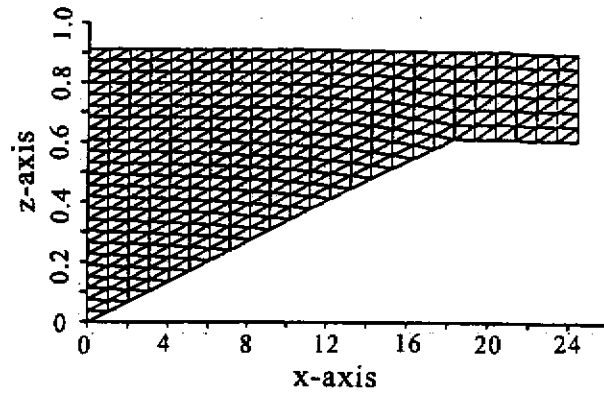
The length of the flume is 24.39 m and it varies in depth from 0.3 m at its inflow end to 0.91 m at its outflow end. It has two different cross-sections; the upper section 1, which is 6.1 m long, has a horizontal bottom and linear variation in width from 0.3 m to 0.91 m; the lower section 2 has a constant width of 0.91 m, and a bottom dropping of 0.61 m over its 18.2 m length. Refer Figs. 3a & 3b for the general layout and Fig. 3c for the associated FEM mesh, which contains 612 linear triangular elements and 342 nodes in the longitudinal-vertical profile.



(a) Plan view



(b) Side view



(c) Finite element mesh

Fig. 3. Schematic diagram of Waterways Experiment Station GRH flume (a) plan view, (b) side view and (c) the finite element mesh.

In order to simulate the underflow type of density current due to the inflow of water at 16.67°C , the flume is filled with water at a uniform temperature of 21.44°C . The water is introduced under a baffle and allowed to flow into the system over the lower 0.15 m region. The outflow of water is removed from the outlet located on the dam 0.15 m from the bottom. The inflow rate of water is the same as the outflow at $0.00063\text{ m}^3/\text{s}$.

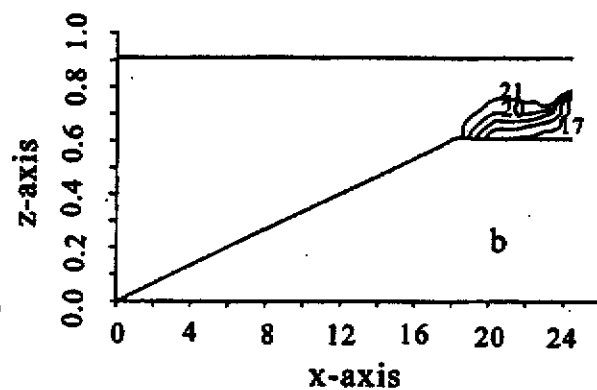
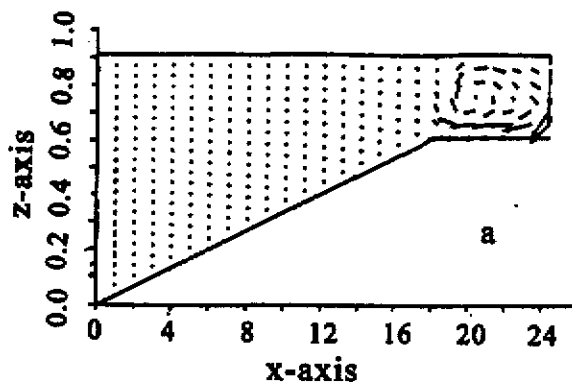


Fig. 4. Structures of (a) density current, and (b) temperature distribution of GRH flume at $t=4$ min.

Because the inflow temperature is lower than the ambient temperature, the underflow type of density current is expected from simulation. The velocity and temperature fields obtained by numerical simulations at time $t=4$ min. are shown in Figs. 4a & 4b, respectively. It is striking that the velocity and recirculation gyre in the inflow are established quickly, as compared with the other homogenous region where the velocity is very low. Thus the model is capable of predicting the establishment of a density underflow. As time goes by, the density current advances along the bottom with the recirculation gyre moving rapidly towards the dam.

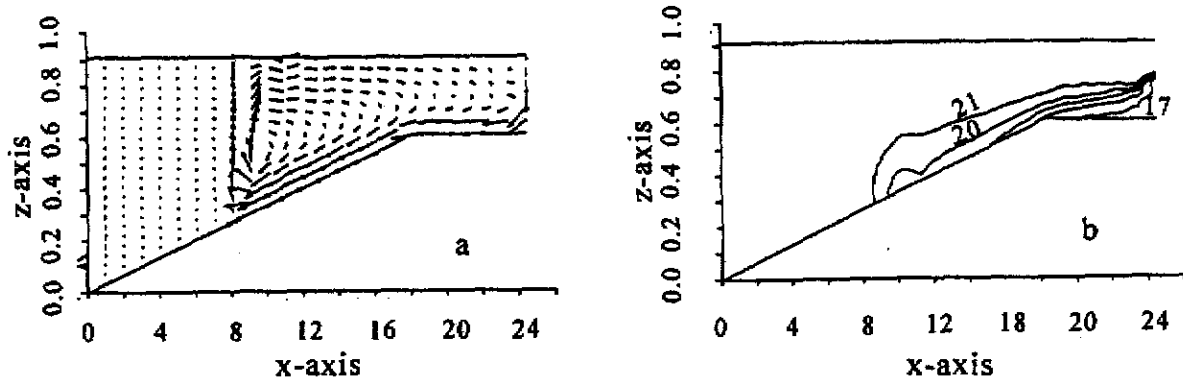


Fig. 5. Structures of (a) density current and (b) temperature distribution of GRH flume at $t=14$ min.

Figure 5 depicts the transient processes of the structures of density current at $t=14$ min. Because the vertical turbulent mixing is reduced by the buoyancy effect, the temperatures vary only in the region near the bottom. After the density current arrives at the dam at $t=50$ min, the flow field becomes more stable and the recirculation gyre occupies the entire region of the flume, as illustrated in Fig. 6.

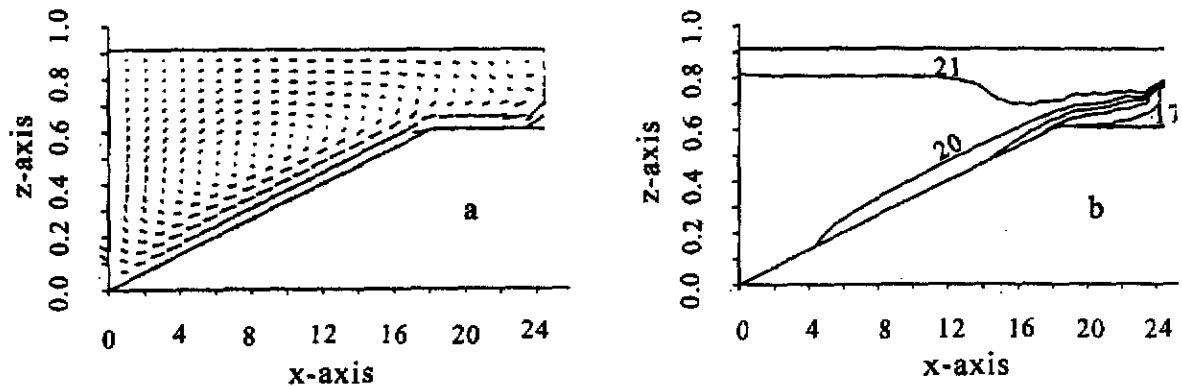


Fig. 6. Structures of (a) density current and (b) temperature distribution of GRH flume at $t=50$ min.

Figure 7 shows the comparison between the numerically calculated and experimental results of the progress of the propagation speed of the density current front. It is interesting to note that the simulated and observed results are very consistent. The numerical results show much smoother variation than the laboratory measurements. However the general trend shows good agreement even for very small velocity in the order of 10^{-2} m/s.

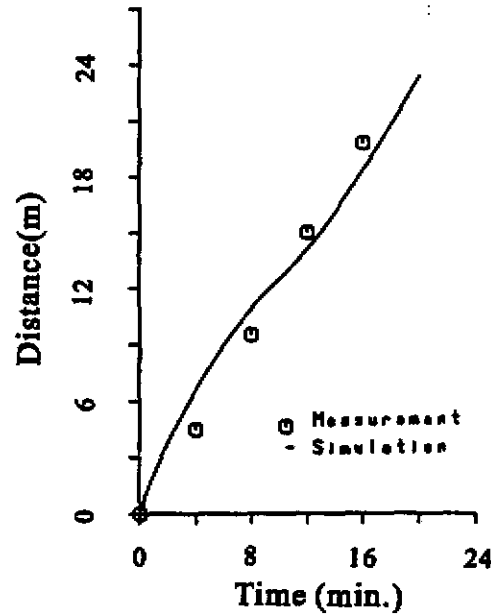


Fig. 7. Comparison of propagation speed of density current front of GRH flume.

6.7 Model application to Te-Chi reservoir

In this section we will present the application of the model to a real reservoir problem.

6.7.1 Description of the Te-Chi reservoir

The usage of measured field data is to test and verify the merit and credibility of the present model to the practical engineering applications. After having the model calibrated and verified with the laboratory data, now the model can be used for the simulations of hydrothermal characteristics of real reservoirs. The Te-Chi reservoir, located at central Taiwan is chosen as a pilot test site. The Te-Chi reservoir surrounded by high mountainous basins in an isle is a very long, narrow and deep reservoir, as shown in Fig. 8a. Due to these topographic

characteristics, it is found to be an ideal reservoir suitable for a laterally averaged two-dimensional stratified lake model simulation. Its longitudinal length is about 13 km, with a major inflow coming from the upstream of the Ta-Chia River and nine other river tributaries. These rivers have been considered as the minor lateral inflow sources. Figure 8b shows the longitudinal-vertical profile and its variation of lateral width. The bottom of the dam is located at 1268 m above the sea level and the maximum water depth is 140 m, with a total storage capacity of $2.5 \times 10^8 m^3$. The intake of selective withdrawal for water utilities is located at a height of 75 m above the bottom of the dam. Numerical simulations for a total period of two years, from 1984 to 1985, are performed and compared with the measured field data.

6.7.2 Hydrological input data

The hydrological input data required for the numerical simulation of the 1984 annual cycle of the reservoir are: the rate of major and minor lateral inflows, outflow rate, and the corresponding inflow temperatures and sediment concentrations. The annual inflow into the reservoir and outflow from the reservoir for the year 1984 are depicted in Figs. 9a and 9b respectively. In dry seasons, that is, in autumn and winter seasons, the inflow rate is very small. On the other hand in spring and summer seasons due to the storms or typhoon rainfalls, the inflow rate is very high. The maximum inflow of $300 m^3/s$ occurs at 156th day of 1984 (January 1 corresponds to day 1 of the year) when the reservoir was assaulted by a typhoon storm of nine days from 150th to 158th day. The watershed lies in the area of vast high mountains, which lie 3000 m above sea

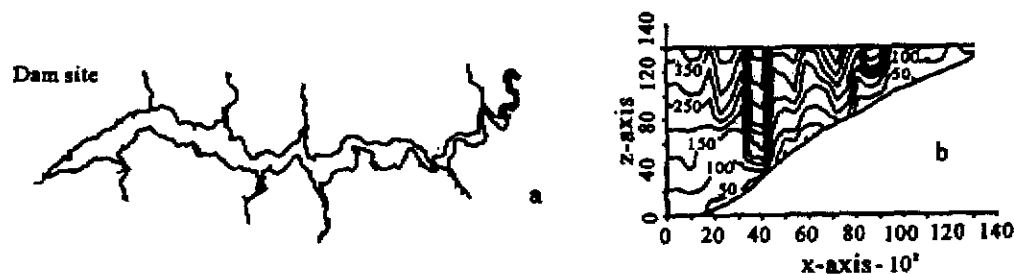


Fig. 8(a). Plan view and (b) longitudinal-vertical profile and width contour of the Te-Chi reservoir.

level. The surface temperature, inflow temperature, as well as intake temperature for the year 1984 are depicted in Fig. 9c. It is interesting to observe that the inflow temperature is always lower than the ambient surface temperature of the reservoir, since the Te-Chi reservoir is located on a high mountain area. Furthermore, by a

regression analysis from the measured data, the sediment inflow concentration has been correlated to the inflow discharge by an exponential function, which will provide the boundary condition for the sediment concentration equation.

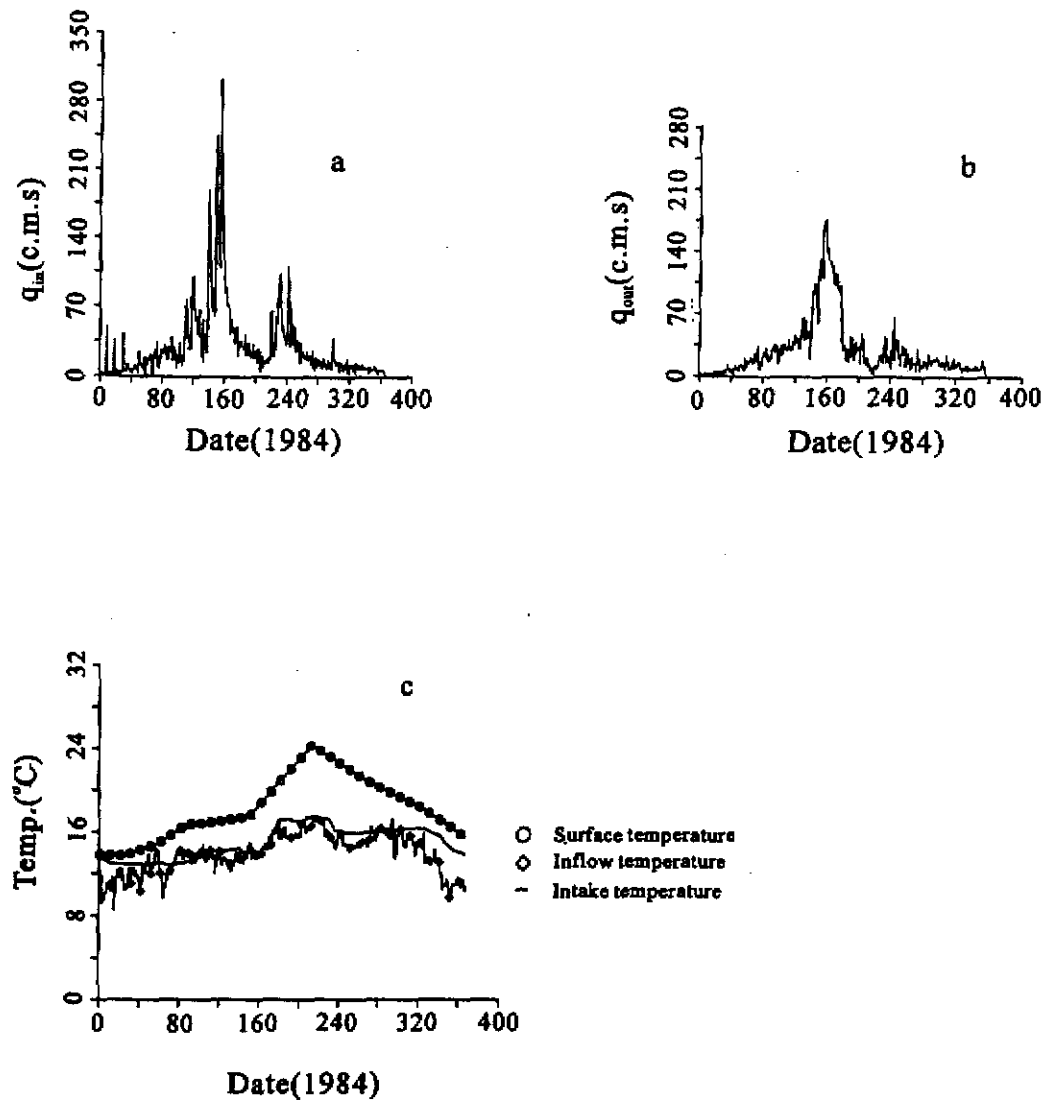


Fig. 9 (a). Inflow, (b) outflow and (c) surface temperature, inflow temperature and intake temperature in 1984 of the Te-Chi reservoir.

6.7.3 Meteorological input data

In addition to the hydrological data, the meteorological data such as the cloud cover, dry bulb temperature, dew point temperature, wind speed, wind direction and solar radiation are also required as input data. The heat flux on the water surface can be obtained by using a thermal equilibrium model from the meteorological data. This model is conceptually based on Newton's law of cooling,

assuming convective heat transfer at the water surface. This law states that the convective heat transfer at a surface is the product of a heat transfer coefficient and the difference between the surface water temperature and the equilibrium temperature obtained from equation (13). The heat flux received by the Te-Chi reservoir for the year 1984 is calculated using the equilibrium temperature model. The heat flux thus calculated is used as the boundary condition at the water surface for the solution of the heat transport equation. Finally, the wind shear stress at the water surface, which is one of the boundary conditions for the momentum equation, is computed from the wind speed by an empirical formula given by equation (10).

6.7.4 Computational domain of the Te-Chi reservoir

The computational domain of the Te-Chi reservoir is discretized into 950 linear triangular elements with 522 nodes. The finite element mesh will move along with the variations of reservoir storage including the free surfaces, with the usage of the ALE method. The types of meshes used at the highest and lowest water levels are shown in Figs. 10a & 10b, respectively.

6.7.5 Results and discussion

Figure 11 shows the comparison between the variations of water levels calculated using the present numerical model and the measured values for the year 1984. The calculated water level is very consistent with the observed one, thus the mass conservation in this model is very well proved. The selective comparisons of the calculated and measured daily water temperature profiles at different cross sections for the year 1984 during the months of January, February, March, April, May and September are illustrated in Figs. 12 & 13. The matching between the calculated and the measured results is excellent except for the month of May,

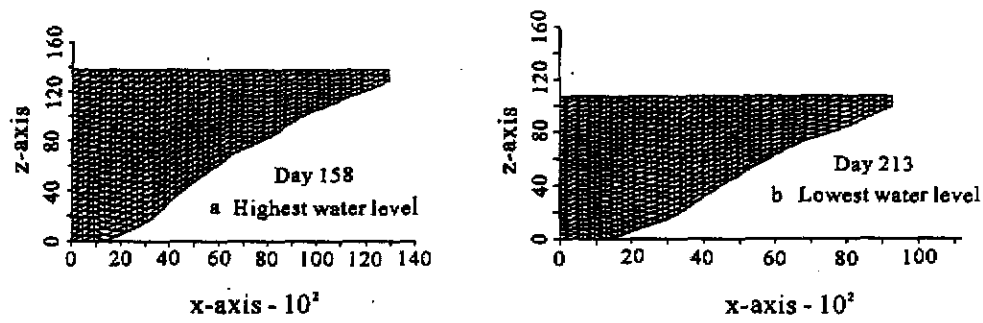


Fig. 10. Moving adaptive finite element grid system of (a) highest water level and (b) lowest water level in 1984 of the Te-Chi reservoir.

where some small deviations are observed. This discrepancy occurs both at the layers of epilimnion and thermocline and more at the layer of epilimnion.

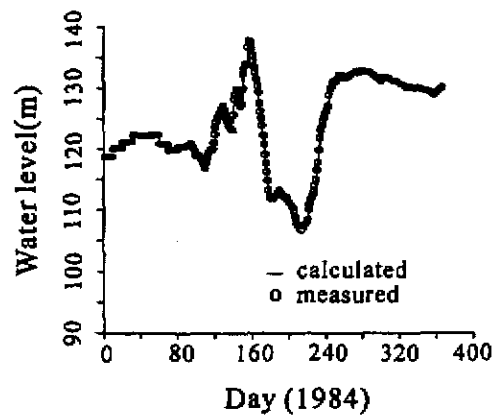


Fig. 11. Comparison of calculated and measured water level in 1984 of the Te-Chi reservoir.

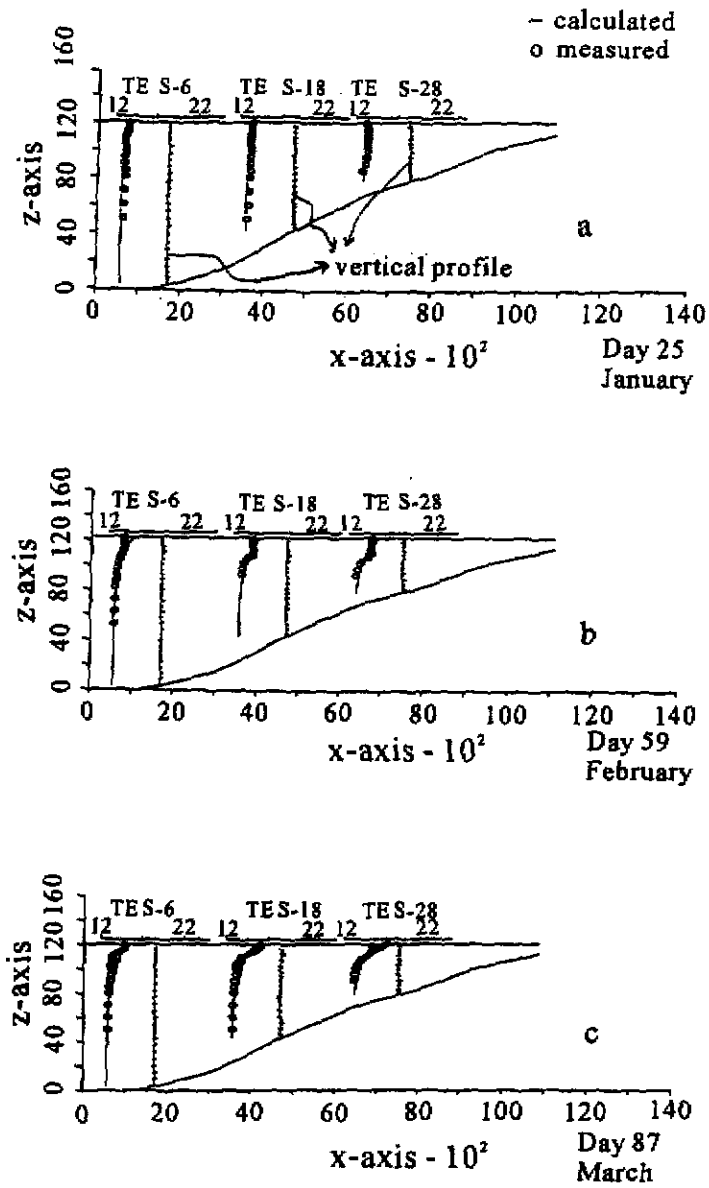


Fig. 12. Comparison of calculated and measured daily temperature profiles at a particular day during the months of (a) January, (b) February and (c) March in 1984 of the Te-Chi reservoir.

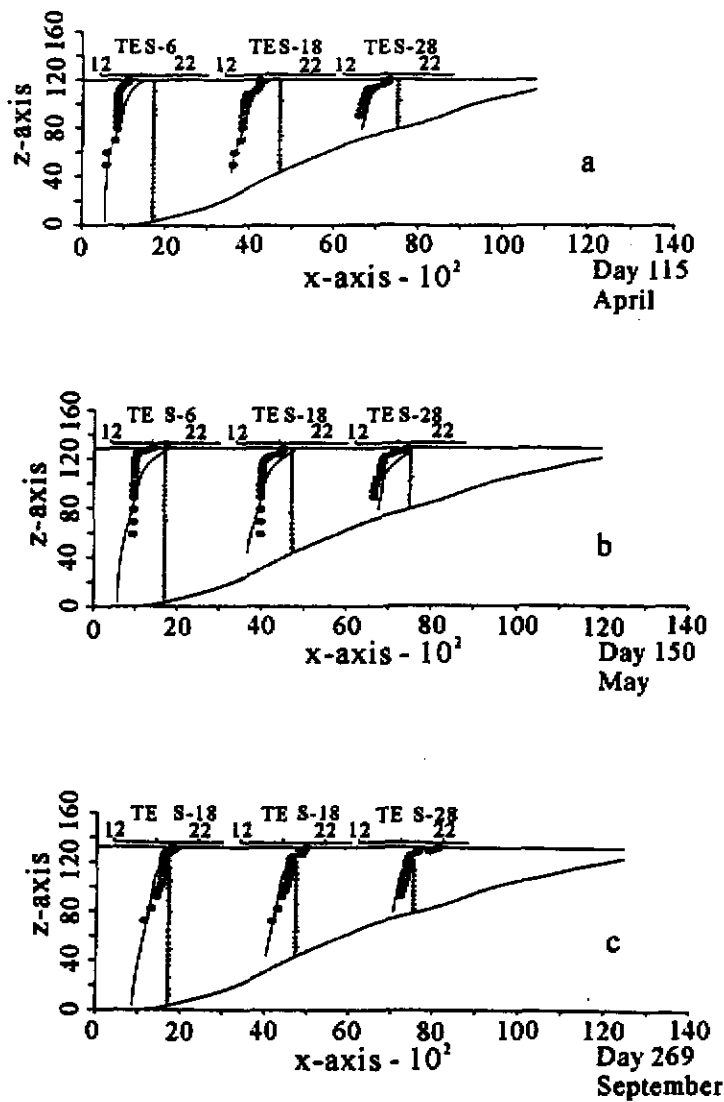


Fig. 13. Comparison of calculated and measured daily temperature profiles at a particular day during the months of (a) April, (b) May and (c) September in 1984 of the Te-Chi reservoir.

As can be observed from Fig. 9c, the inflow temperature of water into the reservoir is always lower than that of the reservoir for the year 1984. Hence an underflow type of density current is expected. Later, the layer of underflow is transformed into turbidity current, due to the presence of suspended sediments in the inflow. When the inflow rate is very small, the strength of turbidity current is very weak. However, while the inflow is very high, as occurring in the event of rainfall during storms, the turbidity current becomes very strong. The heavy rainfalls due to storms occurred from 150th day to 158th day for the year 1984. Figure 14 shows the density currents, temperature and sediment concentration distributions for the 150th day of the year. For the 150th day as depicted in Fig. 14b,

the highest temperature is about 18 °C located at the water surface and the lowest one is about 12 °C occurring near the bottom of the dam. The river inflow temperature is about 15° C which lies between the temperature of the epilimnion and the hypolimnion of the reservoir.

The sediment concentration of the river inflow is about 300 ppm. This results in a higher concentration range near the bed of the reservoir about 6 km away from the dam. The other sediment concentrations are lower than 50 ppm as shown in Fig. 14c. It is worth noting that the boundary condition of complete deposition at the reservoir bed has been used for the sediment transport equation. That is, for any sediment particle being carried into the reservoir, it will deposit at the bed with its settling velocity whenever it touches the bed and does not have any opportunity to be picked up again. Therefore, the sediment concentration decreases along the downstream direction. Due to the higher concentration and lower temperature of river inflows, the density of river inflows is higher than the density of upper layer of reservoir water body. Hence, buoyancy induced plunging phenomenon occurs after the river inflow comes into the reservoir and the underflow density current travels very fast downstream along the bed. Due to the sediment deposit at the bed, the concentration decreases along the downstream direction and the strength of underflow also decreases. Moreover, the selective withdrawal and the type of temperature distribution will affect the density current also. Therefore, the density current leaves the bed about 6 km away from the dam, and then the interflow occurs and advances horizontally to the intake of the selective withdrawal. Besides, due to the underflow and interflow of density currents, there are two circulation gyres generated, in which the upper circulation gyre is stronger than the lower one, as indicated in Fig. 14a.

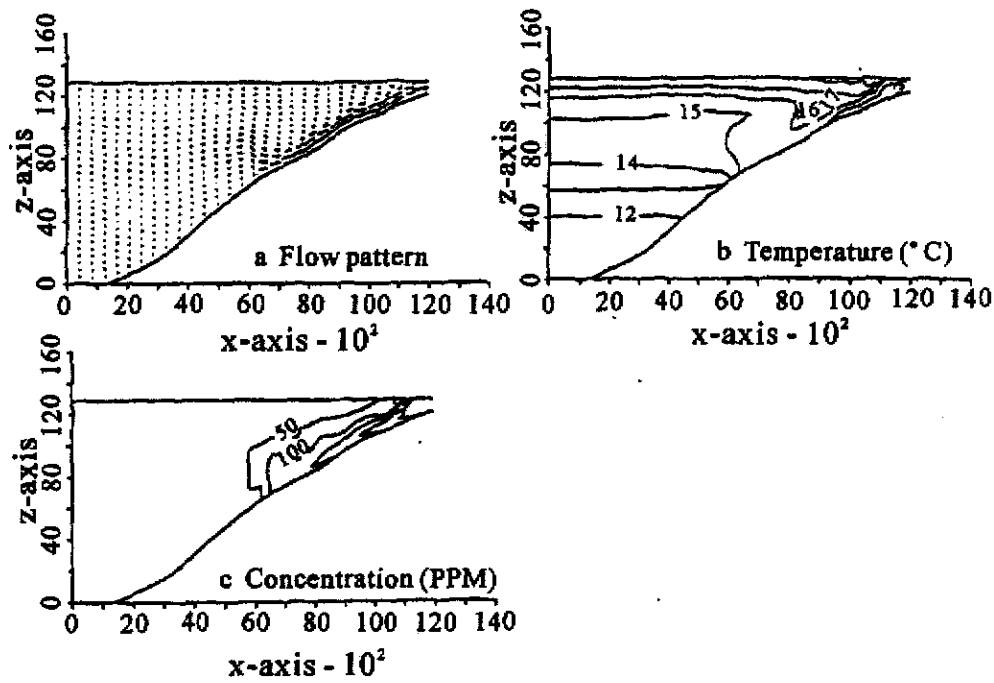


Fig. 14. Structures of (a) density current, (b) temperature, and (c) sediment concentration distributions on 150th day in 1984 of the Te-Chi reservoir.

7. PERSPECTIVE RESEARCH AREAS IN LAKE HYDRODYNAMICS

Real lakes or reservoirs do not satisfy the conditions of laterally averaged two-dimensional models. Hence three-dimensional lake or reservoir model is inevitable when we consider lakes or reservoirs with similar longitudinal and lateral scales, or large lakes or reservoirs, such as the Great Lakes in the northern America. In such models the Coriolis forces have to be included. Also a three-dimensional stratified lake or reservoir model (Simons, 1973) is generally desirable when water quality modeling is concerned.

7.1 Three-dimensional modeling

As far as the sophistication of the level of three-dimensional modeling is concerned, there are two types of models, the 3D Ekman hydrostatic model and the complete Navier-Stokes model. In the 3D Ekman hydrostatic model, the nonlinear inertial force terms as well as the horizontal diffusion terms are considered as secondary effects and are neglected in the model development (Young et al., 2000a). Boundary element method has also been used to reduce the dimension of the

three-dimensional stratified flow modeling. For more details, the work of Young et al. (2000a) can be referred. Another alternative is the extension of the present model to the 3D stratified lake or reservoir model. Of course, the inclusion of Coriolis force in the horizontal momentum equation is necessary. In the mean time, one more horizontal momentum equation has to be added. Three-dimensional modeling is triggered by the need for more accurate predictions of water quality constituents and a better representation of the higher order hydrodynamic processes.

7.2 Improved version of turbulence closure models

In the complete Navier-Stokes 3D stratified lake or reservoir model, the primitive variable approach using the velocity and pressure as major unknowns, is commonly used. The semi-empirical formula or higher order parameter like $k - \epsilon$ model (Spraggs and Street, 1975, and King, 1985b) can be used for the turbulence closure model. However, it is observed that due to the advancement of modeling techniques and computer capacity, more comprehensive turbulence closure models such as DNS or at least LES are becoming more popular and feasible nowadays.

7.3 Velocity-Vorticity formulation

The concept of using velocity and vorticity as primary variables or the so-called velocity-vorticity formulation has been proposed by the author as one of the methods to analyze lake hydrodynamics and some promising programs are underway. For further details the work of Young (1999) and Young et al. (2000b) can be referred. Both finite element and boundary element methods are employed to perform the three-dimensional homogeneous, as well as stratified flow modeling by the velocity-vorticity formulation.

Compared to the traditional 3D primitive variables, the velocity-vorticity formulation allows for an easier three-dimensional modeling. Initially, the Poisson type of equations are considered as the governing equations for the velocity field and once the vorticity field is known, the same equations can be used for both homogeneous and stratified environments. The velocity field is governed by the following Poisson velocity vector equation, which is derived by taking the curl operator of the definition of the vorticity through the usage of the fluid incompressibility.

$$\nabla^2 \bar{\mathbf{u}} = -\bar{\nabla} \times \bar{\boldsymbol{\omega}}$$

where $\bar{\boldsymbol{\omega}} = \bar{\nabla} \times \bar{\mathbf{u}} = \text{vorticity}$.

The vorticity transport equations are obtained by taking the curl operator of the momentum equation of the Navier-Stokes equations and are given as below:

$$\frac{\partial \bar{\boldsymbol{\omega}}}{\partial t} + [(\bar{\mathbf{u}} - \bar{\tilde{\mathbf{u}}}) \cdot \bar{\nabla}] \bar{\boldsymbol{\omega}} = \nu \nabla^2 \bar{\boldsymbol{\omega}} + [(\bar{\boldsymbol{\omega}} + \Omega \bar{\mathbf{k}}) \cdot \bar{\nabla}] (\bar{\mathbf{u}} - \bar{\tilde{\mathbf{u}}}) - \bar{\nabla} \times \left(\frac{\rho}{\rho_r} g \bar{\mathbf{k}} \right)$$

where $\Omega = \text{earth rotational speed}$. The vorticity transport equation provides a clear and thorough picture about the generation, advection, diffusion and dissipation of all the vorticity in the stratified environments. For example, the

Coriolis force effect, $\Omega \bar{\mathbf{k}}$ and the density stratification effect $\bar{\nabla} \times \left(\frac{\rho}{\rho_r} g \bar{\mathbf{k}} \right)$ can be

easily compared with the homogeneous and the non-rotating systems. Therefore, a better dynamic feature can be obtained from this approach. Finally, if the DNS model can be achieved as turbulence closure model, there is no need to provide those turbulent exchange coefficients and DNS will render all the necessary information for the stratified lakes or reservoirs. Even if we cannot afford a DNS model, a LES model may not be a bad substitute at the present stage. It is hoped that in the near future, the DNS model will become available, to be incorporated in a complete 3D stratified lake or reservoir model. With such models, the assumptions and approximations to be made will be reduced and a much better understanding of the hydrodynamics of 3D stratified lakes or reservoirs can be achieved, for both academic research and engineering applications.

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LIST OF FIGURES

- Fig. 1. Schematic diagram of a stratified lake or reservoir showing the transport processes of mass, momentum, heat, and sediment
- Fig. 2. (a) The coordinate system and geometry layout of a stratified lake or reservoir with free surface and moving bed, 2 (b)Elemental control volume
- Fig. 3. Schematic diagram of Waterways Experiment Station GRH flume (a) plan view, (b) side view, and (c) the finite element mesh
- Fig. 4. Structures of (a) density current, and (b) temperature distribution of GRH flume at $t=4$ min.
- Fig. 5. Structures of (a) density current, and (b) temperature distribution of GRH flume at $t=14$ min.
- Fig. 6. Structures of (a) density current, and (b) temperature distribution of GRH flume at $t=50$ min.
- Fig. 7. Comparison of propagation speed of density current front of GRH flume
- Fig. 8. (a) Plan view, and (b) longitudinal-vertical profile and width contour of the Te-Chi reservoir
- Fig. 9 (a) Inflow, (b) outflow, and (c) surface temperature, inflow temperature and intake temperature in 1984 of the Te-Chi reservoir
- Fig. 10. Moving adaptive finite element grid system of (a) highest water level, and (b) lowest water level in 1984 of the Te-Chi reservoir
- Fig. 11. Comparison of calculated and measured water level in 1984 of the Te-Chi reservoir
- Fig. 12. Comparison of calculated and measured daily temperature profiles at a particular day during the months of (a) January, (b) February and (c) March in 1984 of the Te-Chi reservoir
- Fig. 13. Comparison of calculated and measured daily temperature profiles at a particular day during the months of (a) April, (b) May, and (c) September in 1984 of the Te-Chi reservoir
- Fig. 14. Structures of (a) density current, (b) temperature, and (c) sediment concentration distributions on 150th day in 1984 of the Te-Chi reservoir

8. NOMENCLATURE

b	lateral width (m)
C	concentration of suspended sediment (kg/m^3); specific heat capacity (J/kgK)
e	specific internal energy (J/kg)
E	total internal energy (J)
g	acceleration due to gravity (m/s^2)
h	convective heat transfer coefficient ($\text{W/m}^2\text{K}$)
H	water depth (m)
I	solar radiation (W/m^2)
$\dot{m}$	mass flow rate (kg/s)
K	turbulent parameter (eddy viscosity or eddy diffusivity) (m^2/s)
p	pressure (N/m^2)
$\hat{p}$	perturbed pressure due to density stratification (N/m^2)
q	lateral flow ($\text{m}^3/\text{m}^2\text{s}$); heat flux (W/m^2)
Q	total heat energy (J)
t	time (s)
T	temperature (K)
u	flow velocity in the longitudinal direction (m/s)
$\tilde{u}$	mesh velocity in the longitudinal direction (m/s)
$\bar{\tilde{u}}$	average mesh velocity (m/s)
$\overline{ub}$	average lateral velocity flux (m^2/s)
U	wind velocity (m/s)
w	flow velocity in the vertical direction (m/s)
$\tilde{w}$	mesh velocity in the vertical direction (m/s)
W	total work done (J)
x	longitudinal Cartesian coordinate (m)
z	vertical Cartesian coordinate (m)

Non-dimensional numbers

R_i	Richardson number
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Greek letters

β	constant
ρ	density (kg/m^3)
τ	shear stress (N/m^2)

β an empirical constant (0.0026)

Subscripts

a	air
c	sediment
cv	control volume
d	dew point temperature
e	equilibrium
f	inflow/outflow
in	into the control volume
∞	free surface condition
0	bottom condition
out	out of the control volume
s	settling
t	lateral flow
w	pure water
x	longitudinal direction
2	at 2m above the free water surface
10	at 10m above the free water surface
z	vertical direction

Superscripts

C	eddy diffusivity for sediment transport
H	eddy diffusivity for heat transport
M	eddy viscosity

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Two-dimensional simulations of density currents due to sediment-laden inflow into a thermally stratified reservoir

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Abstract

A two-dimensional laterally averaged hydrodynamic model is developed to study the density currents developed in a reservoir due to inflow with sediment concentration. The two-dimensional Navier-Stokes equations are simplified for the stratified flow with free surface under the assumptions of fluid incompressibility, hydrostatic pressure distribution and the Boussinesq approximation. The governing equations are solved using the Galerkin's weighted residual finite element method. The change in the mesh pattern of the computational domain during simulation is taken care of by using Arbitrary Lagrangian-Eulerian method (ALE). The model developed was validated with the experimental results obtained for gravitational underflows of GRH flume of US Army Corps of Engineers. The model is then applied to simulate the field scale of one-year annual cycles of the stratified man-made lake of the Te-Chi reservoir located at central Taiwan. The different regimes of density currents such as, turbidity current, underflow and interflow are predicted for sediment-laden inflow during the days of heavy rainfall due to storm. The numerical results compare favorably well with the observed field measurements.

Introduction

The study of density currents in stratified reservoirs plays an important role in fresh water supply from a reservoir. A reservoir is naturally stratified due to its interaction with atmospheric conditions by means of heat, mass and momentum transport. The inflow water may contain suspended and dissolved solids. Depending upon the temperature and strength of stratification, the sediments or contaminants will be transported to various portions of the stratified reservoir. The outflow from the reservoir is taken at various heights depending upon the applications. In order to ensure the quality of water, the knowledge about the response of density current for various external conditions is essential. The hydrodynamics of stratified lake is a complex phenomenon. Because, the interaction of a reservoir with its surroundings results in turbulent nature of flow circulations varying with space and time in different magnitudes. The salient characteristics of the stratified flows are hydrodynamic instability problems associated with the generation of circulation gyres as well as the formation, maintenance and erosion of thermocline between epilimnion and hypolimnion.

Mathematical modeling of lake hydrodynamics supported by experimental data, has enabled the researchers in this field to understand the physics of the phenomenon in a better way over the years.

In the present study, a laterally averaged two-dimensional model has been used for the simulation of different flow regimes due to the inflow of sediment-laden water. The model is capable of simulating the moving free surface of water during the density current dynamics. The model developed has been validated with the experimental results of GRH flume at the U.S. Army Corps of Engineers. The model is applied to study the hydrodynamics of Te-Chi reservoir situated in central Taiwan. This reservoir is chosen for the present analysis since it satisfies the characteristics of a laterally averaged reservoir. Focus is concentrated on the study of density currents generated in the reservoir due to maximum inflow during the period of heavy rains due to storms. During summer, the inflows to the reservoirs in Taiwan vary widely due to heavy rains caused by storms. Hence knowledge about the response of the lakes is essential during these heavy rain periods for taking the precautionary measures.

For lakes or reservoirs with small aspect ratio (Height/Length), a laterally averaged two-dimensional model (Street, et al., 1977; Edinger and Buchak, 1979; Buchak and Edinger, 1982; King, 1985a; Karpik and Raithby, 1990; Gu et al., 1996; Chung and Gu, 1998; Choi, 1998) can be used to study the density currents. The difference between the density of inflow water and the reservoir water results in a density current. The density current produces different flow regimes such as underflow, plunge, interflow and overflow during the inflow of water into the reservoir. Density flows have been studied for various applications (Akiyama and Stefan, 1984; Alavian et al., 1992). The intrusion or interflow in a linearly stratified reservoir caused the transport of contaminants closer to the surface near the diurnal thermocline, in contrast to the expectation of transport to the bottom of the lake (Fisher and Smith, 1983; Alavian et al., 1992). When the stratification in a reservoir exists for a longer period, the deeper water, i.e. hypolimnetic water is cut off from the atmosphere for any type of interactions. Situations may arise wherein the stratification needs to be altered in order to meet the required outflow conditions (Schladow and Fisher, 1995). Alavian and Ostrowski (1992) proposed a method to control the inflow and outflow from the TVA reservoir in order to meet the stringent condition of outlet water temperature for a power plant. They used a simple two-dimensional model calibrated with field data. If the objective of the study is only to determine the vertical temperature of the lake, where measurements are not available, a simple one-dimensional model can be described using the energy equation for the water column (Hondzo and Stefan, 1993).

The sediment-laden underflow is sometimes called turbidity current. There exists a difference between the density of suspended sediment and the lake water. This causes a reduction in the gravitational acceleration resulting in the motion of turbidity current (Choi,

1998). Lee and Yu (1997) conducted a detailed experimental work to study the characteristics of plunge flow due to turbidity current, without temperature stratification. It is the density difference, which affected the plunge phenomenon rather than the presence of the suspended particles. Chung and Gu (1998) used a laterally averaged two-dimensional hydrodynamic model to study the density currents due to contaminant dispersion in a stratified reservoir. They used hydrostatic pressure equation in the place of vertical momentum equation. They observed that the processes such as plunging, separation, and intrusion occur as a result of contaminant dispersion and they are affected mainly by the negative buoyancy and ambient stratification.

The wind blowing over the water surface of a reservoir also affects the density current stratification. The wind shear acting at the surface causes vertical turbulent mixing of the upper layer. This results in the entrainment of the lower denser fluid into the upper layer (Chu and Soong, 1997; Spiegel and Imberger, 1980). This in turn affects the buoyancy and the horizontal velocity at the layer of thermocline (Kranenburg, 1985) such that the turbulence is suppressed below the layer of thermocline. Hug and Stretch (1995) suggested that the vertical transport could be expressed in terms of dissipation rate of the flow, which is a function of the kinematic viscosity of the fluid and buoyancy frequency. They also found that there might be a critical dissipation rate below which all scales of turbulent motion will be suppressed by buoyancy forces. Sullivan and List (1994) conducted experiments in a laboratory water channel to study mixing at a density interface embedded in a turbulent shear flow. Based on the value of local mean shear Richardson number, the mixing is dominated either by Kelvin-Helmholtz instabilities or shear driven wave breaking. Falconer et al. (1991) studied the wind-driven circulation of a small lake using a three-dimensional hydrodynamic model, neglecting the inflow and the outflow. The drag coefficient C_D in the wind-shear stress expression was assumed to be constant and equal to 0.0026 as given by Munk (1955), since many complex non-linear relationships between C_D and wind speed, gave unrealistic results. They also suggested that future research should concentrate on the development of a more precise and less empirical model for the description of vertical transfer of turbulent momentum. Hsu (1986) also observed that although C_D increases with wind speed, the variation is not linear and C_D depends upon the wave characteristics. Guting and Hutter (1998) used a first order k- ϵ closure model in their study on wind-induced circulation in lakes. They felt that the assumption of constant vertical eddy viscosity does not reflect the true turbulent activity with sudden change in wind speed. The wind blowing over the water surface is not constant. The flow characteristics at the water surface that is caused by turbulent mixing, varies depending upon the strength of the wind. The continuous variation of the flow pattern with varying wind strength cannot be modeled by assigning a constant value for the vertical eddy velocity. With the use of first order k- ϵ model, the turbulent kinetic energy and dissipation

can be computed using the turbulent viscosity obtained by solving the transport equations. In all the works on lake hydrodynamics till now, the temperature regimes of lake sediments has been neglected. Fang and Stefan (1998) has found from their analysis that the heat fluxes between lake water and sediments can be substantial to such an extent causing the shallow lake water warmer by 1-2 °C in the absence of atmospheric heating, i.e. under thick winter cover. Even though number of works is carried out on lake circulation taking into the effect of higher turbulent closure model, three-dimensional effect etc. not much research has been carried out to study the effect of sediment-laden density flow including the energy equation. During a later inflow into a lake, mass, momentum, energy and concentration are also transported into the lake. The interactions of these quantities with the stratified lake completely alter all the transport mechanisms. The present work aims at studying the effect of these transport mechanisms on the density current in a stratified lake. The approach followed for the present analysis is discussed in the following sections.

Mathematical model

A real lake or reservoir is a three-dimensional entity, having complex geometry at the basin. The real physical processes that are taking place in a lake are highly complex and non-linear due to its interaction with the surroundings in varied magnitude. A mathematical model is just a description of "how things work" with our knowledge of physical systems and our understanding. Making assumptions in building models are very common in order to attack a problem starting with a simple tool. In the case of mathematical description of lakes, a lake can be treated as a two-dimensional system when the depth to length ratio is very small and the lake is narrow. The hydrodynamic variables in the vertical and longitudinal directions are significant compared to the lateral directions. In the present work also a mathematical model is developed for the case of a laterally averaged lake or reservoir. The schematic diagram of a lake with the coordinate systems is shown in Fig.1. The conservation equations are obtained by applying the conservation principles of mass, momentum, energy and concentration (sediment) for a control volume of the lake (Lin, 1992).

The vertical momentum equation is replaced by the hydrostatic pressure equation. The Boussinesq approximation is assumed to hold good in the present study. That means the variation of density will appear only in the gravity term, otherwise water is assumed to be incompressible. Laterally averaged vertical and longitudinal velocities are used in the present study. In order to take care of the moving boundaries, mesh velocities in x and z directions are introduced in the convective terms of the transport equations. The governing equations will become complete with the inclusion of equation of state for water, giving the relationship between the density, temperature and sediment concentration and finally the turbulent closure model. Since the major objective of the present work is to solve the

continuity, momentum, energy and concentration as moving boundary problems for sediment-laden flow, a simple turbulent closure model is assumed (Munk and Anderson, 1948). The dependent variables in the present study are u , w , H , T , C , p and ρ and the independent variables are x , z and t . The resulting governing equations are given below. For detailed derivation refer to Young (2002).

Governing equations

Continuity (local)

$$\frac{\partial}{\partial x}(ub) + \frac{\partial}{\partial z}(wb) = q_t \quad (1)$$

Longitudinal Momentum

$$\begin{aligned} \frac{\partial u}{\partial t} + (u - \tilde{u})\frac{\partial u}{\partial x} + (w - \tilde{w})\frac{\partial u}{\partial z} = & -\frac{1}{b} \frac{1}{\rho} \frac{\partial(bp)}{\partial x} \\ & + \frac{1}{b} \frac{\partial}{\partial x}(bK_x^M \frac{\partial u}{\partial x}) + \frac{1}{b} \frac{\partial}{\partial z}(bK_z^M \frac{\partial u}{\partial z}) + \frac{q_t(u_t - u)}{b} \end{aligned} \quad (2)$$

Vertical momentum

$$0 = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g \quad (3)$$

Heat transport

$$\begin{aligned} \frac{\partial T}{\partial t} + (u - \tilde{u})\frac{\partial T}{\partial x} + (w - \tilde{w})\frac{\partial T}{\partial z} = & \frac{1}{b} \frac{\partial}{\partial x}(bK_x^H \frac{\partial T}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z}(bK_z^H \frac{\partial T}{\partial z}) + \frac{q_t(T_t - T)}{b} \end{aligned} \quad (4)$$

Suspended sediment transport

$$\begin{aligned} \frac{\partial C}{\partial t} + (u - \tilde{u})\frac{\partial C}{\partial x} + (w - w_s - \tilde{w})\frac{\partial C}{\partial z} = & \frac{1}{b} \frac{\partial}{\partial x}(bK_x^C \frac{\partial C}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z}(bK_z^C \frac{\partial C}{\partial z}) + \frac{q_t(C_t - C)}{b} \end{aligned} \quad (5)$$

Equation of state for water

$$\rho_w = 999.841 + 6.59585 \cdot 10^{-2}T - 8.45123 \cdot 10^{-3}T^2 + 5.29157 \cdot 10^{-5}T^3 \quad (6a)$$

Ambient fluid density

$$\rho = (1-C) \rho_w + C \rho_c \quad (6b)$$

Turbulent closure model (Munk and Anderson, 1948)

$$K_z^M = K_0^M (1 + 10R_i)^{-0.5} \quad (7a)$$

$$K_z^H = K_0^H (1 + 3.33R_i)^{-1.5} \quad (7b)$$

$$K_z^C = K_z^H \quad (7c)$$

$$\text{where } R_i = \frac{-g \frac{\partial \rho}{\partial z}}{\rho \left(\frac{\partial u}{\partial z} \right)^2}$$

(7d)

Mesh velocities

$$\tilde{u} = \frac{dx}{dt} \quad (8a)$$

$$\tilde{w} = \frac{dz}{dt} \quad (8b)$$

Velocity Boundary conditions

The above governing equations have to be solved with appropriate initial and boundary conditions. In the simulation studies of lake hydrodynamics, it is seldom to have the initial conditions, in general. The computations can be initiated with any accepted initial conditions or homogeneous conditions or even potential flow conditions.

Kinematic free surface

$$\frac{\partial z_\infty}{\partial t} + (u_\infty - \tilde{u}_\infty) \frac{\partial z_\infty}{\partial x} - w_\infty = 0 \quad (9)$$

Dynamic free surface

$$\tau_\infty = C_D \rho_a U_{10} |U_{10}| \quad (10)$$

Bottom of reservoir

$$\frac{\partial z_0}{\partial t} - \tilde{u}_0 \frac{\partial z_0}{\partial x} = 0 \quad (11)$$

Solid boundaries (no-slip)

$$u = u_f, \quad w = w_f \quad (12)$$

Temperature and sediment boundary conditions

Dirichlet boundary conditions are assumed for temperature and concentration at the solid surfaces of the lake (the basin). The specification of temperature at the lake surface does not pose much problem compared to the specification of sediment concentration. In the present work, the sediment concentration in the flow has been correlated to the inflow as an exponential function, instead of a power law relation

used by Cesare et al., (2001), by means of a regression analysis using measured data. Using this correlation the Dirichlet boundary conditions for the sediment concentration equation are specified.

On the free surface, the heat transfer at air-water interface is specified using Newton's law of cooling as given by the following equation.

$$q_w = h(T_e - T_w) \quad (13)$$

where T_e is the equilibrium temperature of water surface.

The water surface temperature, T_w varies depending upon whether it loses heat or gains heat based on the atmospheric conditions. A hypothetical temperature called equilibrium temperature T_e is assumed to exist during the energy balance of the solar radiation and the convective heat transfer at the air-water interface. The expression for the equilibrium temperature is given by equation 14a.

$$T_e = T_a + \frac{I}{h} \quad (14a)$$

In the above expression, h is the convective heat transfer coefficient. This is a function of temperature and flow characteristics at the water surface. The empirical formula proposed by Rimsha and Dochenko (1958) and Brady et al. (1969), are used in the present study.

$$h = 2.32 + \{ 1.56[8.0 + 0.35(T_w - T_a)] + 6.08U_2 \} [\beta + 0.61] \quad (14b)$$

for $T_w < 41^\circ \text{ F}$ (5° C) (Rimsha and Dochenko, 1958)

where $\beta = 0.612 - 0.0204T_m + 0.00049T_m^2$

and $T_m = (T_a + T_w) / 2$, T_a =air temperature, U_2 =wind velocity at 2m above the free water surface

$$h = 15.7 + (\beta + 0.26)(70 + 0.7U_2^2) \quad (14c)$$

for $T_w \geq 41^\circ \text{ F}$ (5° C) (Brady et al., 1969)

where $\beta = 0.255 - 0.085T_m + 0.000204T_m^2$

and T_m is calculated as in the previous expression.

Hydrostatic pressure distribution

The baroclinic internal pressure can be obtained by integrating the vertical momentum equation (3) with the assumption of hydrostatic pressure distribution as given in equation (15).

$$p(x, z, t) = p_w(x, t) + \rho g(z_w - z) + \hat{p}(x, z, t) \quad (15)$$

The internal pressure is the sum of the atmospheric pressure acting at the free surface of water, the hydrostatic pressure due to the position of free surface and the pressure

due to the difference in density of water because of stratification. The pressure due to density stratification is called perturbed pressure and is given as.

$$\hat{p} = \int_z^{z_w} [\rho(x, z, t) - \rho_r] g dz$$

Now the horizontal momentum equation (2) can be rewritten by substituting the expression for pressure gradient $\frac{\partial p}{\partial x}$ from equation (15) as,

$$\begin{aligned} \frac{\partial u}{\partial t} + (u - \bar{u}) \frac{\partial u}{\partial x} + (w - \bar{w}) \frac{\partial u}{\partial z} = & -g \left(\frac{\partial H}{\partial x} + S_0 \right) - \frac{1}{b\rho} \frac{\partial (bp_w)}{\partial x} - \frac{1}{b\rho} \frac{\partial (b\hat{p}_w)}{\partial x} + \frac{1}{b} \frac{\partial}{\partial x} (bK_z^M \frac{\partial u}{\partial x}) \\ & + \frac{1}{b} \frac{\partial}{\partial z} (bK_z^M \frac{\partial u}{\partial z}) + \frac{q_t(u_t - u)}{b} \end{aligned} \quad (16)$$

Where $H = z_w - z_0$ = total water depth; $S_0 = \frac{\partial z_0}{\partial x}$ = bottom slope.

Water depth equation

The variation of water depth H depends on the changes in the free surface, lake bottom and the lateral flow of water into the lake. Hence for the time variation of water depth, an equation can be obtained as given by equation (17), by combining continuity equation (1), kinematic free surface equation (9) and lake bottom equation (11). Also the equation can be made one-dimensional by substituting vertical averaged values of velocity and volume flow rate per unit lateral width.

$$\frac{\partial H}{\partial t} + \left(\frac{\bar{u}\bar{b}}{b_w} - \bar{\tilde{u}} \right) \frac{\partial H}{\partial x} + \frac{H}{b_w} \frac{\partial (\bar{u}\bar{b})}{\partial x} = \frac{q_t}{b_w} \quad (17)$$

where $\bar{u}\bar{b} = \frac{1}{H} \int_{z_0}^{z_w} u b dz$ and

$$\bar{\tilde{u}} = \frac{1}{H} \int_{z_0}^{z_w} \tilde{u} dz$$

For applying the boundary conditions for the vertical velocity w , the vertical momentum equation is ceased to exist, as it is replaced by a simple hydrostatic equation. Hence the local continuity equation (1) is differentiated with respect to z to get the following equation (King, 1985a):

$$\frac{\partial^2 (ub)}{\partial x \partial z} + \frac{\partial^2 (wb)}{\partial z^2} = \frac{\partial q_t}{\partial z} \quad (18)$$

Now, equations (16), (17), (18), (4), (5), (6), and (15) are the final governing equations to be solved for the unknown variables u , w , H or z_w , ρ , T , C , and p .

Numerical scheme

The final governing equations (16), (17), (18), (4), (5), (6), and (15) are solved using the Arbitrary Eulerian-Lagrangian finite element method, which is found suitable for solving moving boundary problems. The variations of reservoir storage and the corresponding fluctuation of free surface as well as the deposition/erosion of the reservoir bottom can be easily captured by the ALE moving boundary technique. The ALE finite element method (FEM) is employed to discretize the computational domain in space. The advantages of Eulerian method such as capturing large distortion of fluid, handling outflow walls and the advantages of Lagrangian method such as exact prediction of material interface, handling free surface boundary condition and curved rigid boundaries, are combined together in the above method (Noh, 1964; Hirt et al., 1974; Donea et al., 1975, 1982; Huges et al., 1981; Ramasamy and Kawahara, 1987; Ramasamy, 1990; Choi, 1998). The existence of free surface causes a severe constraint on the time step while calculating the water depth using equation (17) and hence the time derivative of this one-dimensional equation is discretized using an implicit scheme. Thus the numerical instability condition, called the Courant-Friedrichs-Levy (CFL) is also overcome. The time derivatives of the longitudinal velocity, temperature, and sediment concentration equations (16), (4) and (5) in two-dimensions, are discretized by an explicit scheme. Thus by following the implicitness in one dimension and explicitness in two dimensions, the excess computation is avoided.

While solving the Navier-Stokes equations for lake-hydrodynamic applications two types of numerical instability arise, one is the negative numerical damping caused by the advection-diffusion dominated flows solved by the Galerkin's method and the other one is due to the internal gravity waves. The first numerical instability is overcome by introducing an artificial Balancing Tensor Diffusivity (BTD) (Dukowica and Ramshaw, 1979). The second numerical instability is avoided by adopting the numerical procedures used by Sun (1980) while solving the governing equations. That is, the temperature and sediment concentrations are computed first, after that, velocity field and water depth or free surface are obtained. It is worthwhile to observe that the matrix equations for T , C , and u are all time-invariant as far as the matrix inversion is concerned. In addition, they all possess the property required for symmetric matrix equation solver, except the water depth equation (17), which is nonlinear and needs Newton-Raphson iteration technique. All other variables are uncoupled and can be calculated in a similar way.

The equations (16), (17), (18), (4) and (5) are integrated using Galerkin's

weighted residual method. Time discretization and application of the BTM technique for the above equations are discussed in detail in the appendix.

Validation of the numerical model

The mathematical model developed in the present study is validated by comparing the simulation results with the experimental results of the U.S. Army Corps of Engineers (Johnson, 1980, 1981) in the Generalized Reservoir Hydrodynamics (GRH) flume for gravitational underflow, which is designed to test the behavior of reservoir hydrodynamics. The reservoir data generated by this flume have been used to verify a number of models by earlier researchers in this field (King, 1982; Karpik and Raithby, 1990).

The length of the test flume is (Refer Figs. 1a and 1b) 24.39 m and it varies in depth from 0.3 m at its inflow end to 0.91 m at its outflow end. It has two different cross-sections 1 and 2. The upper section 1, which is 6.1 m long, has a horizontal bottom and linear variation in width from 0.3 m to 0.91 m, whereas the lower section 2 has a constant width of 0.91 m, and the bottom dropping down to 0.61 m over its 18.2 m length, as shown in Figs. 1a & 1b. The associated finite element mesh for the test flume is shown in Fig. 1c. The computational domain is discretized using linear triangular elements with 612 elements and 342 nodes.

Initially some numerical experiments are conducted in order to simulate the density current. For this purpose, the actual data corresponding to the test flume is used as input in the numerical simulation and are given in Table I. The inflow enters the flume under a baffle and allowed to flow into the system over the lower 0.15 m portion of the flume. The outflow water is removed from the outlet located on the dam, 0.15 m from the bottom. Because the inflow temperature is lower than the ambient temperature, the underflow type of density current is observed. Figs. 2a & 2b show the velocity and temperature fields obtained at the end of 8 min. The striking feature observed is that the fluid near the inflow attains high velocity quickly and a recirculation gyre in the inflow is established as seen from Fig. 2a. As the temperature of the inflow water is different from that of the flume water a temperature gradient is set up at the inlet of the flume. This has been predicted exactly as shown in Fig. 2b. As the penetration of momentum of fluid takes place into the neighboring regions, with advance in time, the density current moves forward along the bottom line with the recirculation gyre moving rapidly towards the dam.

Table I

Input data used in the numerical solution for validation of the model

Initial temperature of water in the flume	:	21.44 °C
Inflow water temperature	:	16.67 °C
Volume flow rate of inflow	:	0.00063 m ³ /s
Volume flow rate of outflow	:	0.00063 m ³ /s

Figures 3a, 3b & 4a, 4b depict the structures of density current and temperature transients at $t=16$ min and 28 min. respectively. The development of an elevated density front is clearly observed in Figs. 3a and 4a. This front leads the density current down the slope as also observed by Karpik and Raithby (1990). Though the density transients are set up very fast, the temperature variation is slow as seen from Figs. 3b and 4b. This is because the vertical turbulent mixing is reduced by the negative buoyancy effect and hence the temperature varies only in the region near the bottom as seen from Figs. 3b and 4b. It should be noted that the inflow takes place into a flume, which is not stratified, and hence the temperature variations are observed only in the underflow regions. It is the underflow, which causes the energy exchange to take place between the inflow and the reservoir water near the bed. After the current arrives at the dam say after an hour, the flow field becomes more stable and the recirculation gyre will occupy the entire region in the flume. The longitudinal distance traveled by the density front with time is computed until the density front reaches the end of the flume. The simulated results show good agreement with the measured values and are discussed in a contributed chapter by the author in ASCE nomograms (Young, 2002). The horizontal velocity at the central line near the center of the flume is computed and compared with the experimental results of Johnson (1980 & 1981) and the numerical results of Edinger and Buchak (1979) as shown in Fig. 5. The present numerical predictions show much smoother variation of velocity than the measured values. Even though the present model over predicts the velocities, the difference is less compared to the results of Karpik and Raithby (1990). However the general trend shows good agreement even for very small velocity in the order of 10^{-2} m/s.

Application of the numerical model to Te-Chi reservoir

Description of the Te-Chi reservoir

After the model is validated and verified with the laboratory data, the model is used to simulate the hydrothermal characteristics of a real reservoir, the Te-Chi reservoir, located at 1268m above sea level in central Taiwan. This reservoir is a major source

of fresh water supply with a storage capacity of $2.5 \times 10^8 m^3$. The Te-Chi reservoir surrounded by high mountainous basins in an isle is a very long, narrow and deep reservoir, as shown in Fig. 6a. Its longitudinal length is about 13 km, with maximum water depth of 140 m. The bottom slope of the Te-Chi reservoir is only around 1% and hence the assumption of hydrostatic pressure equation for vertical momentum equation is valid (Chung and Gu, 1998). Hence a laterally averaged two-dimensional model can be used to study the hydrodynamic characteristics of the reservoir. The major inflow to the reservoir comes from the upstream of the Ta-Chia River and besides there are nine other river tributaries, which have been considered as the minor lateral inflow sources. Figure 6b shows the longitudinal-vertical profile and its variation of lateral width as width contours. Numerical simulations of the hydrodynamics of the above reservoir are carried out for the annual cycles of 1984 and 1985.

Hydrological data used as input in the simulation

To simulate the 1985 annual cycle of reservoir hydrodynamics, the required input hydrological data includes the rate of major and minor lateral inflows, outflow rate, and the corresponding inflow temperatures and sediment concentrations. Figures 7a & 7b show the annual inflow and outflow discharge respectively for the year 1985. During dry seasons, that is, in autumn and winter, the inflow rate is very small. However in spring and summer seasons, the inflow rate is very high because of heavy rains due to storms or typhoons. The maximum inflow during 1985 was $245 m^3/s$ and that occurred at 237th day of the year (taking January 1 as 1st day of the year). Figure 7c shows the surface temperature of water in the reservoir, inflow temperature, and intake (withdrawal) temperature for the year 1985. The watershed lies in the area of vast high mountains, which is 3000 m above the sea level. As can be seen from the figure, the inflow temperature is always less than the surface temperature of water in the reservoir throughout the year and hence an underflow or density current is expected during 1985 (Gu et al., 1996).

Meteorological data used as input in the simulation

In addition to the hydrological data, the meteorological data, such as the cloud cover, dry bulb temperature of air, dew point temperature, wind speed and direction and solar radiation are also required as input data for the simulations. The dew point temperature, wind speed and direction and solar radiation that are used for the present simulations for the year 1985 are shown in Figs. 8a, 8b & 8c respectively. The heat

flux on the water surface can be obtained by using a thermal equilibrium model. This model is conceptually based on the assumption of Newton's law of cooling. That is, the surface heat flux can be estimated as the product of a heat exchange coefficient and the difference between the water surface temperature and the equilibrium temperature obtained using equation (13). Figures 9a, 9b & 9c show the calculated values of heat transfer coefficient, equilibrium temperature and heat flux for the year 1984. Finally, the wind shear stress at the water surface, which is one of the boundary conditions for the momentum equation, is computed from the wind speed by the empirical formula given by equation (10).

Discussion on the simulation results of Te-Chi reservoir

The numerical model is calibrated using the data for the year 1984 of the Te-Chi reservoir. Then the model is used to predict the results using the data for the year 1985. The computational domain of the Te-Chi reservoir was discretized using linear triangular elements with 950 elements and 522 nodes. The use of ALE technique enables the finite element mesh to move along with the variations of reservoir storage including the free surface, during computation. The types of mesh used for the highest and lowest water levels are shown in Figs. 10a & 10b. The information about the variation of water level in lakes can be used to estimate the evaporation and rainfall (Nicholson et al., 2000) rates in that region. Figure 11 shows the comparison between the computed and the measured values of water levels for 1985. As can be seen from the figure, the calculated water levels are very consistent with the observed values throughout the year. This means, the present model fully satisfies the mass conservation of the reservoir. It should be noted that the model could predict the water level variations accurately even when the inflow and outflow vary widely over the year (Figs. 7a & 7b). The comparisons of the calculated and measured water temperature profiles at different cross sections of the reservoir, at selective days of the months of January, July, August and November, 1985 are illustrated in Fig. 12. The computed results generally show good agreement with the measured data except the under-prediction for the month of July. In general, the present model is able to predict quite well the hydrothermal structures of the large-scale motion for the real reservoirs or lakes.

The temperature data of inflow to the Te-Chi reservoir shows that the inflow water temperature is always less than that of the reservoir water and hence underflow is formed in the reservoir. The underflow becomes turbidity current due to the presence of sediment particles in the inflow to the reservoir. Since the density of inflow water depends on the sediment concentration in the flow, the strength of turbidity current is

very weak, when the inflow is small. However, while the inflow discharge is very high during heavy rainfall due to storm, strong turbidity currents are formed. It is found from the measured data that the river inflow concentration is about 300 ppm and this results in a higher concentration range near the bed of the reservoir, about 6 km away from the dam. Due to the higher concentration and lower temperature of river inflows, the density of river inflows is higher than the density of upper layer of reservoir water body. Hence, by the effect of buoyancy force, the plunging phenomenon occurs after the river inflow comes into the reservoir and the underflow density current travels very fast to the downstream along the bed. Hence, for any sediment particle being carried into the reservoir, it will deposit at the bed with its settling velocity whenever it touches the bed and does not have any opportunity to be picked up again. As the turbidity current moves downward, the sediment concentration will decrease due to continuous deposition of sediment particles in the reservoir. The decrease in concentration results in the decrease in the impelling force acting on the turbidity current, making the current decelerate. Moreover, the selective withdrawal and the type of temperature distribution will also affect the density current. Therefore, the current leaves the bed about 6km away from the dam and the interflow occurs and advances horizontally to the intake of the selective withdrawal. As far as the thermal stratification of the reservoir is concerned, in the absence of any density current, the reservoir will attain a perfect vertical thermal stratification, having a constant temperature in a given horizontal layer of water. But due to the presence of interflow and underflow type of density currents, the thermal stratification is not straight in the horizontal direction near the sloping portion of the reservoir bed, where the effect of density current is significant.

As time goes by, the flow pattern also changes due to the varying inflow to the reservoir. The predictions of density currents are critical especially for peak inflow. By observing the data for the years 1984 and 1985, it is found that a maximum inflow of 315 m³/s occurs on 156th day of 1984. Hence the simulation results of density currents are obtained for the 156th day of 1984 and are shown in Fig.13a. We are analyzing the density current patterns generated during the period of heavy rain due to storm. Hence when the inflow increases, the underflow density current becomes stronger and travels a long distance along the bed to the neighborhood of the dam. However, when the current leaves the bed, the interflows do not move in the horizontal direction but moves towards the intake of the selective withdrawal, which results in an inverse circulation gyre near the bottom of the dam. Due to the erosive effect of interflow, the temperature distribution (Fig. 13b) becomes more uniform in the hypolimnion of the reservoir except near the intake of selective withdrawal, which is located at 75 m from the bottom of the reservoir. In the meantime, a strong thermal

stratification is also observed, with a lower temperature region called hypolimnion and a high temperature region called epilimnion. It is also found that the epilimnion and hypolimnion regions become narrower with time, due to the effect of density currents. Figure 13c shows the sediment concentration distribution on 156th day. Due to the presence of high sediment concentration in the flow, the impelling force acting on the turbidity current increases, thus forcing it to move downwards faster. Since some of the sediment particles leave during selective withdrawal, the sediment concentration in the downstream of selective withdrawal decreases. The similarity of distribution patterns in temperature and sediment concentration observed in Figs. 13b & 13c can be appreciated. This is expected as the energy and sediment concentration equations consist of similar terms of advection and diffusion.

Conclusion

A two-dimensional density current simulation model was developed to predict the various density flow regimes like, underflow, interflow and turbidity current for a real reservoir. The model was validated with the experimental results obtained for gravitational underflow in GRH flume of US Army Corps of Engineers. The model was successfully implemented for the annual cycle simulation of Te-Chi reservoir located in central Taiwan. The salient characteristics of the stratified lake hydrodynamics, such as the formation, maintenance, and erosion of thermocline as well as the gyre circulation, density current, are captured using the model. The circulation patterns of gyres and the thermocline structures and sediment concentration profiles are all well simulated. The present model accurately predicts the lake water level variations, which are highly useful for estimating evaporation and rainfall data. The model's capability is tested during heavy rainfall conditions in Taiwan. Hence the present model will be a useful tool to predict reservoir hydrodynamics, which will be essential to take precautionary steps during heavy rains due to storms, which is a common feature in Taiwan during summer.

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Appendix

The longitudinal velocity u is decomposed into two parts, $\bar{u}$, and Δu in order to

reduce the treatment of water depth coupling with the longitudinal velocity. This method saves lot of computational effort. Hence the longitudinal velocity u can be written as

$$u^{n+1} = u^{*n+1} + \Delta u^{n+1} \quad (A1)$$

After performing the time discretization by the mixed implicit/explicit finite difference schemes and with the introduction of BTD method, the equations (16), (17), (18), (4) and (5) take the following forms:

Horizontal momentum equation:

$$u^{*n+1} = u^n - \Delta t \left\{ (u^n - \tilde{u}^n) \frac{\partial u^n}{\partial x} + (w^n - \tilde{w}^n) \frac{\partial u^n}{\partial z} - \frac{1}{\rho_0} \frac{\partial p_s^{n+1}}{\partial x} - \frac{1}{\rho_0} \frac{\partial \hat{p}^{n+1}}{\partial x} - \frac{1}{b} \frac{\partial}{\partial x} \left(b K_x^M \frac{\partial u^n}{\partial x} \right) - \frac{1}{b} \frac{\partial}{\partial z} \left(b K_z^M \frac{\partial u^n}{\partial z} \right) - \frac{q_t^{n+1} (u_t^{n+1} - u^n)}{b} - BT D u^n \right\} \quad (A2)$$

$$\Delta u^{n+1} = -\Delta t g \left[\theta_1 \frac{\partial H^{n+1}}{\partial x} + (1 - \theta_1) \frac{\partial H^n}{\partial x} + s_b \right] \quad (A3)$$

Water depth equation:

$$H^{n+1} = H^n - \theta_2 \Delta t \left[\frac{H^{n+1}}{b_s} \frac{\partial \left(\frac{\dot{u}b}{\partial x} \right)^{n+1}}{\partial x} + \frac{\left(\frac{\dot{u}b}{\partial x} \right)^{n+1}}{b_s} \frac{\partial H^{n+1}}{\partial x} - \tilde{u}^n \frac{\partial H^{n+1}}{\partial x} \right] - \theta_2 g \Delta t^2 \frac{\partial}{\partial x} \left\{ \frac{\bar{b}}{b_s} \left[\theta_1 \frac{\partial H^{n+1}}{\partial x} + (1 - \theta_1) \frac{\partial H^n}{\partial x} + s_b \right] H^{n+1} \right\} - (1 - \theta_2) \Delta t \left[\frac{H^n}{b_s} \frac{\partial \left(\overline{ub} \right)^n}{\partial x} + \frac{\left(\overline{ub} \right)^n}{b_s} \frac{\partial H^n}{\partial x} - \tilde{u}^n \frac{\partial H^n}{\partial x} \right] + \frac{\Delta t q_t^{n+1}}{b} \quad (A4)$$

where $\bar{b} = \frac{1}{H} \int_{z_b}^{z_s} b dz$

Differentiated form of continuity equation:

$$\frac{\partial^2(u^{n+1}b)}{\partial x \partial z} + \frac{\partial^2(w^{n+1}b)}{\partial z^2} = \frac{\partial q_i^{n+1}}{\partial z} \quad (A5)$$

Heat energy equation:

$$T^{n+1} = T^n - \Delta t \left[(u^n - \tilde{u}^n) \frac{\partial T^n}{\partial x} + (w^n - \tilde{w}^n) \frac{\partial T^n}{\partial z} - \frac{1}{b} \frac{\partial}{\partial x} \left(bK_x^H \frac{\partial T^n}{\partial x} \right) - \frac{1}{b} \frac{\partial}{\partial z} \left(bK_z^H \frac{\partial T^n}{\partial z} \right) - \frac{q_i^{n+1}(T_i^{n+1} - T^n)}{b} - BTDT^n \right] \quad (A6)$$

Sediment concentration equation:

$$C^{n+1} = C^n - \Delta t \left[(u^n - \tilde{u}^n) \frac{\partial C^n}{\partial x} + (w^n - \tilde{w}^n) \frac{\partial C^n}{\partial z} - \frac{1}{b} \frac{\partial}{\partial x} \left(bK_x^C \frac{\partial C}{\partial x} \right) - \frac{1}{b} \frac{\partial}{\partial z} \left(bK_z^C \frac{\partial C}{\partial z} \right) - \frac{q_i^{n+1}(C_i^{n+1} - C^n)}{b} - BTDC^n \right] \quad (A7)$$

Balancing Tensor Diffusivity:

$$BTD = \frac{\Delta t}{2} \left[\frac{\partial}{\partial x} (u^n - \tilde{u}^n)^2 \frac{\partial}{\partial x} + \frac{\partial}{\partial x} (u^n - \tilde{u}^n) (w^n - \tilde{w}^n) \frac{\partial}{\partial z} + \frac{\partial}{\partial z} (w^n - \tilde{w}^n) (u^n - \tilde{u}^n) \frac{\partial}{\partial x} + \frac{\partial}{\partial z} (w^n - \tilde{w}^n)^2 \frac{\partial}{\partial z} \right] \quad (A8)$$

Where BTD is the operator of balance tensor diffusivity, and w is replaced by $(w - w_s)$ in the sediment equation; Δt =time step at present $n+1$, and previous n states, $0 < \theta_1, \theta_2 = 1$ are the integrating factors for the implicit finite difference scheme.

It is further noted that H and Δu are now one-dimensional equations, while $\tilde{u}$, T , and C are two-dimensional equations. Therefore, we need only one-dimensional elements for computing the free surface effects. The discretized equations for $\tilde{u}$, T , and C are all very similar. Besides, the explicitness of these variables suggests that a very simple and efficient algorithm is possible, since the matrix formed from the finite element analysis is almost identical. After the free surface or the water depth is

determined, and the position of longitudinal movement is assigned, the mesh velocities are implemented by the following definitions:

$$\tilde{u}^{n+1} = \frac{x^{n+1} - x^n}{\Delta t} \quad (A9)$$

$$\tilde{w}^{n+1} = \frac{z^{n+1} - z^n}{\Delta t} \quad (A10)$$

Since the system is coupled and nonlinear in nature, the Newton-Raphson iterative method is adopted. The iterative process will be much benefited from the time marching procedures, which provide a better initial guess for the calculated parameters.

The Galerkin finite element discretization is used to integrate the space domain. First the one-dimensional linear element are chosen to solve Δu and H variables of equations (A2) and (A4), while the two dimensional triangular linear element is adopted to solve the u , w , T and C variables from equations (A1), (A5), (A6), (A7). The resulting FEM matrix equations are listed as follows:

Matrices for 1-dimensional equations to determine Δu and H :

$$M_{lm}^{1D} \Delta u_m^{n+1} = -g \Delta t [\theta_1 G_{lm}^{1D} H_m^{n+1} + (1 - \theta_1) G_{lm}^{1D} H_m^n + M_{lm}^{1D} S_{bm}] \quad (A11)$$

$$\begin{aligned} M_{lm}^{1D} H_m^{n+1} = & M_{lm}^{1D} H_m^n - \theta_2 \Delta t \left[C_{lmn}^{1D} \left(\frac{\left(\frac{*}{ub} \right)^{n+1}}{b_s} - \tilde{u}^n \right) H_m^{n+1} + C_{lmn}^{1D} \left(\frac{H^{n+1}}{b_s} \right)_m \left(\frac{*}{ub} \right)_n^{n+1} \right] \\ & - \theta_2 g \Delta t^2 \left[\theta_1 D_{lmn}^{1D} H_m^{n+1} \left(\frac{\bar{b}}{b_s} H^{n+1} \right)_n + (1 - \theta_1) D_{lmn}^{1D} H_m^n \left(\frac{\bar{b}}{b_s} H^{n+1} \right)_n \right. \\ & \left. + B_{lmn}^{1D} S_{bm} \left(\frac{\bar{b}}{b_s} H \right)_n^{n+1} \right] - (1 - \theta_2) \Delta t \left[C_{lmn}^{1D} \left(\frac{\overline{ub}^n}{b_s} - \tilde{u}^n \right) H_m^n + C_{lmn}^{1D} \left(\frac{H^n}{b_s} \right)_m \left(\frac{*}{ub} \right)_n^n \right] \end{aligned}$$

$$+ \Delta t M_{lm}^{1D} \left(\frac{q_i^{n+1}}{b_s} \right)_m \quad (A12)$$

$$M_{lm}^{1D} = \int_C N_l N_m ds$$

$$G_{lm}^{1D} = \int_C N_l \frac{\partial N_m}{\partial x} ds$$

$$C_{lmn}^{1D} = \int_C N_l \frac{\partial N_m}{\partial x} N_n ds$$

$$D_{lmn}^{1D} = \int_C \frac{\partial N_l}{\partial x} \frac{\partial N_m}{\partial x} N_n ds$$

$$B_{lmn}^{1D} = \int_C \frac{\partial N_l}{\partial x} N_m N_n ds$$

Matrices for two-dimensional equations to determine u , T and C :

$$\begin{aligned} M_{ij}^{*n+1} u_j^{*n+1} &= M_{ij}^{*n} u_j^{*n} - \Delta t (C_{ij} + K_{ij}^M + \tilde{K}_{ij}) u_j^n + \frac{\Delta t}{\rho_0} G_{ij} p_j^{n+1} + \frac{\Delta t}{\rho_0} G_{ij} \hat{p}_j^{n+1} \\ &+ \Delta t M_{ij} \left[\frac{q_i^{n+1} (u_i^{n+1} - u_i^n)}{b} \right]_j + \Delta t F_i^u \end{aligned} \quad (A13)$$

$$u_i^{*n+1} = u_i^{*n} + \Delta u_i^{*n+1} \quad (A14)$$

$$K_{ij}^1 u_j + K_{ij}^2 w_j = F_i^w \quad (A15)$$

$$M_{ij} T_j^{*n+1} = M_{ij} T_j^{*n} - \Delta t (C_{ij} + K_{ij}^T + \tilde{K}_{ij}) T_j^n + \Delta t M_{ij} \left[\frac{q_i^{n+1} (T_i^{n+1} - T_i^n)}{b} \right]_j + \Delta t F_i^T \quad (A16)$$

$$M_{ij} C_j^{*n+1} = M_{ij} C_j^{*n} - \Delta t (C_{ij}^C + K_{ij}^C + \tilde{K}_{ij}^C) C_j^n + \Delta t M_{ij} \left[\frac{q_i^{n+1} (C_i^{n+1} - C_i^n)}{b} \right]_j + \Delta t F_i^C \quad (A17)$$

$$M_{ij} = \int_{\Omega} N_i N_j d\Omega$$

$$C_{ij} = \int_{\Omega} \left[(u^n - \tilde{u}^n) \frac{\partial N_j}{\partial x} + (w^n - \tilde{w}^n) \frac{\partial N_j}{\partial z} \right] d\Omega$$

$$C_{ij}^C = \int_{\Omega} \left[(u^n - \tilde{u}^n) \frac{\partial N_j}{\partial x} + (w^n - w_s - \tilde{w}^n) \frac{\partial N_j}{\partial z} \right] d\Omega$$

$$K_{ij}^M = \int_{\Omega} \left[\left(K_x^M \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + K_z^M \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) \right] d\Omega$$

$$\begin{aligned} \tilde{K}_{ij} = \frac{\Delta t}{2} \int_{\Omega} & \left[(u^n - \tilde{u}^n)^2 \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + (u^n - \tilde{u}^n)(w^n - \tilde{w}^n) \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial z} \right. \\ & \left. + (w^n - \tilde{w}^n)(u^n - \tilde{u}^n) \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial x} + (w^n - \tilde{w}^n)^2 \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right] d\Omega \end{aligned}$$

$$G_{ij} = \int_{\Omega} N_c \frac{\partial N_i}{\partial x} d\Omega$$

$$K_{ij}^1 = \int_{\Omega} b \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial x} d\Omega$$

$$K_{ij}^2 = \int_{\Omega} b \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} d\Omega$$

$$F_i^u = \int_C N_i \tau_s ds$$

$$F_i^T = \int_C N_i q_s ds$$

$$F_i^C = \int_C N_i q_c ds$$

$\tilde{K}_{ij}^c$ is obtained by $\tilde{K}_{ij}$, if w^n is replaced by $w^n - w_s$.

Where N_e , N_s = shape functions, q_e = sediment flux on the boundary.

The stiffness matrices, such as $M_{em}^{1D}, \dots, M_{ej}, \dots, F_i^u, \dots$, etc can be computed from the standard procedures of finite element analysis, once the shape functions, N_i, N_m, N_n, N_l, N_j are determined. The details can be obtained from any FEM text, such as Gallagher (1976), Zienkiewicz (1977). Since the water depth equation is nonlinear, Newton-Raphson method is used to compute H and all other variables are decoupled and hence can be calculated in a segment way.

Nomenclature

- b lateral width (m)
- C concentration of suspended sediment (kg/m³); specific heat capacity (J/kgK); coefficient
- g acceleration due to gravity (m/s²)

h	convective heat transfer coefficient ($\text{W/m}^2\text{K}$)
H	water depth (m)
I	solar radiation (W/m^2)
$\dot{m}$	mass flow rate (kg/s)
K	turbulent parameter (eddy viscosity or eddy diffusivity) (m^2/s)
p	pressure (N/m^2)
$\hat{p}$	perturbed pressure due to density stratification (N/m^2)
q	lateral flow ($\text{m}^3/\text{m}^2\text{s}$); heat flux (W/m^2)
t	time (s)
T	temperature (K)
u	flow velocity in the longitudinal direction (m/s)
$\tilde{u}$	mesh velocity in longitudinal direction (m/s)
$\bar{\tilde{u}}$	average mesh velocity (m/s)
$\overline{ub}$	average lateral velocity flux (m^2/s)
U	wind velocity (m/s)
w	flow velocity in the vertical direction (m/s)
$\tilde{w}$	mesh velocity in the vertical direction (m/s)
x	longitudinal Cartesian coordinate
z	vertical Cartesian coordinate

Non-dimensional numbers

R_i Richardson number

Greek letters

β	constant
ρ	density (kg/m^3)
τ	shear stress (N/m^2)

Subscripts

a	air
c	sediment
d	dew point temperature
e	equilibrium
f	inflow/outflow
∞	free surface condition
0	bottom condition
s	settling

t	lateral flow
w	pure water
x	longitudinal direction
2	at 2m above the free water surface
10	at 10m above the free water surface
z	vertical direction

Superscripts

C	eddy diffusivity for sediment transport
D	drag
H	eddy diffusivity for heat transport
M	eddy viscosity

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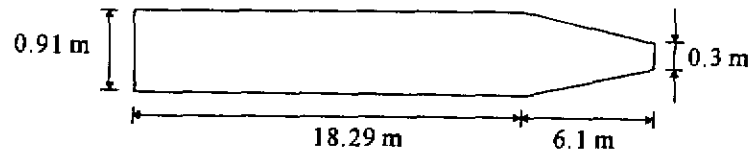
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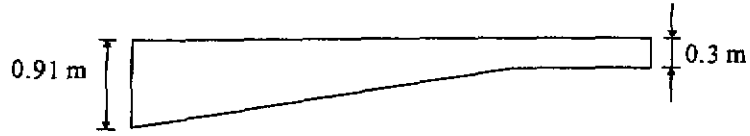
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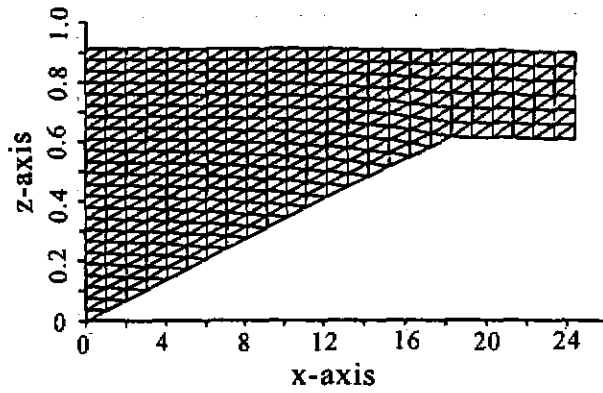
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(a) Plan view



(b) Side view



(c) Finite element mesh

Fig.1 Schematic diagram of Waterways Experiment Station GRH flume (a) plan view, (b) side view and (c) the finite element mesh.

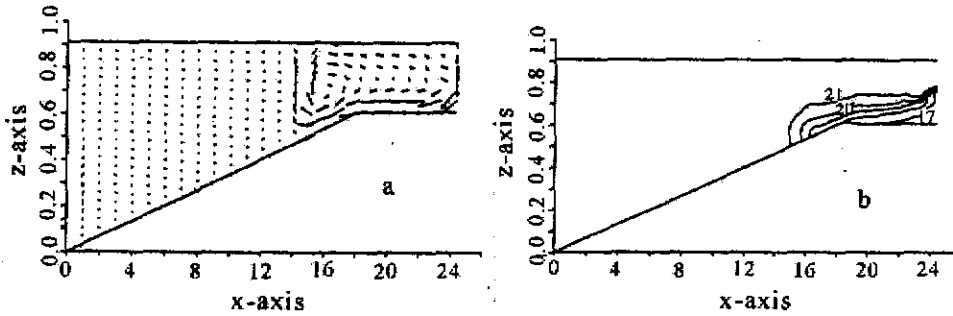


Fig.2 Structures of (a) density current and (b) temperature distribution of GRH flume at $t=8$ min.

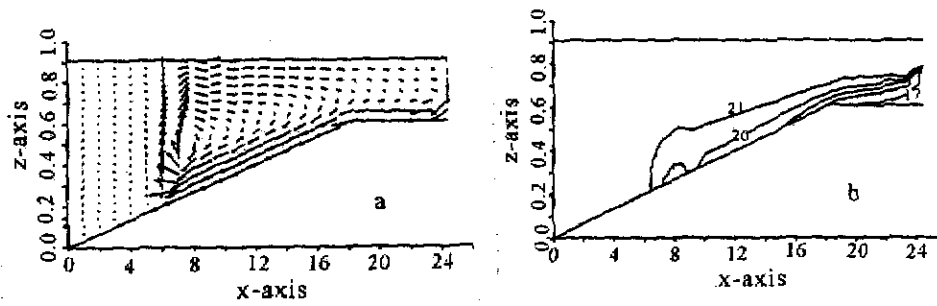


Fig.3 Structures of (a) density current and (b) temperature distribution of GRH flume at $t=16$ min.

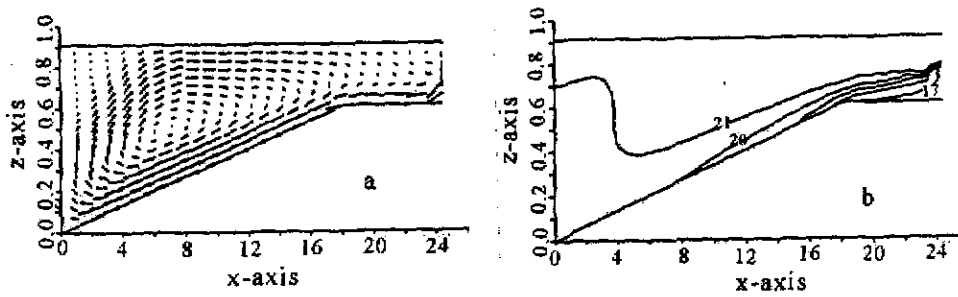


Fig.4a Structures of (a) density current and (b) temperature distribution of GRH flume at $t=28$ min.

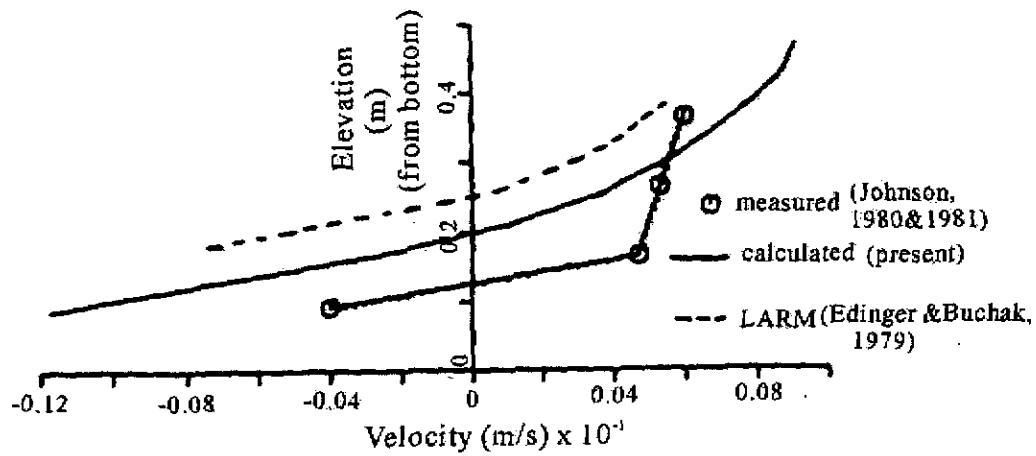


Fig.5 Comparison of longitudinal velocity distribution at the central section of GRH flume.

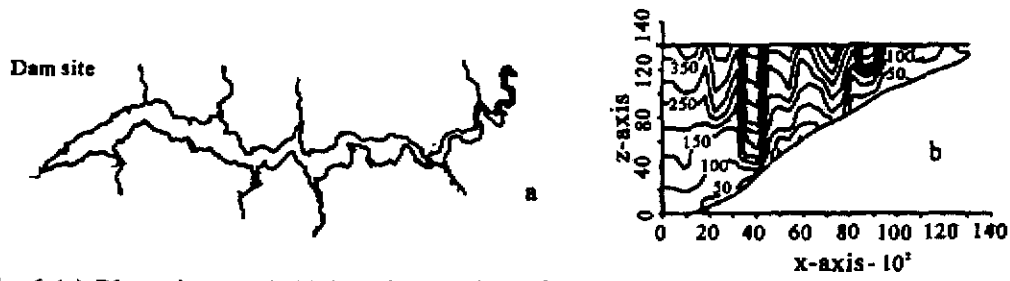


Fig.6 (a) Plan view and (b) longitudinal vertical profile and width contour of the Te-Chi reservoir

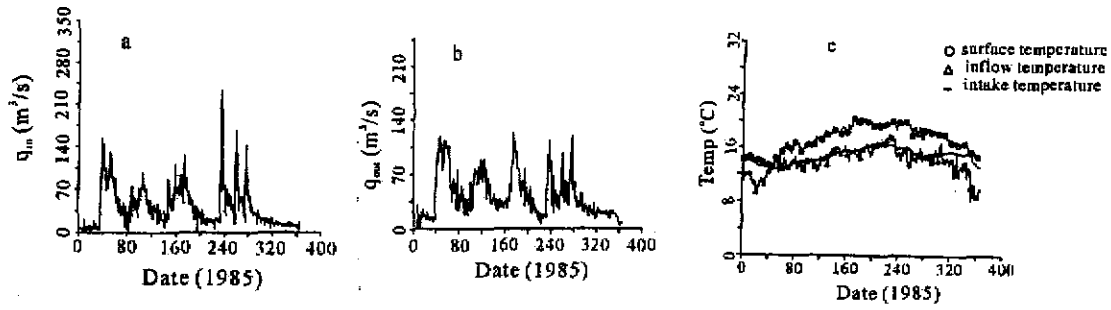
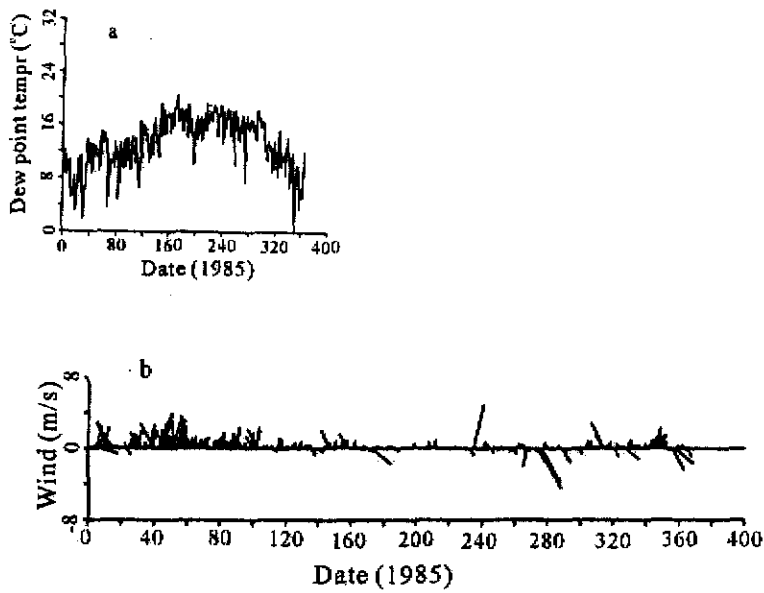


Fig.7 (a) inflow, (b) outflow and (c) surface temperature, inflow temperature and intake temperature in 1985 of the Te-Chi reservoir.



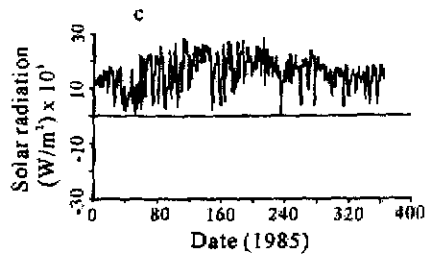


Fig.8 (a) Dew point temperature, (b) wind speed and direction, and (c) solar radiation in 1985 of the Te-Chi reservoir.

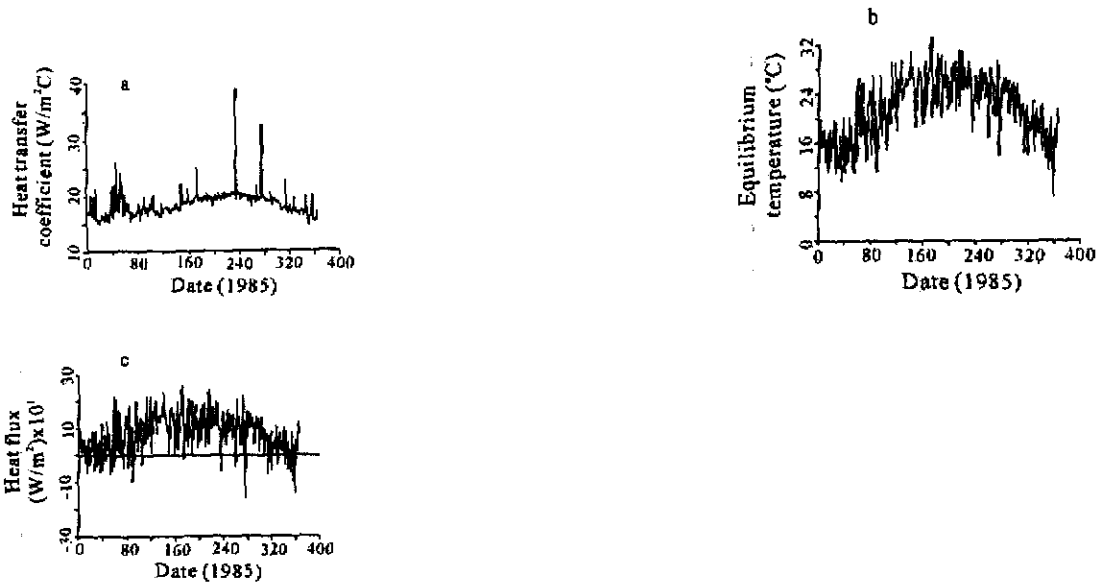


Fig.9 (a) heat transfer coefficient, (b) equilibrium temperature and (c) heat flux on the water surface in 1985 of the Te-Chi reservoir.

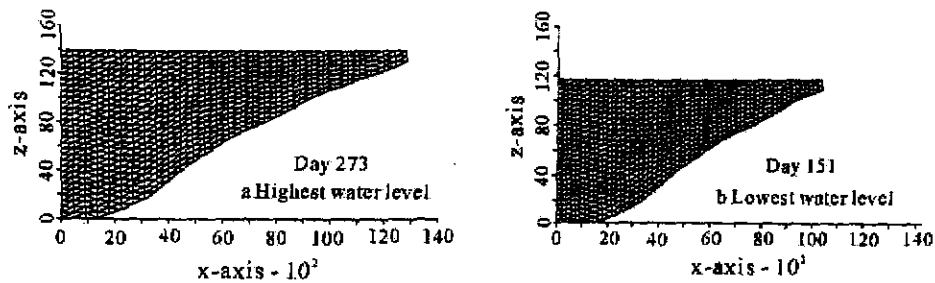


Fig.10 Moving adaptive finite element grid system for (a) highest water level and (b) lowest water level in 1985 of the Te-Chi reservoir.

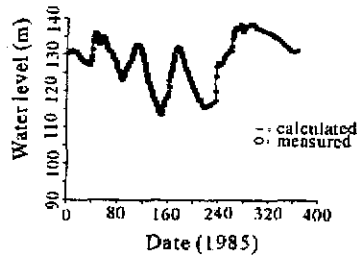


Fig.11 Comparison of calculated and measured values of water levels of the Te-Chi reservoir in 1985.

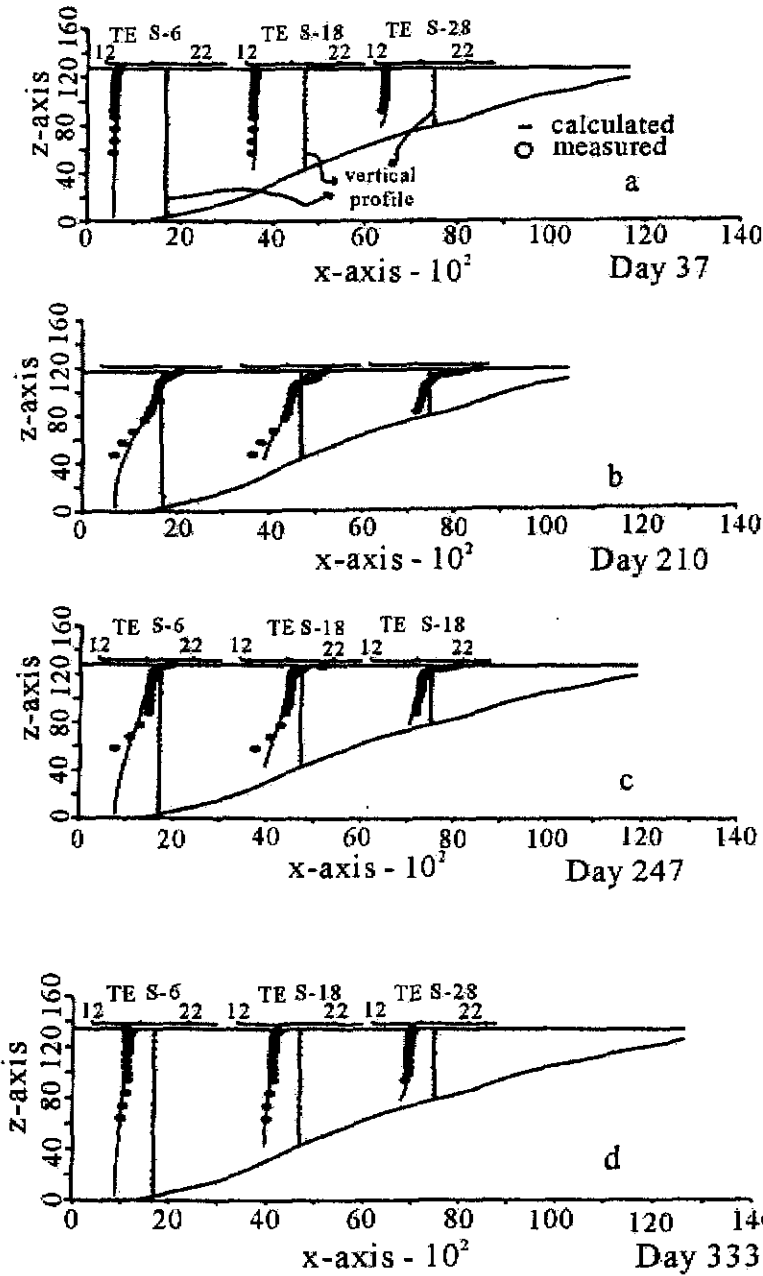


Fig.12 Comparison of calculated and measured values of daily temperature profiles at

a particular day during the month of (a) January, (b) July, (c) August, and (d) November in 1985 of the Te-Chi reservoir.

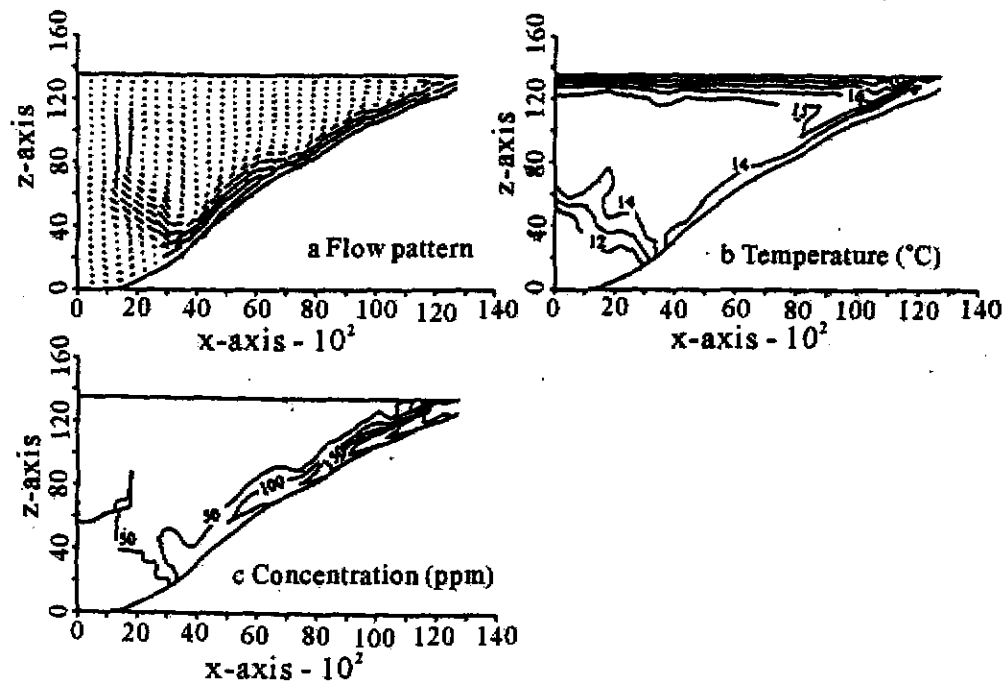


Fig.13 Structures of (a) density current, (b) temperature and (c) sediment concentrations on 156th day in 1984 of the Te-Chi reservoir

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Arbitrary Lagrangian-Eulerian Finite Element Analysis of Free Surface Flow Using a Velocity-Vorticity Formulation

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The main purpose of present study aims at the establishment of a numerical model for the moving boundary free surface flow problems. In order to comprehend the motion of the fluid flow, the Navier-Stokes equations through the velocity-vorticity formulation are adopted to deal with free surface flows. It should be noted that the pressure field can be eliminated by taking the curl of the Navier-Stokes equations. This paper proposes a new velocity-vorticity method for solving the unsteady free surface flow problems. The governing equations for the velocity field are deduced to the linear Poisson equations and the vorticity field is the vorticity transport equation which will be solved by the finite element method. The free surface kinematic boundary condition is imposed on the free surface position, while the velocity on the free surface are solved by using the free surface dynamic boundary condition and continuity equation. In the numerical techniques, the interior flow equations are basically treated by finite element, free surface boundary conditions are solved by using the Crank-Nicolson finite difference scheme. Present study naturally gives more reasonable results on problems including the maximum run-up of a solitary wave reflected from a vertical wall, the interactions between solitary wave and the seiche phenomenon in a rectangular reservoir. These applications reveal that the finite element is very powerful approach in the realm of computational fluid mechanics.

KEY WORDS: arbitrary Lagrangian-Eulerian; free surface flow, Velocity-Vorticity formulation; free surface kinematic boundary condition, free surface dynamic boundary condition.

1. INTRODUCTION

In many fluid mechanics problems the boundary is not contained in a fixed domain just as free surface flow. Finite element method (FEM) is very convenient and most promising for handling mechanics problems with complex geometries. The arbitrary Lagrangian-Eulerian method is adopted so that the irregular computational domain can be easily discretized and the moving mesh technique. For flows with a free surface the computational mesh is fitted to the free surface boundary at each time step, with the free surface elevation and velocity satisfying a kinematic and dynamic boundary condition.

Numerical methods to simulate the flow with a free surface can be classified into three categories, namely, the Eulerian, Lagrangian, and arbitrary Lagrangian-Eulerian (ALE) methods. The Eulerian method uses a fixed grid system which is generated over the entire domain and is not changed until the completion of computation. The methods known as volume tracking methods are based on marker quantities which are used to indicate the state of the cells used to discretize the domain of interest. They have the advantage of simplification and economy to deal with a free surface boundary conditions but gives a rather free surface. A method known as the MAC method has been developed [10, 24]. In the Lagrangian method, the free surface is tracked by a coordinate system which moves with a fluid particle. The mesh boundaries agree with the free surface, it qualitatively gives accurate free surface shapes and easy to implement the free surface boundary condition. However, the mesh is twisted overly due to the change of fluid domain may result in numerical

errors. As with the Lagrangian approach, the implementation of this method in three dimensions would be very difficult indeed. The Lagrangian formulation has been used by many authors for solving fluid flow problems [2]. Combinations of Lagrangian-Eulerian methods with different modifications are in common use. One of the most efficient Lagrangian-Eulerian methods in practice is arbitrary Lagrangian-Eulerian (ALE) technique, based on the arbitrary movement of the reference frame, which is continuously rezoned in order to allow a precise description of moving interfaces. In the ALE method, the nodes in the interior of the domain are displaced in an arbitrary prescribed way to obtain a mesh of proper shape to avoid mesh crossing. The ALE method can be considered of as a moving deformable control volume problem. It is noted that in the ALE, the node velocity is difference of the fluid velocity. The ALE formulation has been used by various investigators for solving moving boundary problems [4, 7, 11, 12, 18, 19, 20].

Numerical simulation of viscous free surface flow are well known for primitive variable of pressure-velocity. This formulation have been thoroughly invested by various numerical method such as finite difference (FDM) [23], finite element (FEM) [6, 9, 17, 25] and Finite volume method (FVM) [13]. The velocity-vorticity form of the Navier-Stokes equations pioneered by Fasel [8] has been established as an effective formulation for the solution of incompressible viscous flow problems. The velocity-vorticity formulation which eliminates pressure calculation, is well developed and established viscous incompressible flow with a stationary domain by many investigators [26-27]. In tradition, the most investigators solve free surface flow problems using primitive variable method or Vorticity-Stream function method. Present developments primarily concern the solution of the free surface flow problem. Moreover, the governing equations are not necessary to compute the pressure field no matter interior equations or free surface kinematic and dynamic equations. The ALE

scheme is employed to deal with the moving boundary, such as the motion of a solitary wave run-up and run-down from a vertical wall. Using the present model, by Crank-Nicolson scheme FDM is adopted to deal with boundary conditions and FEM using ALE scheme for the moving boundary.

In the computational methodology of unsteady incompressible viscous fluid flows, the fractional step methods have been proven to be effective. In the present study, a new computational procedure is developed to solve the incompressible viscous free surface flow problems. This model is based on the velocity-vorticity method of the Navier-Stokes equations. Each time step the free surface position and velocity are satisfied the FSKBC and FSDBC. The Semi-implicit FEM and by using ALE scheme for moving boundary, such as the motion of two opposite solitary waves interactive processes, a solitary wave maximum run-up from a vertical wall

The free surface flow problems are simulated using the present model. The contents of the paper are organized as follows. Section 2 presents the free surface governing equations, the main variables of the equations is velocity, vorticity and free surface elevation. In Section 3, we employ a semi-implicit FEM for interior field of velocity and vorticity distribution. Moreover, the free surface boundary conditions is moving at each time step, we transform a physical coordinate to computation coordinate system, then using the FDM to calculate free surface boundary conditions. Section 4 outlines the flow chart for the numerical model. The feasibility and accuracy of the developed numerical scheme has been verified in section 5, by comparing with other numerical schemes available in literature. Section 6 contains our main conclusions.

2. GOVERNING EQUATIONS

2.1 Incompressible Viscous Flow

The partial differential equation set governing viscous, laminar flow of an incompressible fluid is a subject class of the familiar nonlinear Navier-Stokes

equations system. Let Ω be the fluid domain, which is surrounded by a piecewise smooth boundary Γ . By using the vector form, the corresponding basic equations of conservation of mass, and momentum are [19-20]

Continuity

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

Momentum

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \vec{u} \quad (2)$$

where $\vec{u}$ is the velocity vector, p is the pressure, Re is the Reynolds number and t is the time. Equation (1) and (2) represent the Navier-Stokes equations in the pressure-velocity formulation.

The vorticity vector $\vec{\omega}$ can be expressed as:

$$\vec{\omega} = \nabla \times \vec{u} \quad (3)$$

By taking the curl of both sides of Eq. (2) and using Eqs. (1) and (3), we can obtain the vorticity transport equation as follows:

$$\frac{\partial \vec{\omega}}{\partial t} + \vec{u} \cdot \nabla \vec{\omega} = \vec{\omega} \cdot \nabla \vec{u} + \frac{1}{\text{Re}} \nabla^2 \vec{\omega} \quad (4)$$

By taking the curl of Eq. (3) and using Eq. (1) we get,

$$\nabla^2 \vec{u} = -\nabla \times \vec{\omega} \quad (5)$$

which is the vector form of Poisson equation for $\vec{u}$.

Equation (4) and (5) with $\vec{u} = (u, v, w)$ as velocity vector and $\vec{\omega} = (\omega_x, \omega_y, \omega_z)$ as vorticity vectors are known as Velocity-Vorticity formulation of the Navier-Stokes equations and can replace Eqs. (1) and (2) in which $\vec{u}$ and p are primitive variables.

The two-dimensional velocity-vorticity formulation for the incompressible flows can be derived from the Eqs. (4) and (5) as following:

$$\frac{\partial \omega}{\partial t} + u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} = \frac{1}{\text{Re}} \nabla^2 \omega \quad (6)$$

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (7)$$

$$\nabla^2 v = \frac{\partial \omega}{\partial x} \quad (8)$$

For the Navier-Stokes equations, the solution of vorticity transport equation in Eq. (6), in combination with the velocity Poisson equations, (7) and (8), gives the velocity and vorticity distributions all over the domain at the concerned time step.

We seek a solution in the domain Ω which satisfies the initial conditions,

$$u = u_0, v = v_0; \omega = \omega_0 \quad \text{at} \quad t=0 \quad (9)$$

and no-slip boundary conditions of velocity on the boundary Γ of Ω .

2.2 Free Surface condition

Free surface flows can be considered two-phase flows and assumption that both density and viscosity of the adjacent fluid is impermeable at the interface. An interesting effect of the displacement of the free surface is that the position of the upper boundary is not known a priori in the free surface flow problems. The mathematical expression for free surface kinematic boundary condition can be derived from the equation which describes the surface that constitutes the boundary. An moving surface can be written in terms of a mathematical expression of the two-dimensional form as following.

$$F(x, y, t) = y - \eta(x, t) = 0 \quad (10)$$

Rewrite the equation (10), the height method used the kinematic condition as the governing equation of the free surface position as follows:

$$\frac{\partial \eta}{\partial t} = v - u \frac{\partial \eta}{\partial x} \quad (11)$$

where η is the height of free surface.

The dynamic boundary condition represent the continuity of stress on the free surface.

Neglecting the surface tension on the free surface, the free surface dynamic boundary condition is as follows

$$\left[u_t + uu_x + vu_y - \frac{1}{\text{Re}}(u_{xx} + u_{yy}) \right] + \eta_x \left[v_t + uv_x + vv_y + 1 - \frac{1}{\text{Re}}(v_{xx} + v_{yy}) \right] = 0 \quad (12)$$

which are also valid for rotational and viscous flow

The above equation (12) have two unknown variables of velocities(u & v), in order to solve velocities(u & v), so we add continuity equation to iterative the FSDBC and continuity equation. The continuity equation can be written as follows:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (13)$$

As far as vorticity boundary condition is concerned, it is not known *a priori*. In general, as the velocity field is determined, the bottom velocity distribution may be approximated to high order approach. It can be written as follows,

$$u(y) = a_0 + a_1 y + a_2 y^2 + a_3 y^3 + a_4 y^4 + \dots \quad (14)$$

From the vorticity definition, the vorticity boundary conditions can be written as,

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (15)$$

2.3 Arbitrary Lagrangian-Eulerian description

The arbitrary Lagrangian-Eulerian method originally developed by Hughes et al.[12]. In ALE, let $\Omega(X_i, t)$ represents the material domain (Lagrangian), $\Omega(x_i, t)$ represents the spatial domain (Eulerian) and $\Omega(\xi_i, t)$ represents the referential domain. Then the Lagrangian-Eulerian mapping can be described by $x_i = x_i(X_i, t)$ and the Eulerian-referential mapping can be described by $x_i = x_i(\xi_i, t)$. Consider a physical property $f(x_i, t)$ expressed in a spatial domain. We can write the time derivative of f as

$$\frac{\partial f}{\partial t}(X_i, t)|_{x_i} = \frac{\partial f}{\partial t}(\xi_i, t)|_{\xi_i} + c_i \frac{\partial f}{\partial t}(x_i, t) \quad (16)$$

c_i is the convective velocity described as

$$c_i = u_i - \hat{u}_i \quad (17)$$

Where u_i is the material velocity and $\hat{u}_i$ is the mesh velocity. In the Lagrangian description, $u_i = \hat{u}_i$, In the Eulerian description, the mesh velocity $\hat{u}_i = 0$.

For the numerical analysis of a moving boundary, the ALE method is adopted in this paper. The governing equations of incompressible flow with free surface considering mesh velocities are given by following:

$$\frac{\partial \omega}{\partial t} + (u - \hat{u}) \frac{\partial \omega}{\partial x} + (v - \hat{v}) \frac{\partial \omega}{\partial y} = \frac{1}{\text{Re}} \nabla^2 \omega \quad (18)$$

where u and $\hat{u}$ are the particle and mesh velocities in x-axial direction,

v and $\hat{v}$ are the particle and mesh velocities in y-axial direction.

$(u - \hat{u})$ and $(v - \hat{v})$ mean the convective velocity defined by the difference between the particle and mesh velocities.

In the ALE form, the height method used the kinematic condition as the governing equation of the free surface position as follows:

$$\frac{\partial \eta}{\partial t} = v - (u - \hat{u}) \frac{\partial \eta}{\partial x} \quad (19)$$

where η is the height of free surface.

The equation (12) can be written as:

$$\left[u_t + (u - \hat{u})u_x + (v - \hat{v})u_y - \frac{1}{\text{Re}}(u_{xx} + u_{yy}) \right] + \eta_x \left[v_t + (u - \hat{u})v_x + (v - \hat{v})v_y + 1 - \frac{1}{\text{Re}}(v_{xx} + v_{yy}) \right] = 0 \quad (20)$$

3. NUMERICAL FORMULATION

As mentioned earlier, in the solution of two-dimensional free surface flow using the velocity-vorticity formulation, the vorticity transport and the Poisson-type velocity equations are solved using the finite element method. The free surface boundary conditions and vorticity transport boundary condition are solved by finite difference scheme. In this section, the numerical formulation is briefly described.

3.1 FINITE ELEMENT FORMULATION

The linear triangular element is easily discretized by the finite element method, in this study the linear triangular element is employed to calculate the local element. The geometry of quadrilateral for substructuring is shown in fig.1. The arbitrary quadrilateral can be divided into four triangular elements. In order to add the accuracy of calculation and keep the element symmetry, we can eliminate the central point of arbitrary quadrilateral, the equation (21-a) can be written as the form of equation (21-b) is shown following

$$K_{ij}\phi_j = f_j \quad i = 1,5 \quad j = 1,5 \quad (21-a)$$

$$K'_{ij}\phi_j = f'_j \quad i = 1,4 \quad j = 1,4 \quad (21-b)$$

The arbitrary element velocity and vorticity are approximated as (By using indicial notation and summation convention for repeated indices)

$$\omega_j = N_j \omega_j \quad (22)$$

$$u_j = N_j u_j \quad (23)$$

$$v_j = N_j v_j \quad (24)$$

where N_j denotes the interpolation or shape function of vorticity and velocity. The weak formulations of equation (18), is obtained by using the standard Galerkin method

$$0 = \iint \Omega \left(\frac{\partial \omega}{\partial t} + (u - \hat{u}) \frac{\partial \omega}{\partial x} + (v - \hat{v}) \frac{\partial \omega}{\partial y} - \frac{1}{\text{Re}} \left(\frac{\partial^2 \omega}{\partial^2 x} + \frac{\partial^2 \omega}{\partial^2 y} \right) \right) d\Omega \quad (25)$$

and using a time integration for the time derivative of ω , Eq.(25) can be written as,

$$\begin{aligned} 0 = & \sum \iint \Omega N_i N_j \frac{d\omega_j}{dt} d\Omega + \sum \iint \Omega (N_k (u_k - \hat{u}_k) N_i \frac{\partial N_j}{\partial x} + N_k (v_k - \hat{v}_k) N_i \frac{\partial N_j}{\partial y}) \omega_j d\Omega - \\ & \sum_{S^e} \int q_n N_i d\Gamma + \frac{1}{\text{Re}} \sum \iint \Omega \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \end{aligned}$$

(26)

where $q_n = \frac{\partial \omega}{\partial x} n_x + \frac{\partial \omega}{\partial y} n_y$

For two-dimensional flows, if $q_n = 0$ or ω is specified on the boundary, then the surface integration vanishes. Equation (26) can be written in the form,

$$\sum [M_{ij}^*] \left\{ \dot{\omega}_j \right\} + [L_{ij}^*] \{\omega_j\} + \frac{1}{\text{Re}} [K_{ij}^*] \{\omega_j\} = \{0\} \quad (27)$$

where

$$\begin{aligned} M_{ij}^* &= \iint N_i N_j d\Omega \\ L_{ij}^e &= \iint \left(N_k (u_k - \hat{u}_k) N_i \frac{\partial N_j}{\partial x} + N_k (v_k - \hat{v}_k) N_i \frac{\partial N_j}{\partial y} \right) d\Omega \\ K_{ij}^* &= \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega \\ \dot{\omega} &= \frac{\omega^{n+1} - \omega^n}{\Delta t} \end{aligned} \quad (28)$$

The fractional step methods have been proven to be effective, in the meantime semi-implicit FEM method has rendered some advantages of stability and simplicity.

So the Eq.(28) can be written as follows:

$$\left\{ \frac{1}{\Delta t} [M_{ij}^{(*)}] + \theta \left[L_{ij}^{(*)} + \frac{1}{\text{Re}} K_{ij}^{(*)} \right] \right\} \{\omega_j\}^{n+1} = \left\{ \frac{1}{\Delta t} [M_{ij}^{(*)}] - (1-\theta) \left[L_{ij}^{(*)} + \frac{1}{\text{Re}} K_{ij}^{(*)} \right] \right\} \{\omega_j\}^n \quad (29)$$

Equation (29) confirms that the needed additional data are integration time-step size

Δt , integration factor θ , and the known data $\{\omega_j\}^n$ at any time t^n .

$\theta = 0$ means explicit method (always instable)

$\theta = 1$ means fully-implicit method

In this model, $\theta = \frac{1}{2}$ is chosen.

Consider the Poisson type velocity equation in u and assuming that the vorticity and its derivatives are known, Eq(7) can be written as follows:

$$\nabla^2 u = -\frac{\partial \omega}{\partial y} \quad (30)$$

using the method of weighted residuals and Galerkin criterion, Eq. (30) can be written as,

$$0 = \iint N_i \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial \omega}{\partial y} \right) d\Omega \quad (31)$$

$$\Rightarrow 0 = \sum \iint \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) d\Omega - \sum \iint \left(N_i \frac{\partial N_j}{\partial y} \right) \omega_j d\Omega \quad (32)$$

$$\Rightarrow \left[K_{ij}^{(e)} \right] \{ u_j \} + \left[P_{ij}^{(e)} \right] \{ \omega_j \} = \{ 0 \} \quad (33)$$

where

$$P_{ij}^{(e)} = -\sum \iint \left(N_i \frac{\partial N_j}{\partial y} \right) d\Omega \quad (34)$$

Similar formulation is performed for the v component.

3.2 FINITE DIFFERENCE FORMULATION

The free surface boundary conditions are solved in Velocity-Vorticity variables using a finite difference method based on boundary -fitted coordinates. Using boundary-fitted coordinates , it means that mapping the arbitrary physical space(x, y, t) to a uniform computational space(ξ, η, τ). In this study, the boundary conditions are imposed on the body-fitted coordinates. The fig. 2 shows the body-fitted coordinate system of physical space and computational space. However, the grid space Δx and Δy are both non-uniform everywhere, and the grid is not orthogonal. This problem can be eliminated by transforming the non-uniform non-orthogonal physical space illustrated in Fig. 2a into the uniform orthogonal computational space illustrated in Fig.2b. In the finite difference scheme, the ξ direction is adopted by central difference scheme, but the time of τ and space of η are solved backward difference scheme. For example as following,

$$\frac{\partial f}{\partial \xi} = \frac{[f_{i+1,j} - f_{i-1,j}]}{2\Delta\xi}, \quad \frac{\partial f}{\partial \eta} = \frac{[f_{i,j} - f_{i,j-1}]}{\Delta\eta}, \quad \frac{\partial f}{\partial t} = \frac{f_{i,j}^{n+1} - f_{i,j}^n}{\Delta\tau} \quad (35)$$

the computational rule of equation (35), the second order accuracy of the Crank-Nicolson method is adopted to solve the free surface boundary conditions, the free surface kinematic condition can be written as,

$$\eta_i^{n+1} + 0.5 \cdot (u_i - \hat{u}_i) \left(\frac{\eta_{i+1}^{n+1} - \eta_{i-1}^{n+1}}{2\Delta x} \right) \Delta\tau = \Delta\tau \cdot \left[v_i - 0.5 \cdot (u_i - \hat{u}_i) \left(\frac{\eta_{i+1}^n - \eta_{i-1}^n}{2\Delta x} \right) \right] + \eta_i^n \quad (36)$$

similar formulation is performed for the FSDBC,

Using the boundary-fitted coordinate system, the equation (20) can be written as follows ;

$$u_\tau x_\xi + v_\tau y_\xi + \left[(u - \hat{u})u_\xi + (v - \hat{v})v_\xi \right] + \omega \left[(u - \hat{u})y_\xi - (v - \hat{v})x_\xi \right] + y_\xi + \frac{1}{\text{Re}} \left[\left(\frac{x_\xi^2 + y_\xi^2}{J} \right) \omega_\eta - \left(\frac{x_\xi x_\eta + y_\xi y_\eta}{J} \right) \omega_\xi \right] = 0 \quad (37)$$

where $J = (x_\xi y_\eta - y_\xi x_\eta)$ is the Jacobian coefficient,

The continuity equation can be written as follows,

$$(v_\eta u_\xi - y_\xi u_\eta) + (v_\eta x_\xi - v_\xi x_\eta) = 0 \quad (38)$$

As far as the velocity are solved by Poisson equations, the vorticity boundary condition must be concerned, From the vorticity definition, the vorticity boundary condition can be written as, fig. 3 shows the coordinate system of computational space.

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \frac{[(y_\eta v_\xi - y_\xi v_\eta) - (u_\eta x_\xi - u_\xi x_\eta)]}{J} \quad (39)$$

4. SOLUTION PROCEDURE

Here an iterative scheme is used in the solution of free surface flow using the velocity-vorticity formulation of the Navier-Stokes equations. In most of the

incompressible viscous flow problems, the most natural boundary conditions arise when the velocity is prescribed all over the boundaries of the problem. The vorticity boundary conditions are originated from the Stokes theorem or vorticity definition. In the present model, the velocity Poisson equations are initially solved to get the vorticity boundary conditions which are used in the solution of the vorticity transport equation. In free-surface part, the position of free surface is tracked by FSKBC, while the free surface velocities boundary conditions are solved by combination the continuity equation and FSDBC. The solution procedures adopted here include the following iterative steps:

1. Get initial condition and boundary condition.
2. Solve the free surface η by FSKBC and allocate new mesh distribution .
3. Calculate the mesh velocity.
4. Combination the continuity equation and FSDBC to solve the unknown of free surface velocity until the velocity is iterated to converge.
5. Solve the velocity Poisson Equation using FEM.
 - a. Calculate the velocity distribution at all nodal points.
 - b. Determine the new vorticity boundary values.
6. Solve the vorticity transport equation.
 - a. Get the unknown vorticity values through out the domain.
 - b. Calculate the derivatives of the vorticity to be used in the velocity Poisson equations.
6. Check for the convergence of the velocity and vorticity components in the present iteration, If convergence criterion is satisfied, then stop and proceed to the next time step, otherwise go to step 2.

In the successive time step, we use the velocity and vorticity components from the previous time step as initial conditions and use the iterative procedures, steps 2 to 6.

The procedures are repeated until the prescribed time step is reached.

5. NUMERICAL EXAMPLES

5.1 Analysis of a solitary wave propagation

The proposed free surface model has been applied on a test problem to confirm the feasibility of the model. The test problem is a solitary wave reflected from the vertical wall, for which many numerical results are available in the literature. In this model results are compared with the results of a series solution, such as a analysis solution of Byatt-Smith (1971) [3], experimental result [5,15] and the numerical simulation (Sung, 1999) [21]. Calculations are performed for a time increment $\Delta t = 0.02$ and for initial heights of the wave $\frac{H}{d} = 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5$ Byatt-Smith (1971) [3] obtained the maximum run-up height analytically by the method of superposition

$$\frac{R_{\max}}{d} = 2 \frac{H}{d} + \frac{1}{2} \left(\frac{H}{d} \right)^2 + o \left(\frac{H}{d} \right)^3 \quad (40)$$

The wave reaches the highest run-up along the right side vertical wall will be computed as shown in Fig. 4, the calculated values are agreed exactly with the results of investigators. The Fig. 5 is shown the numerical simulation were carried in from $t=0$ to 25 with $Re=10^3$, 5×10^4 and inviscid flow. For $Re=5 \times 10^4$ the amplitude decay rate was found to be smallness, and the wave height approach the inviscid flow. Because of viscous effect, the lower Reynolds number may cause viscous damping. The vorticity contour was shown in Fig 6. This illustrates the fact that viscous forces is confined only to the boundary layer and free surface, and the wave height was caused viscous damping and phase delay. It is noted that the Reynolds number for the example in this section is more significant when Re is higher or lower. This is due to the characteristic lengths taken for Reynolds numbers.

5.2 The interaction of two opposite solitary wave

In this section, collisions between two solitary waves are simulated using a

numerical scheme. The previous investigators of Su & Mirie (1980) [22] considered an inviscid and incompressible fluid of two solitary waves head-on collisions by a perturbation method up to the third order of approximation. In 1982, Mirie & Su [16] calculated the collisions of two solitary waves to confirm the generation of secondary waves as predicted in former paper. They found that the solitary waves having experienced changes of their phases and were trailed by a dispersive wave train while two solitary waves head-on collisions. The maximum amplitude run-up during the collision is obtained by their verification was shown as follows.

$$\text{Maximum run-up} = A_L + B_R + \frac{1}{2} A_L B_R + \frac{1}{4} (A_L B_R^2 + B_R A_L^2) \quad (41)$$

Where the A_L, B_R is the initial amplitude of solitary waves in left and right hand side.

We consider the collision of two solitary waves with different amplitudes. The initial amplitudes of two solitary waves are equal to 0.4 (left hand side) and 0.2 (right hand side). The two solitary waves interactive process is shown in Fig. 7. The grid size was $\Delta x = 0.2, \Delta t = 0.02$ and the range consisted of 4000 grid points. In this moving grid, the Δx is fixed but Δy is changed by free surface dynamic condition. The maximum run-up calculated is (0.641) while equation (37) gives (0.652). The calculation of this example is equal to second-order accuracy. The Fig. 8 and 9 show that the velocity distribution of two solitary waves interactive processes. The results are in agreement with the analysis and numerical solutions of Su & Mirie. We also found that after the collision of two solitary waves, the solitary waves recuperate almost all of their original amplitude for the length of time in our computation.

5.3 water oscillation in a rectangular reservoir

In many reservoir or lake has often the seiche phenomenon. The oscillating free surface computation is further tested by uninode standing wave shown in Fig 8. In this

study, the mean water level d equal to 5m and the half wave length L is set to 98m and the amplitude of the wave is set to many situation. The initial conditions of wave velocity is equal to zero and wave position can be written the curvilinear oscillating free surface.

$$y_s = A \cdot \cos\left(\frac{\pi x}{L}\right) + d \quad (42)$$

Where A is the initial amplitude, L is half wave length, d is the mean water level, y_s is the free surface position. The flow is considered to be inviscid so that the exact linear solution can be easily to verify. The flow velocity of analytical solution can be written as following,

$$\begin{aligned} u' &= \frac{A\sqrt{gd}}{d} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi\sqrt{gd}t}{L}\right) \\ v' &= -\frac{A\sqrt{gd}\pi y}{dL} \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi\sqrt{gd}t}{L}\right) \end{aligned} \quad (43)$$

In this paper, the governing equations are all dimensionless. However, the case of water oscillating in a reservoir shown in dimension. In order to exchange the dimensionless for dimension, the programming output data must be satisfied the follows stipulation(Table 1. shows dimension physical quantity in exchange for dimensionless).

$$\text{Characteristic time } t^* = \frac{d}{\sqrt{gd}} = \frac{t'}{t} \Rightarrow t = \frac{t'}{(d/\sqrt{gd})}$$

$$\text{If } d=5\text{m, } g=9.8 \text{ m/s}^2 \Rightarrow t = 1.4t'$$

$$\text{Characteristic length } H^* = \frac{d}{h}$$

$$\text{Characteristic velocity } u^* = \sqrt{gd} = \frac{u'}{u}, v^* = \sqrt{gd} = \frac{v'}{v}$$

Where d is the actual water level(unit: m), h is the non-dimension of static water level

t' is the actual time(unit: sec), t is the non-dimensional time

u is the actual velocity (mm/s), and a similar formulation is performed for v and w

	Length	Time	Period(T)	Velocity(u)	Velocity(v)
Dimensionless	1	1	39.2	1	1
Dimension	5(m)	0.71428(sec)	28(sec)	7m/sec	7m/sec

Table 1: The dimensionless physical quantity is transformed into dimension

The amplitude of the wave is set to 0.1 m is confirmed the accurate of the model. The flow is considered to be tiny viscous of fluid ($Re=5 \times 10^4$) so that the oscillation in the reservoir is agreement with linear analysis and has a little decay as shown in Fig. 10. While the initial amplitude is equal to 0.5m or 2m, the nonlinear effect in the free surface flow is more significant. Fig 11 and 12 shows the history of water wave oscillating in middle, left and right wall free surface position. Because of the initial wave shape is so sloping, the nonlinear effect on the flow is very obviously. Fig. 13 shows the free surface profile and velocity vectors of fluid in a reservoir due to a surge motion while the initial amplitude is equal to 2 m. Fig. 14 shows the moving boundary and moving mesh for the seiche phenomenon in a rectangular reservoir. It is found that due to the effect of gravity from free surface dynamic condition, the fluid velocity is urged by gravity and inertia force. It is noted that the boundary condition can introduce velocity and vorticity into the flow.

6. CONCLUSIONS

A numerical solver of the incompressible Navier-Stokes equations using the Velocity-Vorticity form for flows with free surface has been developed and verified. The Poisson-type velocity equations and vorticity transport equation are solved using the finite element technique, then interior domain velocity and vorticity are determined. The velocity and position of free surface are solved by FSKBC and FSDBC. For flows with a free surface an arbitrary Lagrangian-Eulerian (ALE) is

u' is the actual velocity(unit: m/s), u is the non-dimensional velocity

similar formulation is performed for v' and v

	Length	Time	Period(T)	Velocity(u)	Velocity(v)
Dimensionless	1	1	39.2	1	1
Dimension	5(m)	0.71428(sec)	28(sec)	$7m/sec$	$7m/sec$

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adopted to calculate the flows with free surface at every time step. The free surface flows using Velocity-Vorticity formulation has been found to be feasible and adequate.

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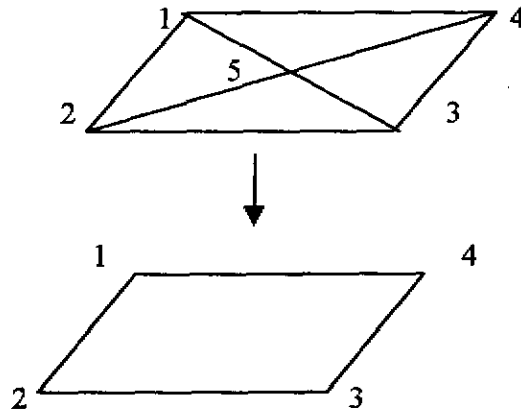


Fig. 1: The geometry of quadrilateral for substructuring

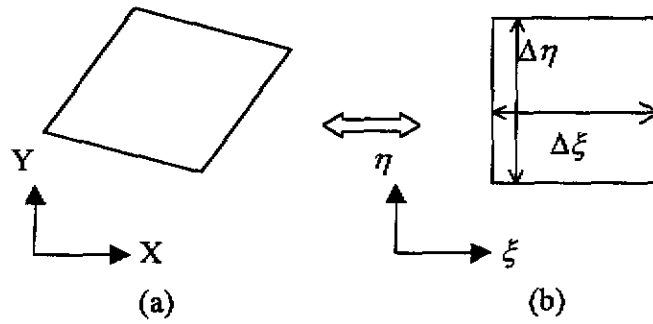


Fig. 2: Body-fitted coordinate system(a) physical space (b)computational space

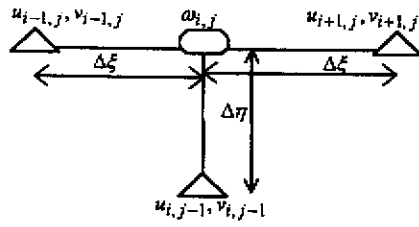


Fig. 3: The coordinate system of computational space for vorticity boundary condition

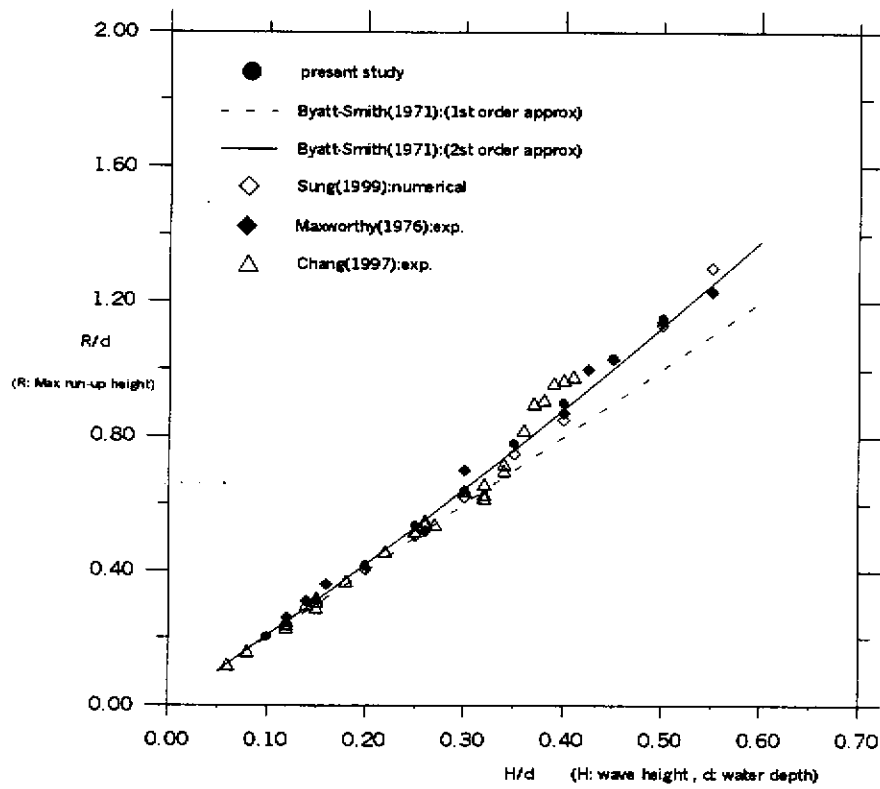


Fig. 4: Maximum run-up height versus incident wave amplitude

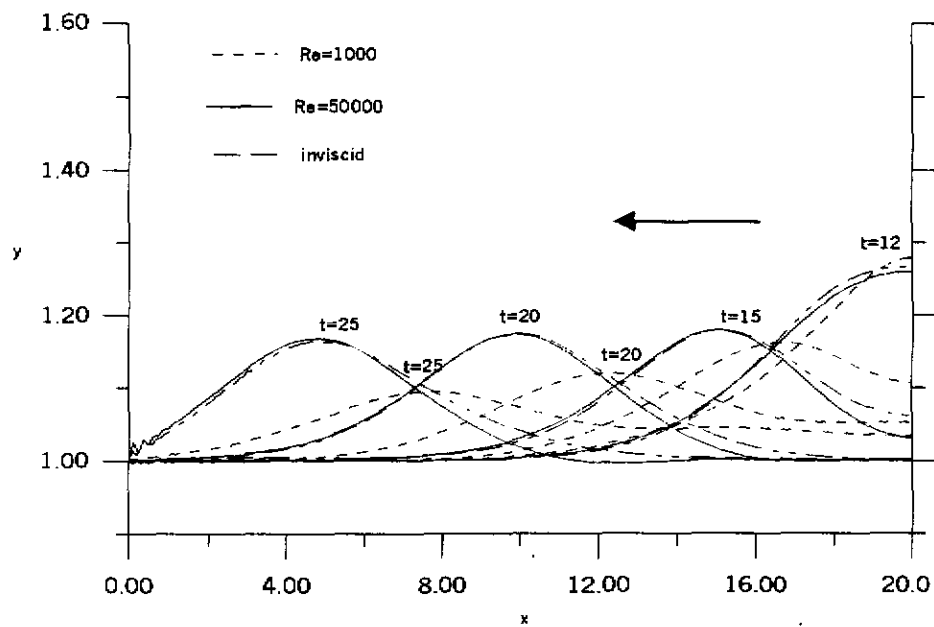
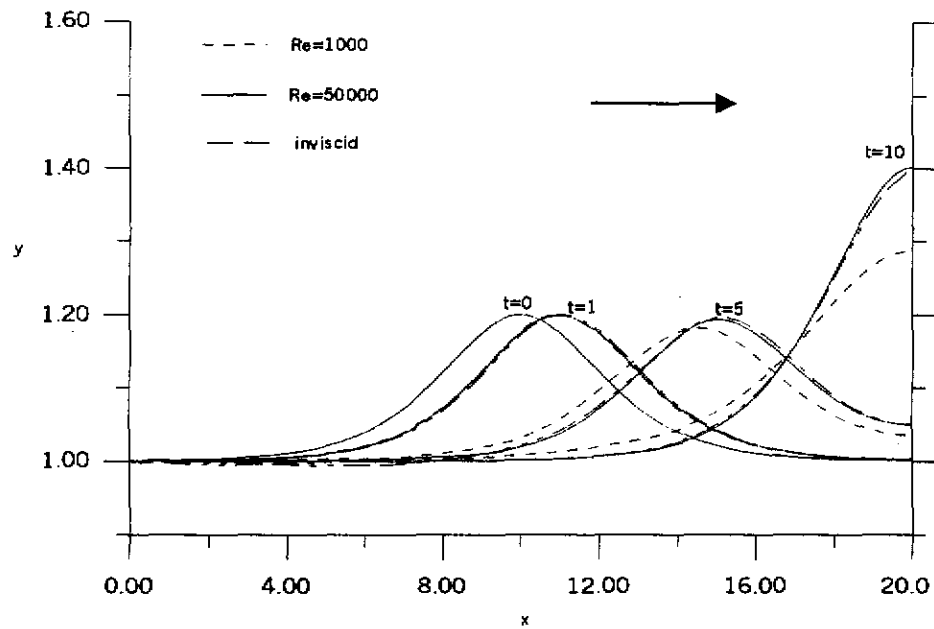


Fig 5: The solitary waves reflected from a vertical wall

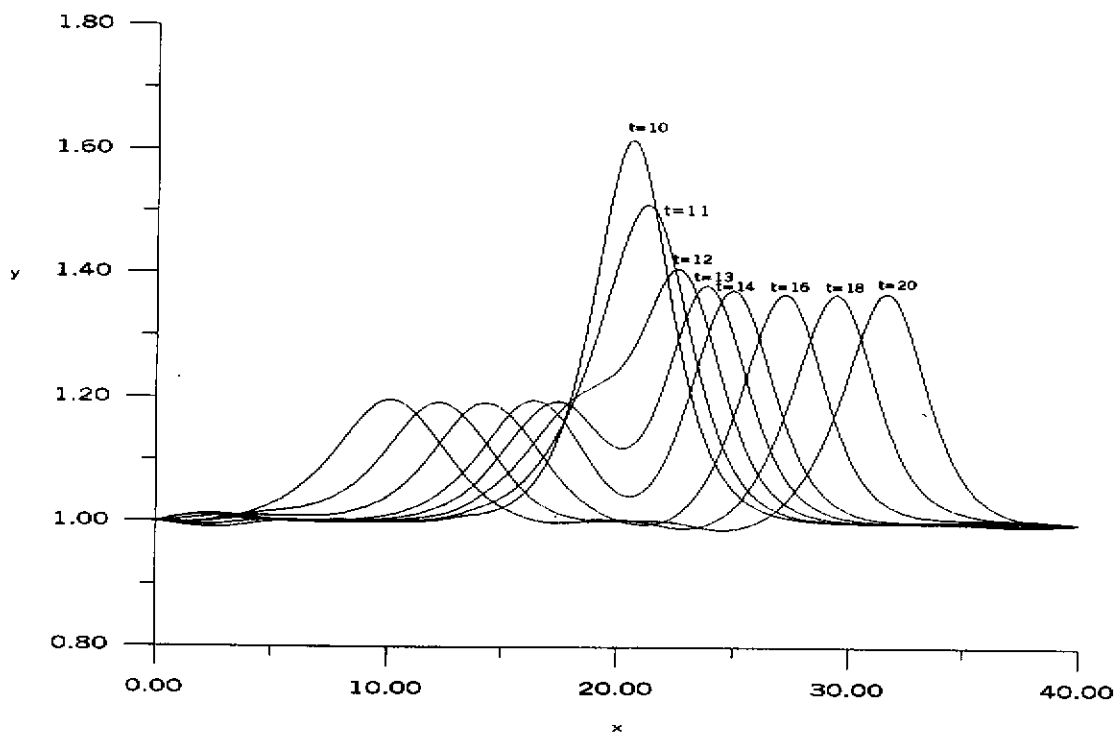
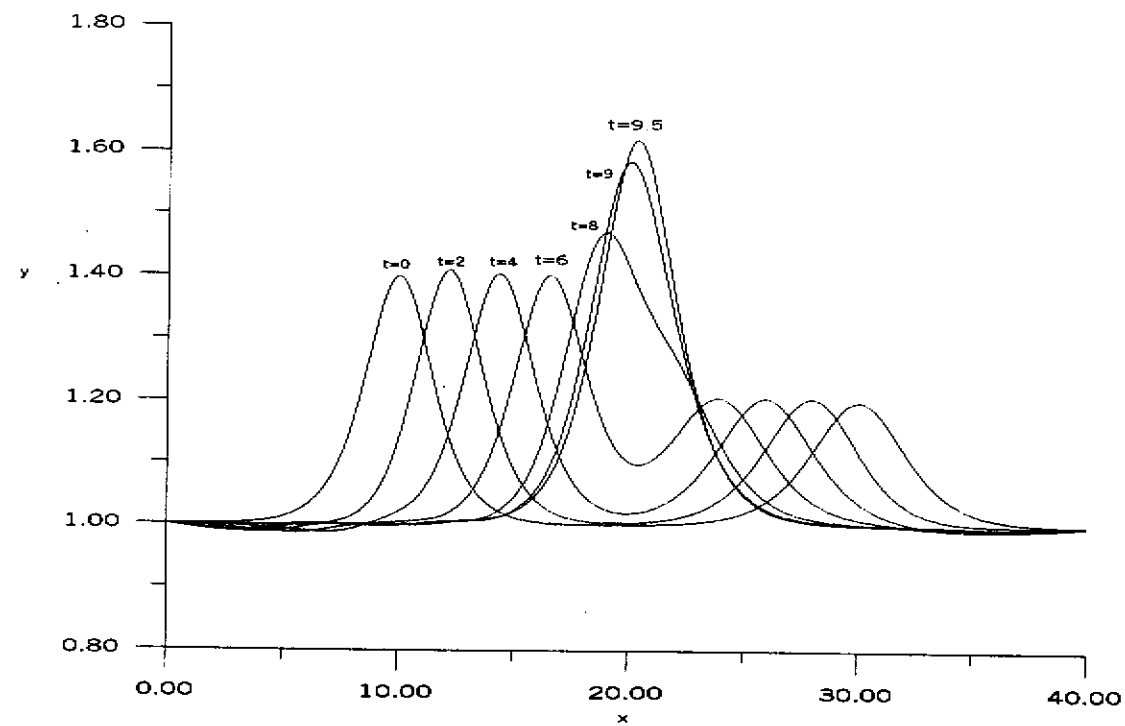


Fig 7: Two solitary waves travelling in opposite directions(Left hand side $A=0.4$, Right hand side $A=0.2$)

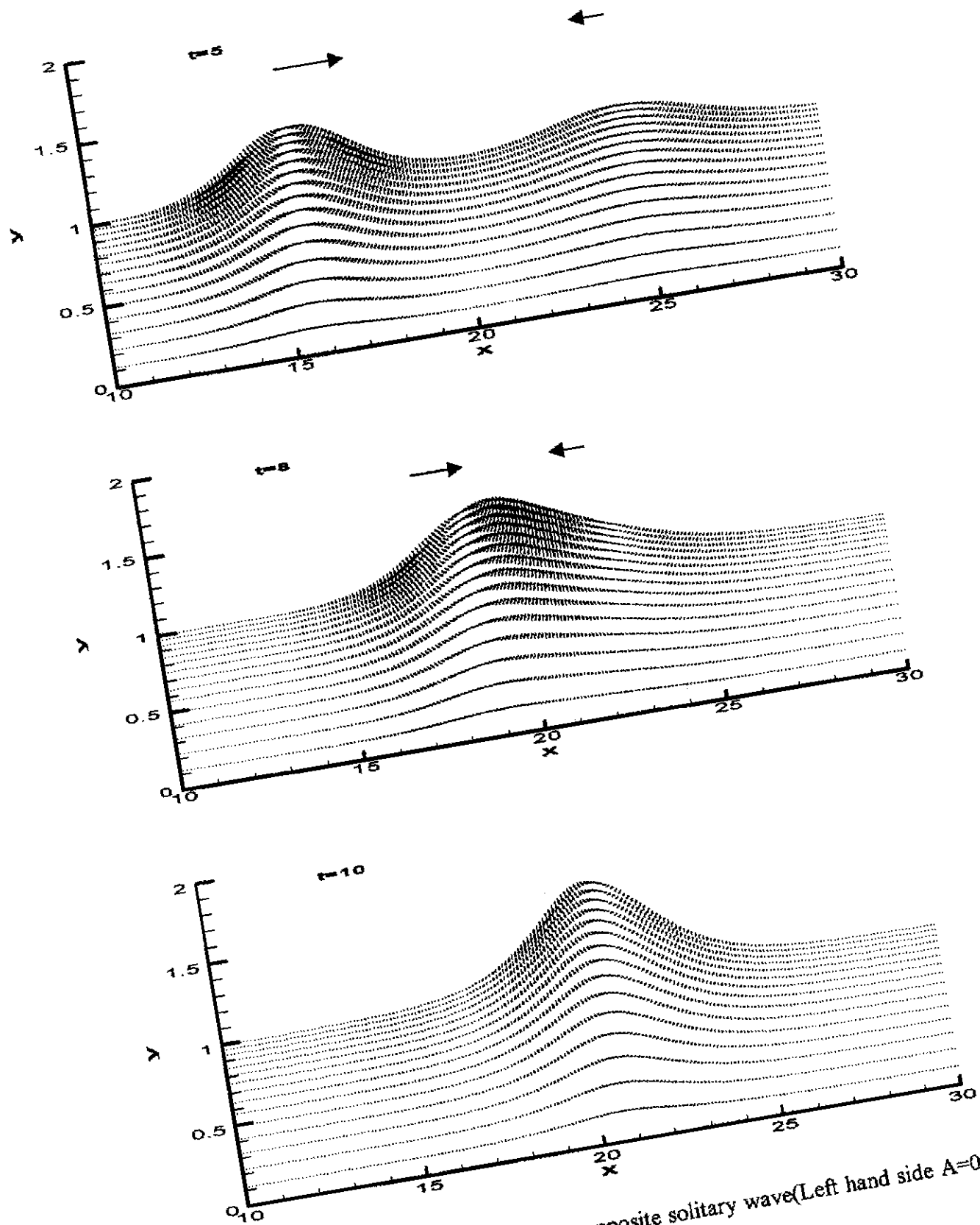


Fig. 8: The interactive processes of two opposite solitary wave (Left hand side $A=0.4$, Right hand side $A=0.2$)

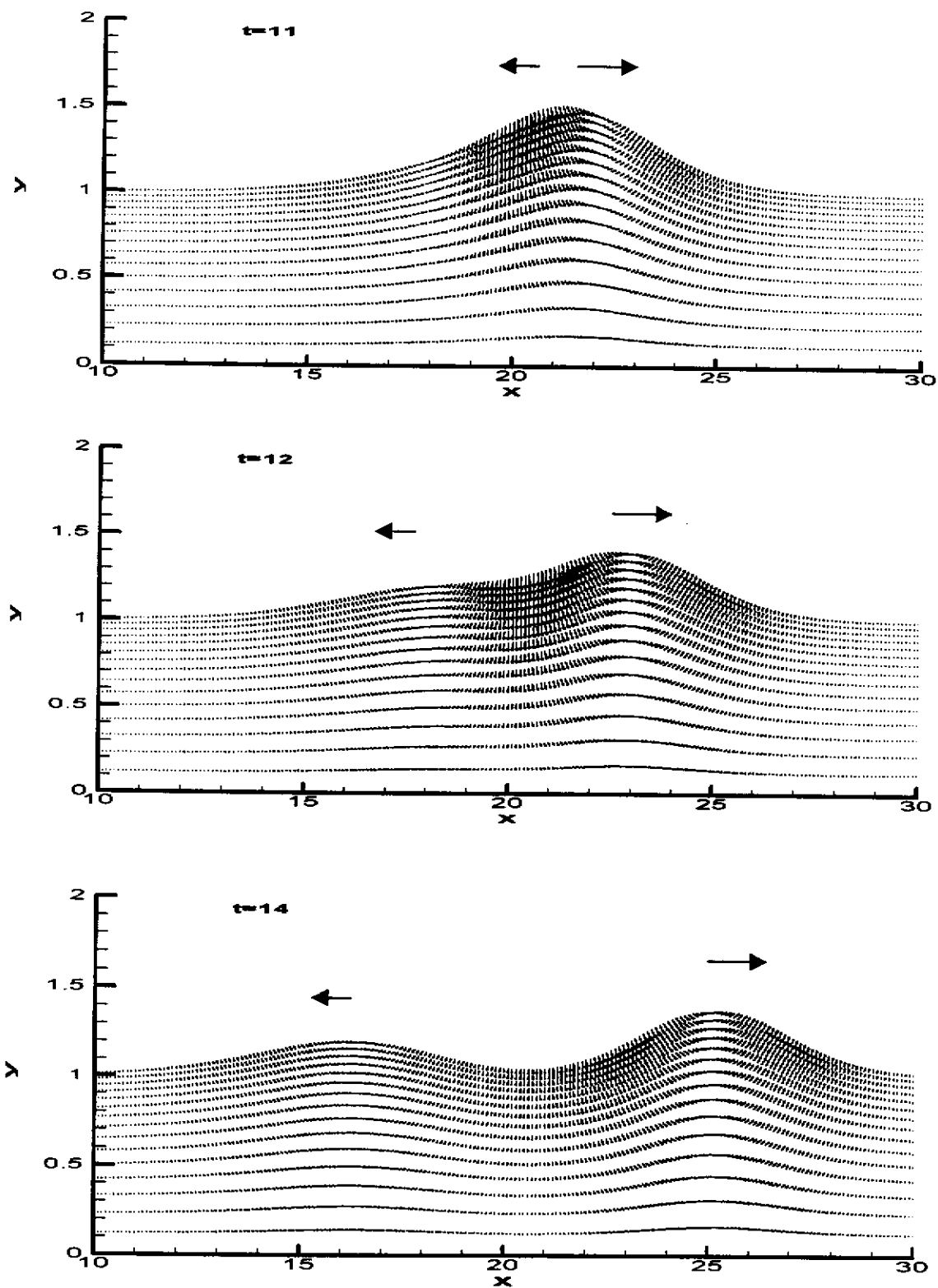


Fig. 9: The interactive processes of two opposite solitary wave(Left hand side $A=0.4$, Right hand side $A=0.2$)

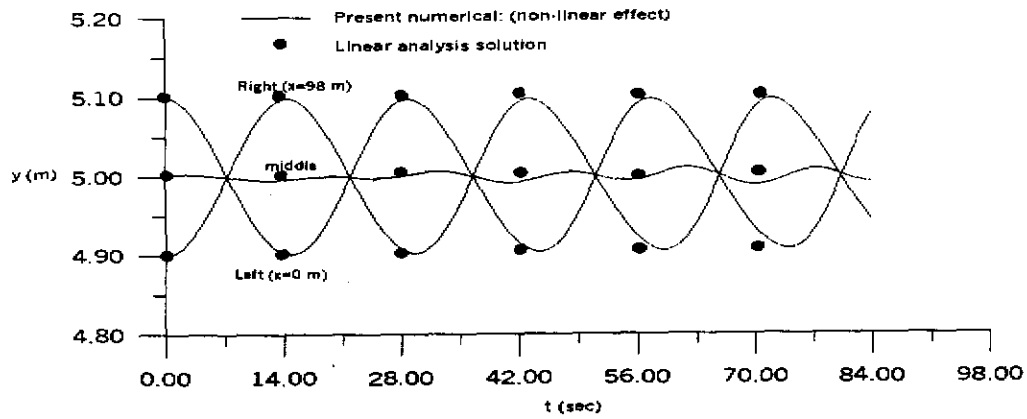


Fig. 10: The history of surface elevation for amplitude equal to 0.1 m

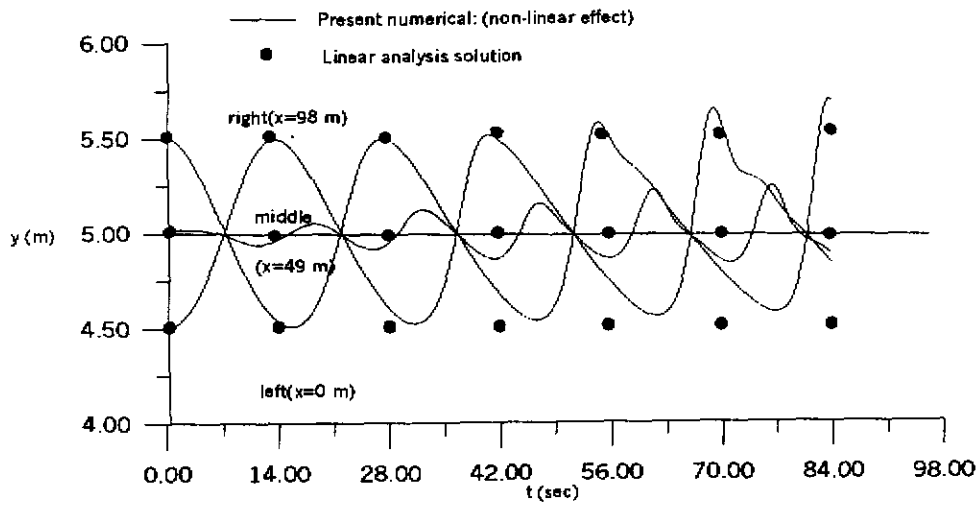


Fig. 11: The history of surface elevation for amplitude equal to 0.5 m

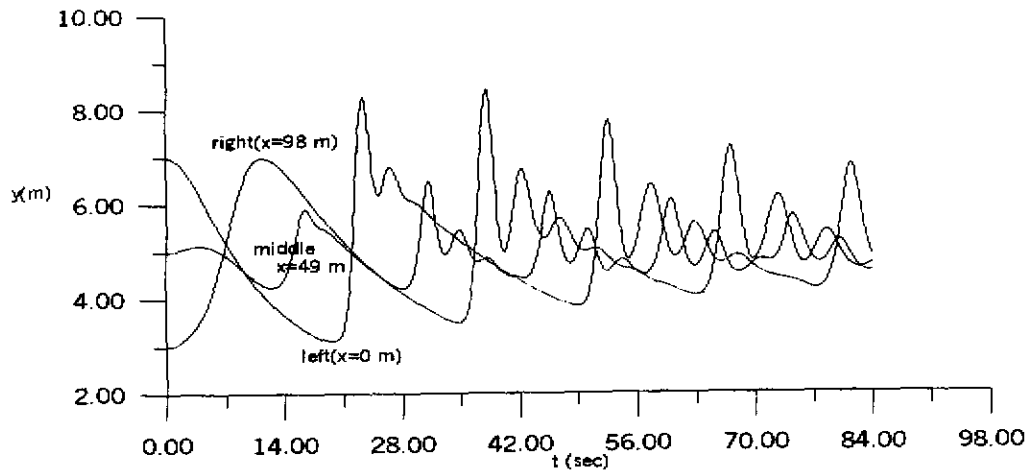


Fig. 12: The history of surface elevation for amplitude equal to 2 m

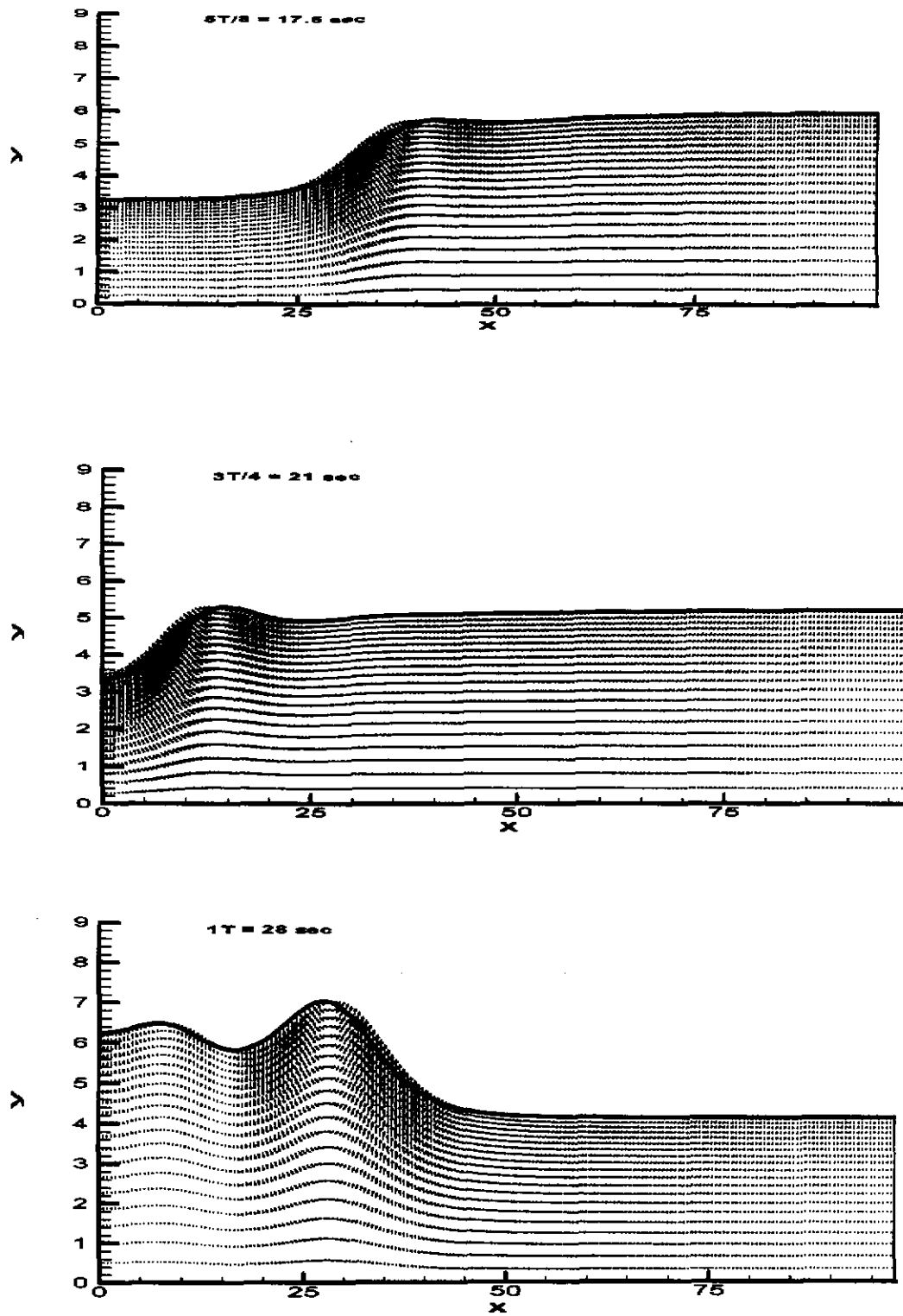


Fig.13: The velocity vectors for the seiche phenomenon in a rectangular reservoir($A=2$ m)

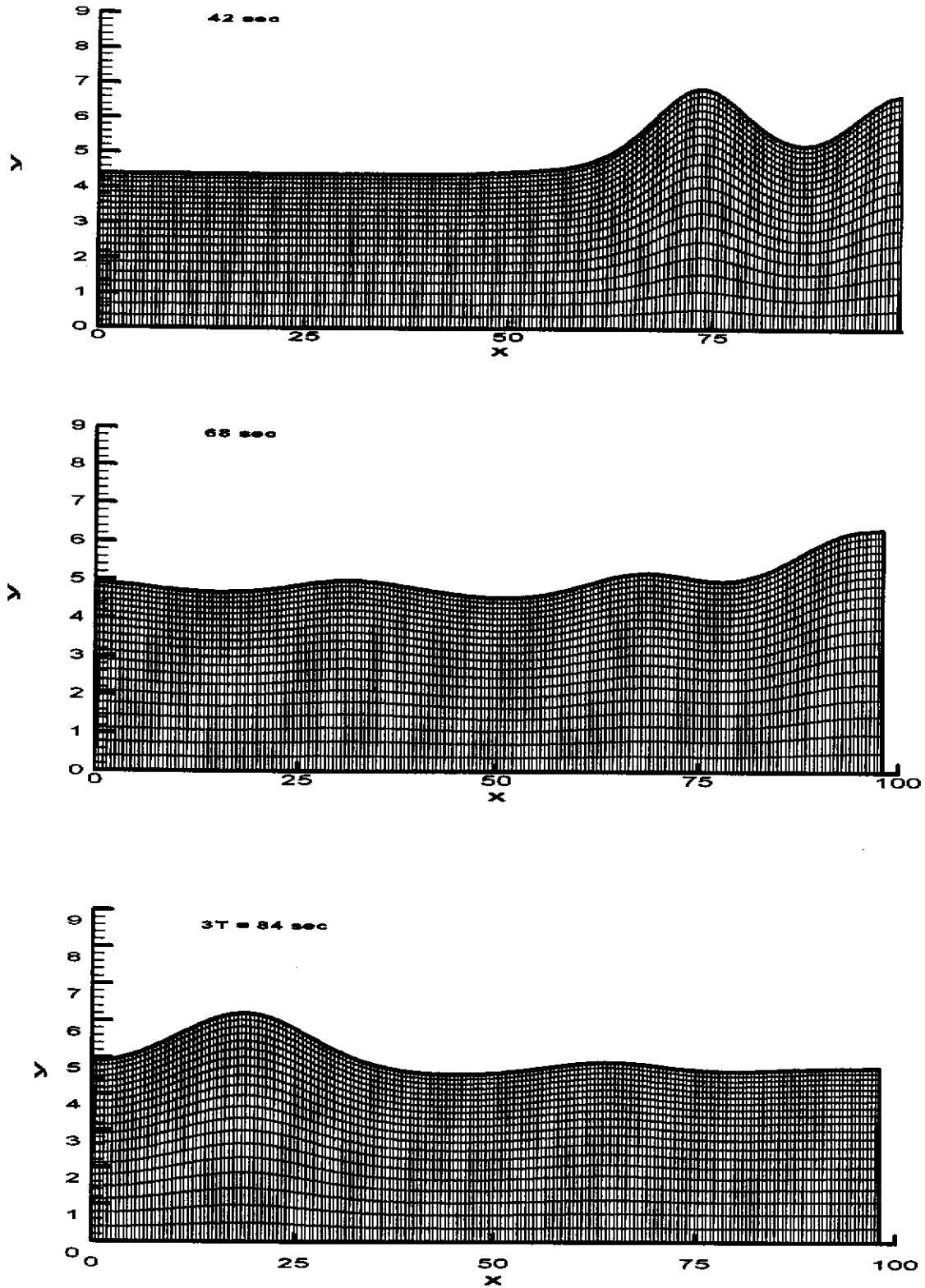


Fig.14: Moving boundary and moving mesh for the seiche phenomenon in a rectangular reservoir($A=2$ m)

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Effect of mass lumping in the study of Three-dimensional diffusion problem using isoparametric elements

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Abstract

The transient three-dimensional diffusion problem is solved using Galerkin finite element method to study the temperature variation at the center of a cube during sudden cooling. Linear and parabolic three-dimensional isoparametric elements are used using mass lumping for the capacitance matrix. A convergence study is also carried out to verify the effect of mass lumping on the temperature predictions using 8-node linear and 20 nodes parabolic elements. The limitation of mass lumping with 20-node elements has been discussed by comparing the predicted results with analytical solution.

Introduction

In the study of transient field problems, the time derivative is normally approximated using finite difference methods resulting in various schemes such as Crank-Nicholson, explicit, implicit and Galerkin. The use of above techniques will result in consistent capacitance matrices. Except for the explicit scheme, all the other schemes require matrix inversion while solving the simultaneous equations for getting solutions with time. When solving multi-dimension problems with higher order isoparametric elements, the size of capacitance matrix increases and hence use of matrix inversion results in higher computation effort. Mass lumping has been found to be an alternate to avoid the matrix inversion for certain type of problems. The name is derived from the original usage of mass lumping analysis used in mechanics [2]. In mass lumping procedure, all the nodal values in the given row of a capacitance matrix are added and assigned at the diagonal of the row.

Hence the capacitance matrix is reduced to a diagonal matrix. A derivation using a local shape coordinate shape function for time derivative has been discussed by Segerlind [9]. With mass lumping the simultaneous equations can be easily solved without matrix inversion for diffusion type of problems and this procedure results in an explicit time marching scheme. Whenever the given problem demands the use of an explicit time marching scheme, the mass lumping technique can be exploited in order to reduce the computation. Even though mass lumping reduces the computational effort very much, the suitability of the method has to be studied for a given problem.

Fried and Malkus [4] have found in their studies that mass lumping does not affect the accuracy of numerical computations. Gresho et al. [5] observed that mass lumping gives reasonable results for pure diffusion but the presence of advection the results may become unstable. and Mizukami and Tsuchiya [8] used mass lumping technique for the solution of three-dimensional Navier-Stokes equations. The authors have solved the transient Three-dimensional Navier-Stokes equations using fractional step method. The capacitance matrix for the transient velocity terms are mass lumped in both the time levels. The entrance flow in a square duct has been studied using 8-node isoparametric brick elements. Mass lumping is also applied successfully for solving multidimensional advection-diffusion equations. Wu [13] in his work on the use of wave equation model, solved the three-dimensional advection of Gaussian cylinder and a sphere using finite element method with mass lumping. Their results indicate that mass lumping has not degraded the numerical solution in contrast to the view expressed by Strang and Fix [10]. Moreover lumping reduces the computational effort. Hence wherever possible the capacitance matrix can be mass lumped in order to reduce the computational effort. Since the mass lumping assumes uniform capacitance within an element, a numerical test has to be carried out in order to verify how far this assumption holds well when higher order elements are used for discretizing the computational domain. The present work aims at

performing numerical experiments on the limitation of use of lumping technique as far as the type of elements are concerned. The problem of sudden cooling of a cube is considered as a test problem in the present work. Carslaw [3] reports the analytical results for such problem and Zienkiewicz and Parekh [12] report the numerical results. The above transient three-dimensional diffusion problem is studied using 8-node as well as 20-node isoparametric brick elements. Numerical results are obtained to understand the suitability of lumping technique with respect to convergence of results with mesh size as well as for the type of above mentioned isoparametric elements.

Governing equations

The following linear transient heat conduction equation in three-dimension is considered for the numerical experiment.

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) \quad (1)$$

where T- temperature, t-time, α -diffusion coefficient

The solid is subjected to dirichlet boundary condition as given by

$$T=T_b \text{ on part of the boundary} \quad (2)$$

Where T_b temperature at the boundaries

The governing equation (1) is integrated using Galerkin weighted residual finite element method. Let the variable T be represented by a shape function as follows:

$$T = \sum_1^n N_i(x,y,z)T_i(t) \quad (3)$$

where N_i are the shape functions defined for the spatial discretization. Since isoparametric formulation is concerned in the present work, the above it shape function will be used to discretize the variable T also. The index n takes value of 8 for an 8-node isoparametric element and 20 for 20-node isoparametric element. Applying the Galerkin weighted

residual technique for equation (1) using the shape function defined in equation (3), we get the following equation.

$$\int N_i \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) dx dy dz = 0 \quad (4)$$

After integration by parts [], we can write the final equation in matrix form as follows:

$$[C] \left\{ \dot{T} \right\} + [K] \{T\} + \{F\} = 0 \quad (5)$$

where $C_{ij} = \int_V N_i N_j dV$ and

$$K_{ij} = \int_V \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) dV \quad (6)$$

$\{F\}$ - load vector. The detailed derivation of the above equations can be obtained from references 6,11 and 12.

Numerical Solution

The final equation (5) is solved to obtain solution for temperature at different time levels. The time derivative is discretized using Crank-Nicholson scheme. This scheme is used to validate the code for the problem of sudden cooling as discussed by Zienkiewicz and Parekh [12]. Later results are obtained for the same problem by mass lumping the capacitance matrix. Two types of isoparametric elements with 8-node (linear) and 20-node (parabolic) are considered in the present study. This is in order to verify how lumping is effective when isoparametric elements with center nodes, such as in 20-node elements are considered.

The cooling of a cube initially at unit temperature is taken as a test problem [12]. The linear and parabolic three-dimensional isoparametric elements are used to study the temperature variation inside the cube. The cube initially at unit temperature is suddenly

exposed to zero surface temperature. It is required to study the temperature variation at the center of the cube side 'a' ($x=y=z=0$).

The boundary conditions are:

At $t=0$, $-a < x < a$, $-a < y < a$, $-a < z < a$, $T=1.0$

at $t>0$, $-a < x < a$, $-a < y < a$, $-a < z < a$, $T=0.0$

The surface boundary conditions are applied by considering the symmetry of the element in x,y and z directions. That means adiabatic boundary conditions are considered on the surfaces of the slice of the element considered.

Results and discussion

Initially the code developed for the study of three-dimensional transient diffusion problem using 8-node and 20-node isoparametric elements is validated with the results obtained by Zienkiewicz and Parekh [12]. Figures 1 and 2 show the comparison of the present results with the results of the above authors and the analytical solution, for 8-node and 20-node isoparametric elements respectively. It can be observed from both the figures that our predictions are in good agreement with the predictions of Zienkiewicz and Parekh [12]. The temperature variation during sudden cooling of cube is non-linear in nature. Hence linear isoparametric elements (8-node) are not sufficient to trace the temperature variations accurately. With the use of parabolic isoparametric elements (20-node) the temperature predictions are almost coinciding with the analytical solution as seen from Fig.2. All the above results are obtained using Crank-Nicholson scheme for discretization of time domain.

Now the capacitance matrix is lumped by adding all the elements in the row and assigning the result at the diagonal of the respective row. This process reduces the original consistent capacitance matrix to a diagonal matrix. Hence the solution procedure is much simplified. Without matrix inversion, the temperature can be predicted in an explicit time

marching method. Adding all the elements in the row does not pose any problem for the case of 8 nodes element, but in the case of 20-node element having mid side nodes, this technique does not work because of some negative entries in the capacitance matrix. Hence the alternate lumping procedure suggested by Hinton et al. [7,1] is followed for lumping in the case of 20-node elements. Before getting the results for temperature evolution, a test for the rate of convergence is carried out for both 8-node and 20-node elements. The results reported by Zienkiewicz and Parekh [12] correspond to 'a' and 'a/2' cases. The subdivision of the elements is continued further to 'a/3', 'a/4'...up to 'a/10' for the case of 8-node elements. For the case of 20-node elements the element length is subdivided only up to 'a/5' since there is a mid side node. The temperatures are predicted with time for different element length sizes. The difference between two consecutive set of element length size is taken as a criteria for convergence. When this difference becomes very small, then the results obtained will be consistent. These results are plotted in Figs. 3 to 6 for 8-node and 20-node elements for the complete transients. Figures 3 shows the rate of convergence for 8-node elements for time intervals from 0.1 to 0.5 and Fig.4 show the above results for time intervals from 0.6 to 1.0. For the initial transients up to the time level 0.5, the difference in the results become closer to zero beyond 343 elements (a/6). But for the later part of the transients, little oscillations in the difference are observed as seen from Fig.4. The difference is initially high with less number of elements and this decreases with increase in number of elements, in other words with finer mesh, for all the transients as expected.

The convergence results for 20-node elements are shown in Figs.5 and 6. The difference in temperature between two consecutive elements decreases as the number of elements increases up to 125 elements ('a/5') and beyond this the difference increases as against the trend observed in the case of 8-node elements. Moreover, the difference does not approach minimum for all the time levels from 0.1 to 0.5, as the time increases the difference also increases as seen from Fig.5. But in the case of 8-node elements the

difference becomes minimum for all the transients. For the time levels from 0.6 to 1.0, the difference becomes minimum up to 125 elements. When the mesh becomes very fine beyond this ($a/5$), the results diverge. These results indicate that mass lumping for capacitance matrix has some limitation when higher order elements are used. In order to have completeness in the convergence test, results are also obtained using Crank-Nicholson scheme for 8 nodes elements for all the transients. Figure 7 shows the results for time levels from 0.1 to 0.5 and Fig.8 shows the results for time levels from 0.6 to 1.0. It can be observed from both the figures that the convergence is obtained even from 8 elements itself and also the difference continues to decrease from the maximum for one element and reaches almost zero for 27 elements for all the transients. This behavior is expected since the time derivative is approximated with second order accuracy in the case of Crank-Nicholson scheme.

From the convergence test results it is observed that 8-node element are found to be suitable for the prediction of transient temperatures for a sudden cooling of a cube, compared to 20-node elements using mass lumped capacitance matrix. The temperature variations with time for different mesh sizes are shown in Figs. 9 and 10 for the case of 8 nodes elements. With one element, the temperature variations could not be predicted as the behavior of the analytical solution as seen from Fig. 9. When the number of elements are increased beyond one, the temperature transients follow the path of the analytical solution and the results deviate from the analytical solution when the mesh is coarse. With increase in number of elements, the numerical results become very close to the analytical results as indicated by Fig. 10. This trend is observed for 125 elements itself. Figure 11 shows the temperature transients for the case of 20-node elements. With one element, a temperature beyond the initial value of 1.0 is predicted at the beginning of the transient and with the highest number of elements, the latter part of the transients is observed to reach even negative values. In between the very coarse and very fine meshes, the temperature

transients follow the analytical solution with some differences. Unlike in the case of 8-node elements, even with finer meshes, the results do not become very close to the analytical solution for 20-node elements as seen from Fig. 11. The reason for getting negative temperature values for the finest mesh may be the lumping might have resulted in too much softening of the material.

Conclusion

Numerical experiments are carried out to study the effect of lumping for the case of sudden cooling problem of a cube using three-dimensional 8-node and 20-node isoparametric elements. The code developed has been validated with the results reported by Zienkiewicz and Parekh. A convergence test with different finite element meshes shows that 8 nodes lumped system predicts consistent results for all the transients; whereas the 20-node lumped system predicts consistent results only in the latter part of the transients. During the initial part of the transients, the results are not consistent. The 8-node lumped system predicts the temperature transients in accordance with the behavior of the analytical solution as the mesh becomes fine. Even though it is expected that 20-node lumped system should predict the results with more accuracy compared to the 8 nodes elements, the present study shows that 20-node lumped system give less accurate results because of over softening and hardening of the system with 20-node elements.

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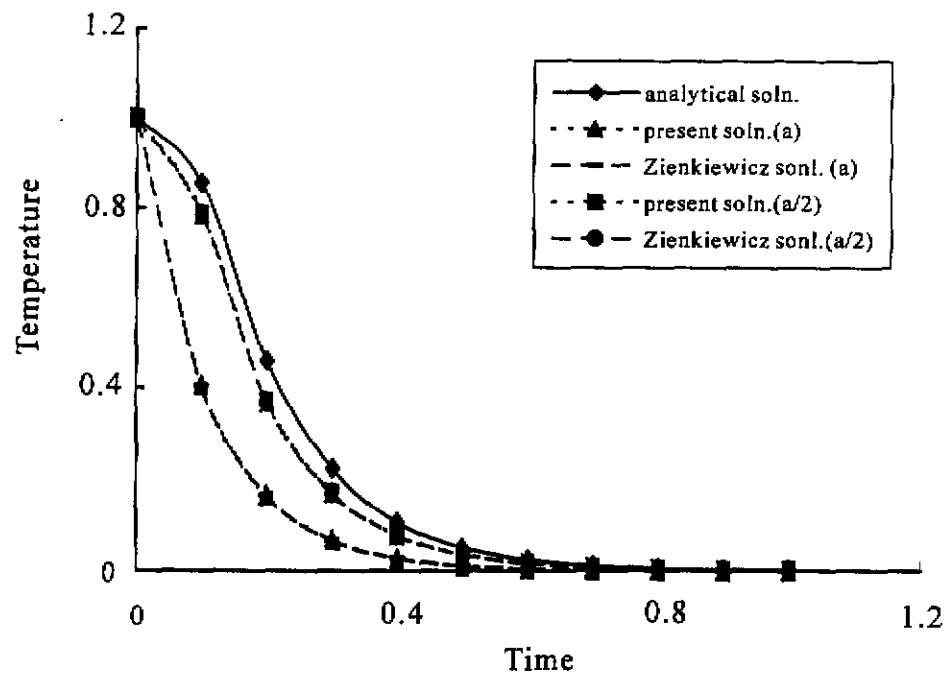


Fig. 1 Comparison of results with Zienkiewicz and Parekh for 8-node elements

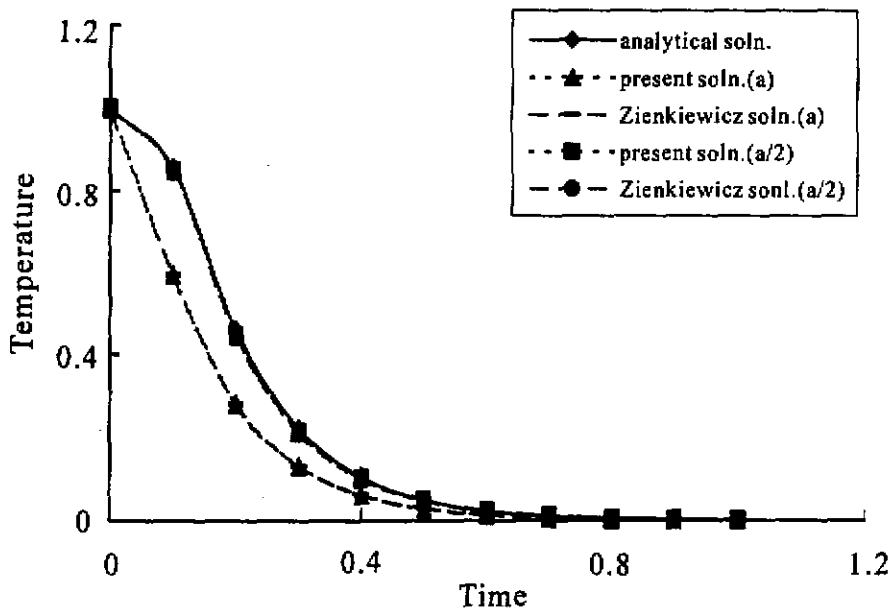


Fig.2 Comparison of results with Zienkiewicz and Parekh for 20-node elements

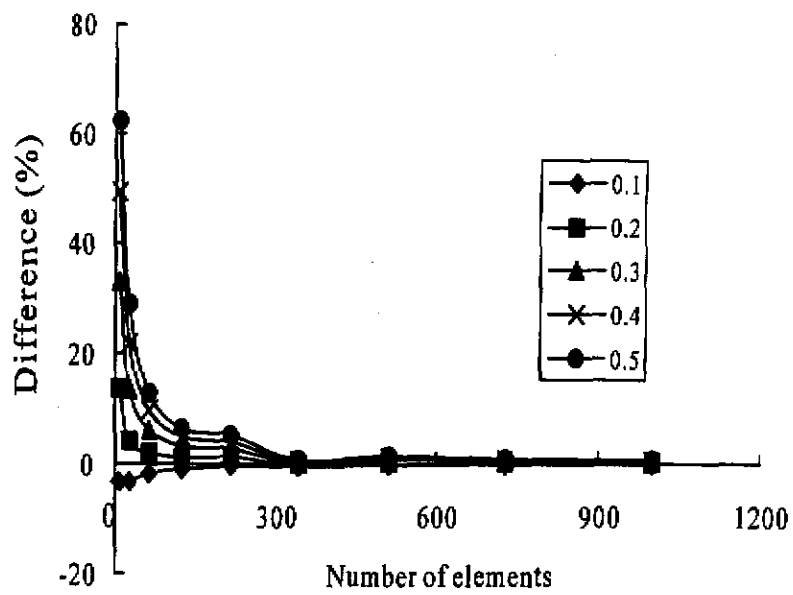


Fig. 3 Convergence results for 8-node lumping for time intervals from 0.1 to 0.5.

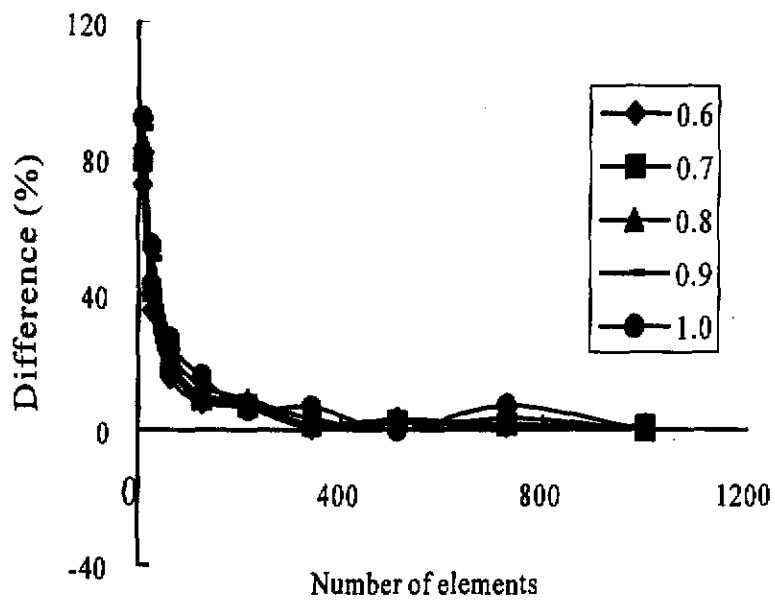


Fig. 4 Convergence results for 8-node lumping for time intervals from 0.6 to 1.0

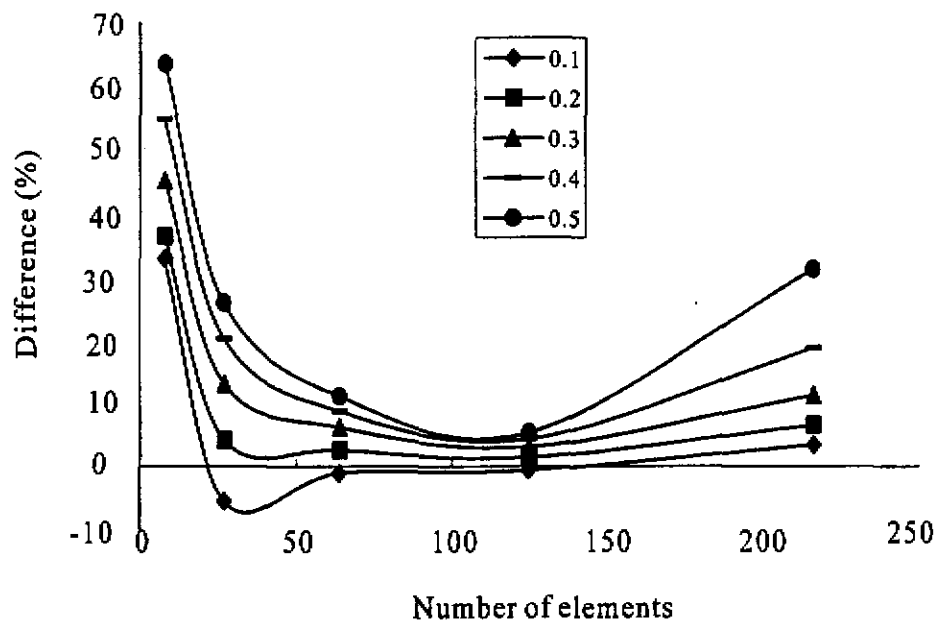


Fig.5 Convergence results for 20-node lumping for time intervals from 0.1 to 0.5

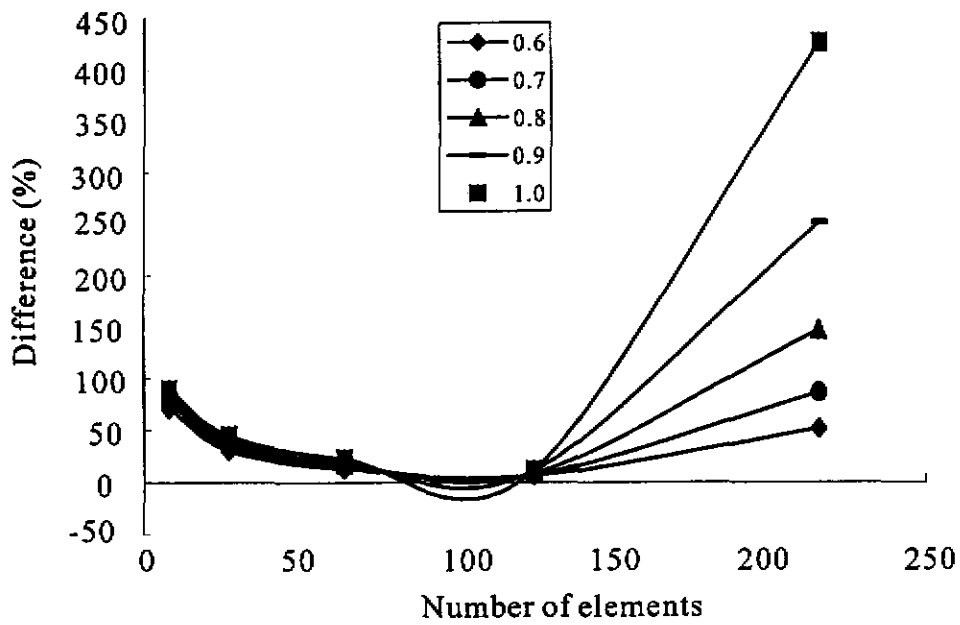


Fig.6 Convergence results for 20-node lumping for time intervals from 0.6 to 1.0

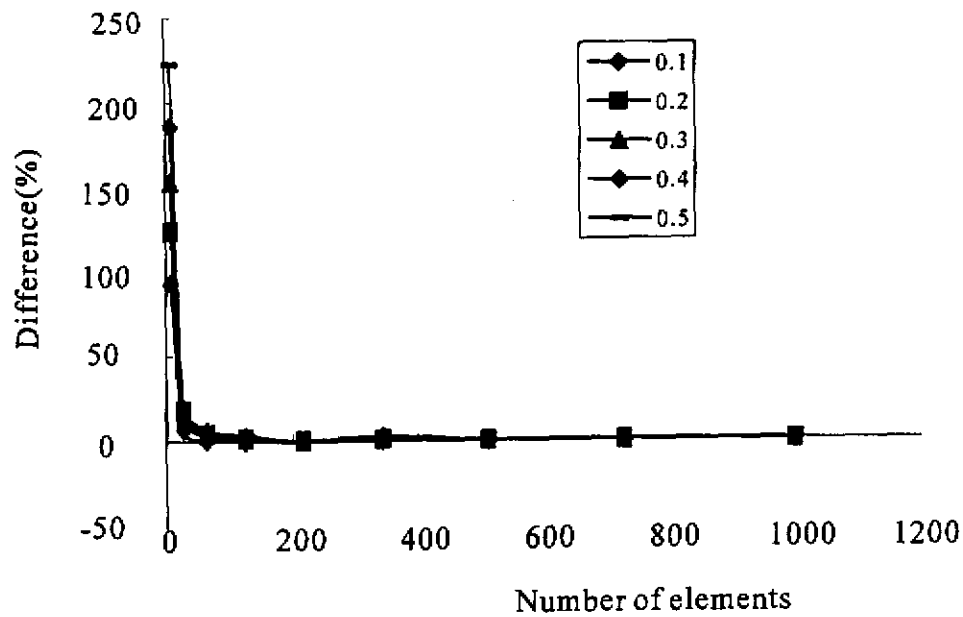


Fig.7 Convergence results for 8-node Crank Nicholson scheme for time intervals from 0.1 to 0.5

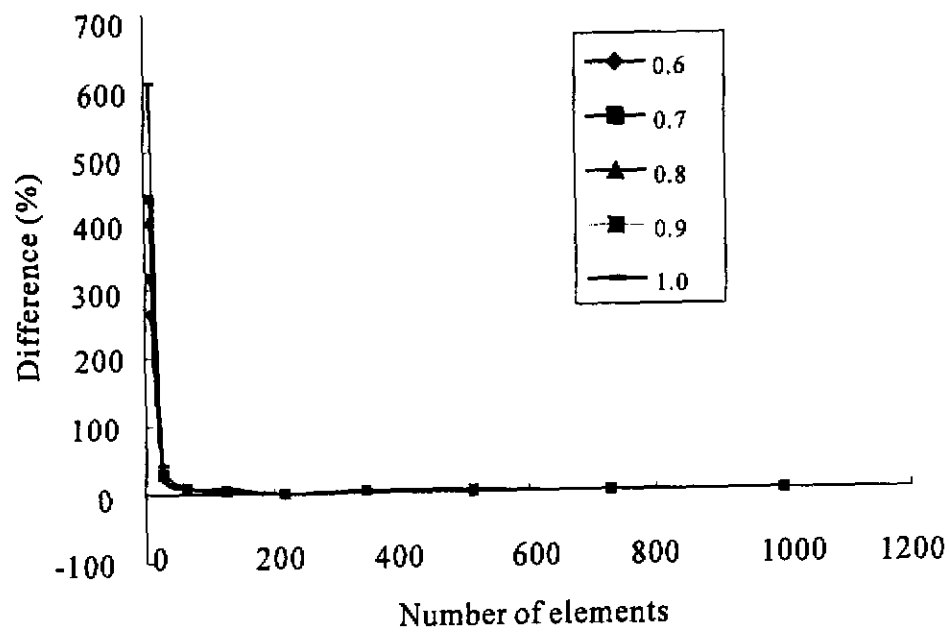


Fig.8 Convergence results for 8-node Crank-Nicholson scheme for time intervals from 0.6 to 1.0

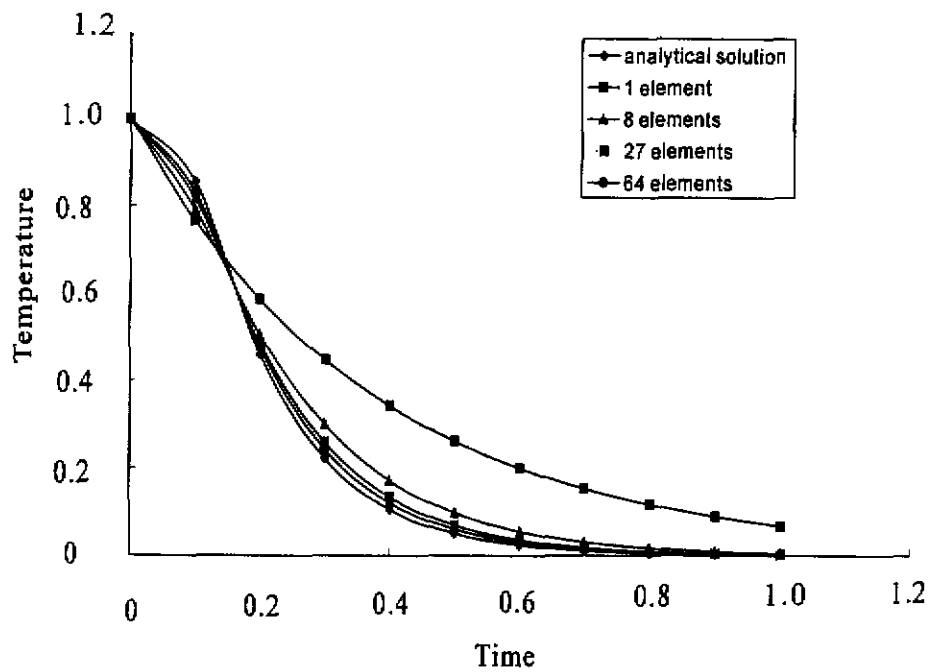


Fig.9 Temperature evolution results for 8-nodeelements for Crank-Nicholson for different number of elements

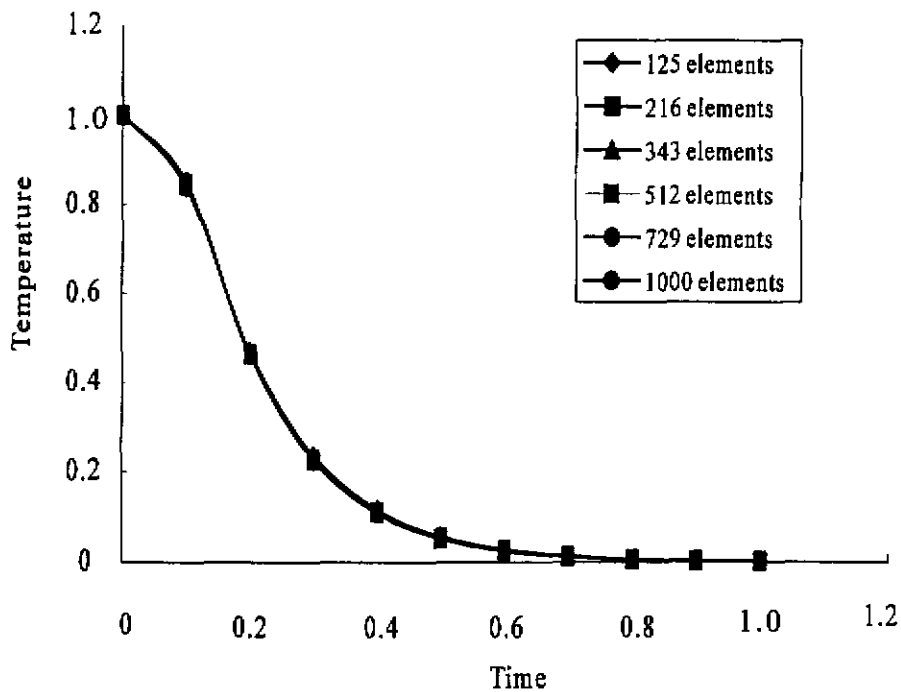


Fig. 10 Temperature evolution results for 8-node elements for Crank-Nicholson scheme for different elements

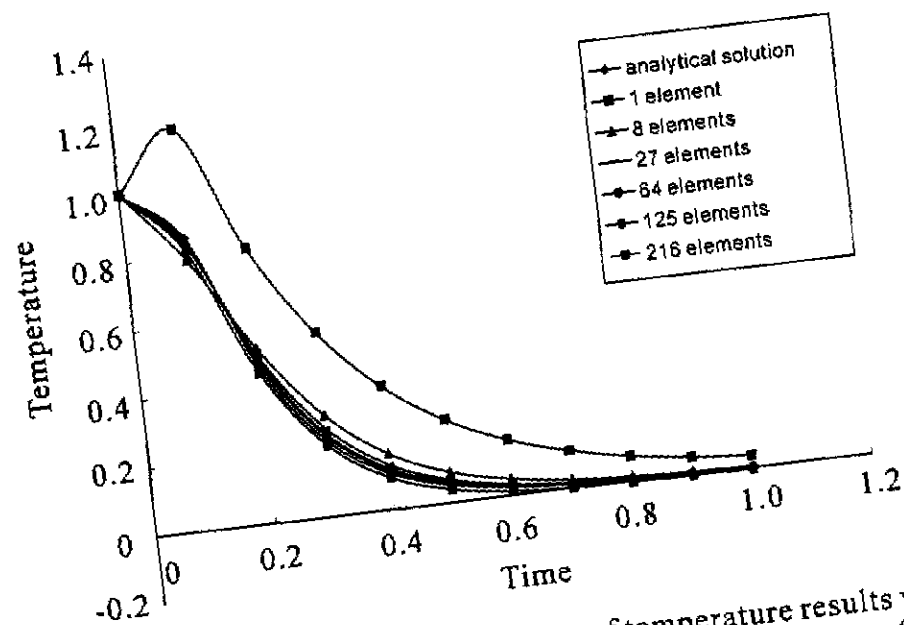


Fig.11 Comparison of time evolution of temperature results with analytical solution for 20-node lumping for different number of elements

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非線性三維河口污染物擴散模式之研究

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摘要

本文之研究目的，在於建立非線性三維河口污染物擴散之數學模式。為了儘量減低處理非線性方程式，我們在水理模式採用了以速度－渦度觀念，使得在處理速度分佈，祇為分離之線性 Poisson 方程式，而在渦度場方面，則為傳統之傳輸－擴散－反應方程式。為了達到降低維度，我們仍然使用了邊界元素法（ELBEM），以求解渦度、溫度、鹽度及污染物之傳輸－擴散－反應方程式。因此本研究重點，即著重於線性 Poisson 方程式之邊界元素及有限元素模式的建立及速度－渦度觀念之可行性。為了慎重起見，吾人先以二維之 Stokes 及 Navier-Stokes 之流場為例，模擬二維穴室流。由結果顯示，Stokes 及 $Re=2000$ 的 Navier-Stokes 之流場均能獲致準確之結果。雖然在此低的 Re 數下，仍能計算出週期運動及渾沌現象。此點顯示非線性之河口，與線性模式相比較，其水理之差異是有天壤之別的。其次，在三維的模擬上，三維 Stokes 穴室流也已獲得初步不錯的結果。吾人相信，以速度－渦度法來模擬河口水理的新觀念，是很有潛力的方法。

關鍵詞：河口水理，污染物傳輸與擴散，速度－渦度法，邊界元素法，有限元素法，三維，非線性模式。

Nonlinear 3D Mathematical Modeling of Pollutant Transport in Estuaries

Der-Liang Young¹ Sheng-kai Yang² Ying-Hong Liu²

Abstract

The main purpose of present study aims at the establishment of a mathematical model for predicting the pollutant transport in a nonlinear 3D estuary. To reduce the handling of nonlinear partial differential equations, the concept of velocity-vorticity formulation is adopted to model the estuary hydrodynamics. Thus the governing equations for the velocity field are deduced to the linear Poisson equations. As far as solution of vorticity is concerned, we have successfully developed an Eulerian-Lagrangian Boundary Element Method (ELBEM) to attack the advection-diffusion-reaction equation. To further lower the dimension, the BEM is again applied to solve the velocity Poisson equation. The distribution of pollutant, temperature, as well as salinity are all solved by the ELBEM algorithm as well as the the feasibility of the concept of velocity-vorticity

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formulation.

To test the basic methodology, we choose the 2D Stokes and Navier-Stokes equations for simple flows as a firm starting. The results reveal that the Stokes and Navier-Stokes flows with Re as high as 2,000 have both rendered very encouraging outcomes. Even in very lower Re flows, the periodic, aperiodic and chaotic flow structures have been obtained. The nonlinearity has demonstrated to play a vital role in the estuary hydraulics, as comparing with the linear model. The more complex flow structure is not found in the linear model. We are now in a position to investigate the 3D velocity Poisson equation.

The 3D stokes cavity flow is again used to illustrate the numerical simulation. The reasonable outcomes also convince us that the velocity-vorticity method will become an innovative algorithm to model the pollutant transport in a nonlinear 3D estuary.

(Keywords: Estuary hydrodynamics, Pollutant advection-diffusion, Velocity-Vorticity method, Boundary element method, Finite element method, 3-dimension, Nonlinear model)

一、緒論

台灣地區地狹人稠四面環海，河口及沿海之開發日益頻繁，集中之人口及不斷成長之工業對水域之水質與環境造成負面之影響，水質規畫與管理之工作成為重要的課題，然而，河口及沿海水域之污染物傳輸與擴散機制深受河川流量及水質、海洋潮汐、洋流運動、風力、地球自轉之科氏力、海水密度層變及河口與海岸地形等因素所影響。欲瞭解河口及沿海水域複雜污染物對流、擴散與反應現象，水理與水質數值模擬應是最佳之分析方法。

前三年在國科會的資助下, Young and Wang (1994), Young and Wang (1995), 楊德良、何柏釗(1996), Young and Lin(1994), Young and Lin (1996), 「三維河口污染物擴散模式之研究」以建立三維時變之線性水理及水質數值模式，透過數值模擬測試，已可明瞭河口及沿海大尺度之淺水流場受海洋潮汐作用產生之週期運動、受科氏力影響之愛克曼螺旋機制、風剪力拖曳效應及海水密度層變之影響。模式應用邊界元素法（邊界積分法）以克服三維模擬之龐大計算容量與計算時間，並降低數值擴散及數值延散之產生。

本計畫再將線性模式推廣到非線性之水理與污染物之數值模式，我們已成功的發展一套利用邊界積分法來解決非定常性之污染物的傳輸擴散模式，對於降低維度與減少數值擴散與數值延散，均有良好之結果，如此，對於以前未考慮慣

性力與水平擴散之水理模式，可以獲得更圓滿的解決。對於河口污染物擴散之研究，將可更上一層樓。研究方向將分三個階段進行，第一階段進行沒有密度層變之非線性水理與污染物邊界積分數值模式之建立並與目前線性模式互相比較，以瞭解慣性力與水平擴散向對於水理之影響。第二階段則著重有密度層變之非線性三維河口污染物之擴散模式研究，最後階段則著重能以現場資料，尤其是淡水河口為例，探討模式之可行性。

二、數學模式

2.1 水理模式

本研究為非線性極強之廣義 Navier-Stokes 方程式及連續方程式，為避開處理壓力及降低非線性與希望達成分割(decoupling)而有利於平行計算(parallel computing)，今以速度渦度法(velocity-vorticity method)來求解均值(即沒有密度層變)之河口水理。其基本方程式為

$$\nabla^2 \bar{u} = -\bar{\nabla} \times \bar{\omega} \quad (1)$$

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \bar{\nabla} \bar{\omega} = \nu \nabla^2 \bar{\omega} + (\bar{\omega} + f\hat{k}) \cdot \bar{\nabla} \bar{u} \quad (2)$$

式中 $f = 2\Omega \sin \theta$, $\bar{\omega} = \bar{\nabla} \times \bar{u}$

2.2 污染物傳輸模式

描述污染物傳輸模式，一般以所謂之傳輸(advection)、擴散(diffusion)及反應

(reaction) 方程式為之，即

$$\frac{\partial \bar{C}}{\partial t} + \bar{u} \cdot \nabla^2 \bar{C} = k_r \nabla^2 \bar{C} + \bar{S}_r(\bar{C}, \bar{x}, t) \quad (3)$$

配合以前之研究-「三維河口污染物擴散模式」之研究，我們已成功的發展一套非線性之歐拉-拉格蘭吉邊界元素法，Eulerian-Lagrangian Boundary Element Method (ELBEM)，如果能將整個系統改成(3)式之標準式，觀念上已完全解決了本研究計畫，因為在第二階段有密度層變(density stratification)之計畫中，吾人只要在第(2)式中增加因密度而增加之渦度即可。

$$\frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \nu \nabla^2 \bar{\omega} + (\bar{\omega} + \bar{f}\bar{k}) \cdot \bar{\nabla} \bar{u} + \bar{\nabla} \times \left(-g \frac{\rho - \rho_0}{\rho} \bar{k} \right) \quad (4)$$

及狀態方程式

$$\rho = \rho(T, S, \bar{C}) \quad (5)$$

及溫度方程式

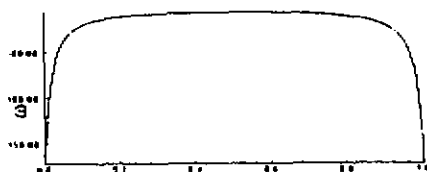
$$\frac{\partial T}{\partial t} + \bar{u} \cdot \bar{\nabla} T = k_T \nabla^2 T + S_T(T, \bar{x}, t) \quad (6)$$

及鹽度方程式

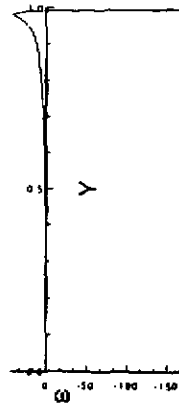
$$\frac{\partial S}{\partial t} + \bar{u} \cdot \bar{\nabla} S = k_s \nabla^2 S + S_s(S, \bar{x}, t) \quad (7)$$

三、數值模擬結果

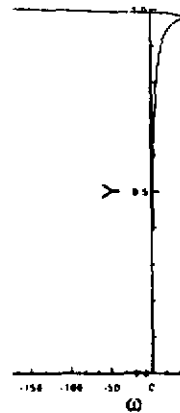
本文為研究速度-渦度法以求解速度場及渦度場之觀念是否正確可行，為顧及計算量之龐大與複雜性，先以二維之 Stokes 及 Navier-Stokes 流場為試驗。在速度場求解，係以邊界元素法(BEM)為主軸，分別求解 u 及 v 之速度分向。而在渦度場之解法，則是利用以前所發展之(ELBEM)方



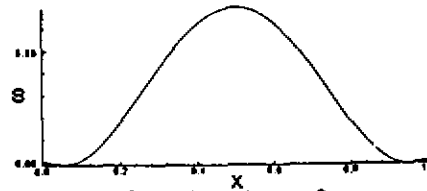
1. Vorticity along y=1



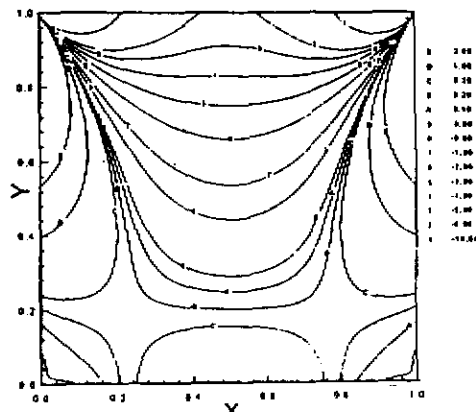
2. Vorticity along x=0



4. Vorticity along x=1



5. Vorticity along y=0



3. Vorticity contours

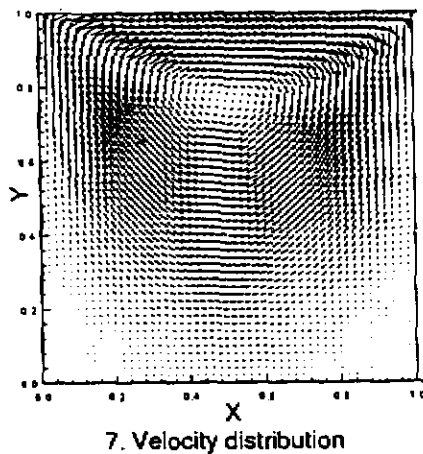
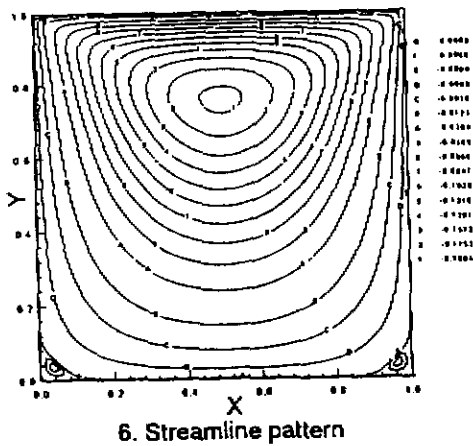
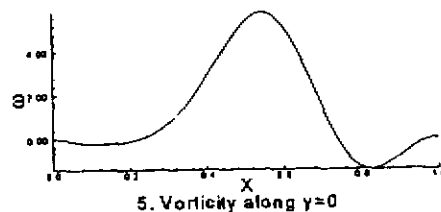
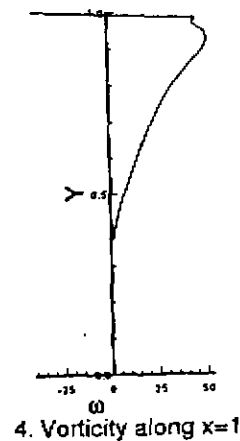
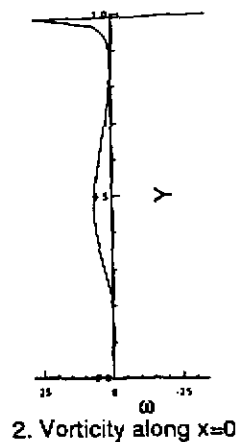
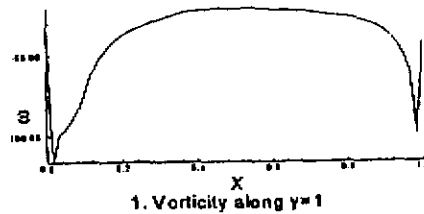
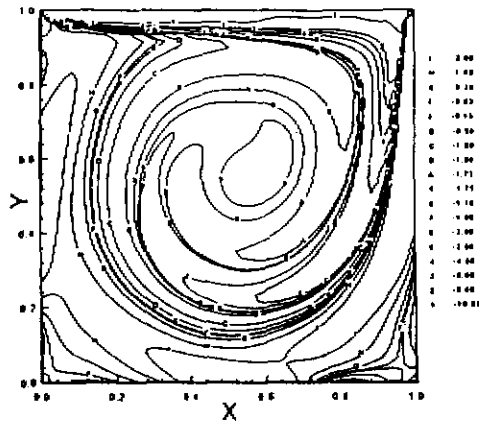


圖 1:二維穴室流場之物理特性

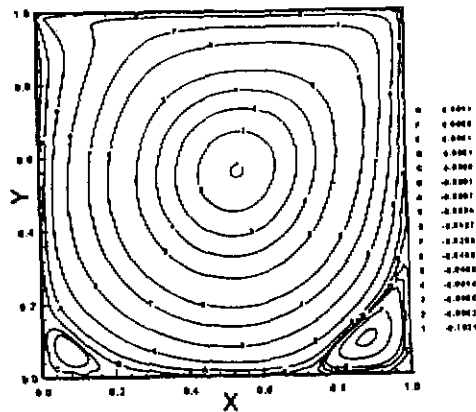
法,以求解渦度之傳輸與擴散過程。圖 1 為 Stokes 流場中上邊界速度 $u=1$ 之等渦度線,及邊界渦度、流線及速度分佈圖,為瞭解渦度邊界條件對流場之影響,利用四種不同之邊界條件設定方法,發現穴室流中移動上之邊界與兩側壁交接處之奇異點分佈,對流場有甚大之影響。經由與增加奇異點附近之節點密度,可將流場環流量逼近至 -1.001,與解析環流量值 -1 間相對誤差小於 0.2%,連續方程式則滿足到 (-14),與理論值 0 相差極小。計算渦心位置 (0.500, 0.760),渦心強度為 -3.12,流線值 -0.0995,均與前人之研究結果甚為相符。至於計算二維黏性不可壓縮流,由雷諾數 0.001 到 2000,將中線速度分佈,渦心強度,渦度值與角窩大小等流場重要特徵與 Burggraf, Ghia, Pan, Young, 廖清標 (1997), 等人用其他計

算流力方法比較,本研究亦得到相當好的結果。圖 2 為 $Re=2000$, Navier-Stokes 流場中上邊界條件 $u=1$ 之等渦度線及邊界渦度、流線及速度分佈圖。

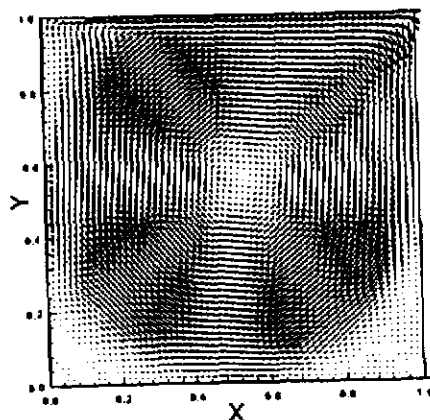




3. Vorticity contours

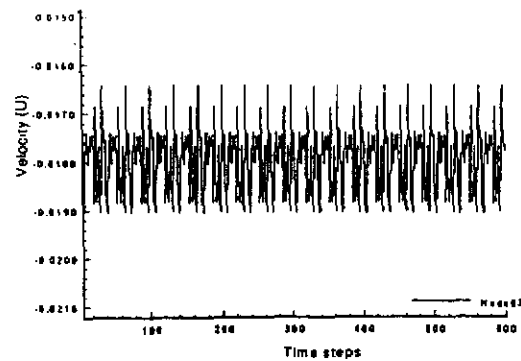


6. Streamline pattern

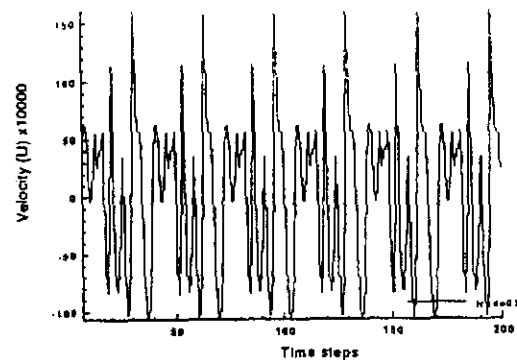


7. Velocity distribution

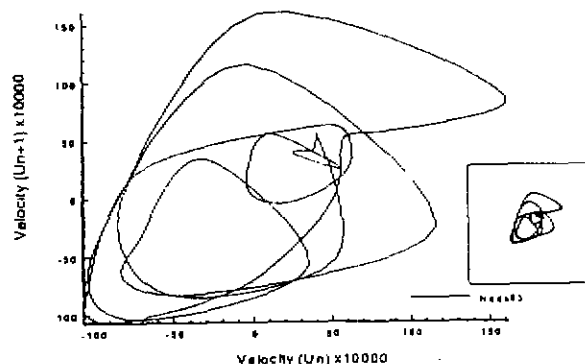
爲了更進一步探討低雷諾數之渾沌動力現象，本文發現在 $Re=1$ 及 $Re=10$ 時均開始有所謂週期循環解存在。向穴室流移動，流場動力現象會越來越複雜，甚至存在著包含 10 個以上頻率之和諧解，圖 3 爲 $Re=1$ 節點 3 之水平速度 u 之混沌特性。如把雷諾數提昇到 $Re=10$ ，發現流場仍有混沌現象存在，但以較 $Re=1$ 回穩不少，和諧現象依然存在，但包含頻率已降到 4 個左右，圖 4 爲 $Re=10$ 節點 3 之水平速度 u 之混沌特質。



(1) Time history of velocity (U) (original scale)

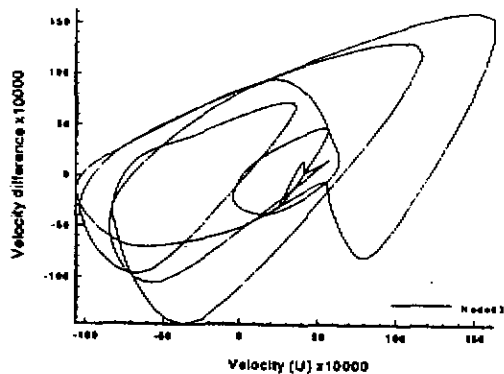


(2) Time history of velocity (U) (zoom in)

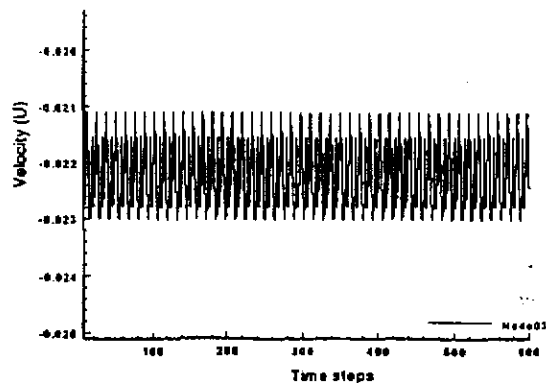


(3) Phase plane of velocity (U) on time n and $n+1$

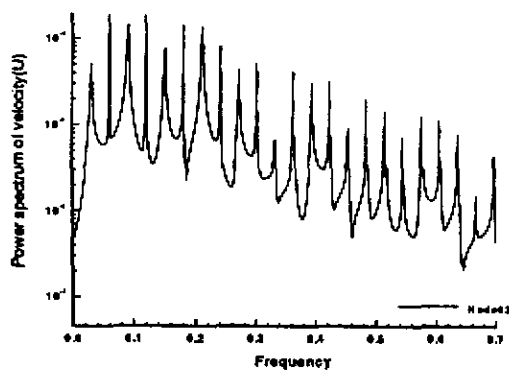
圖 2: 二維穴室流場在 $Re=2000$ 之物理特性



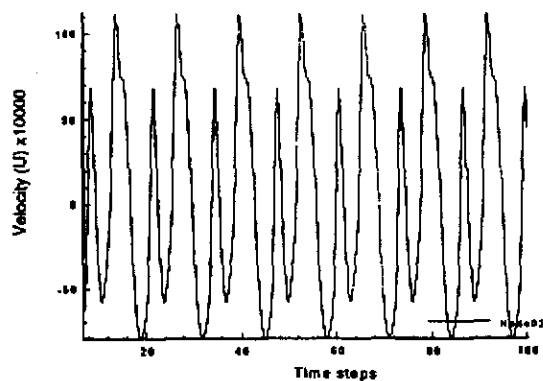
(4) Phase plane of velocity(U) and velocity difference



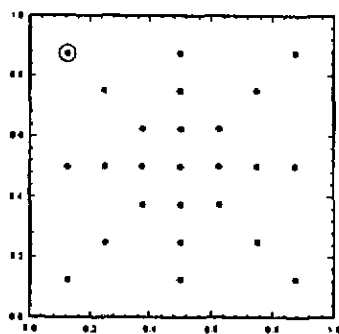
(1) Time history of velocity (U) (original scale)



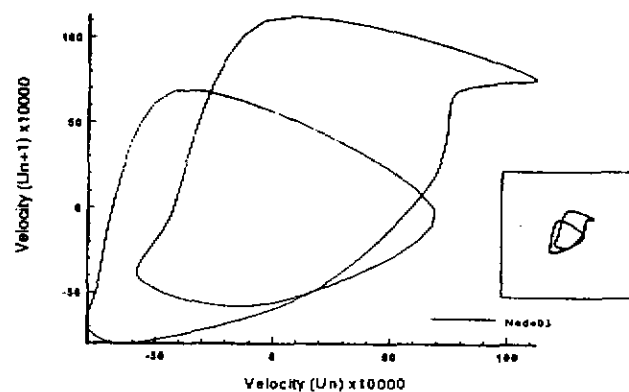
(5) Power spectrum of velocity(U)



(2) Time history of velocity (U) (zoom in)

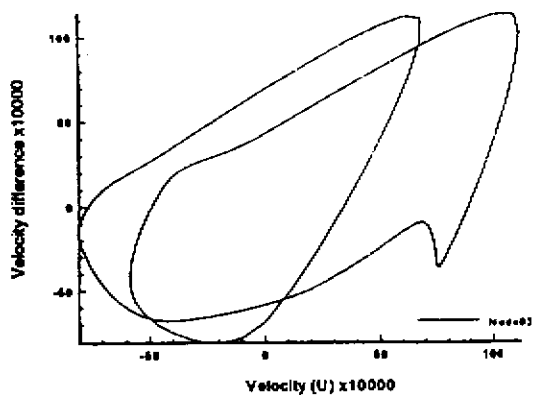


(6) Location of the present node

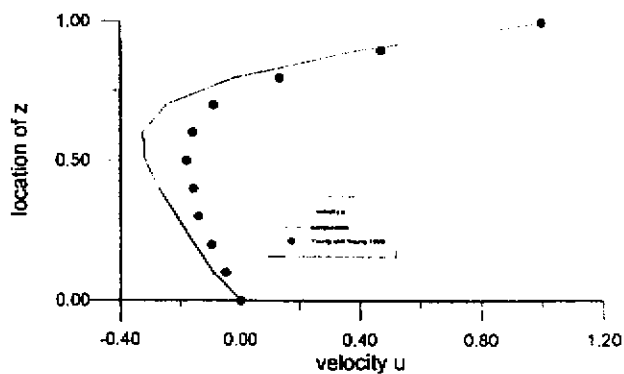


(3) Phase plane of velocity(U) on time n and n+1

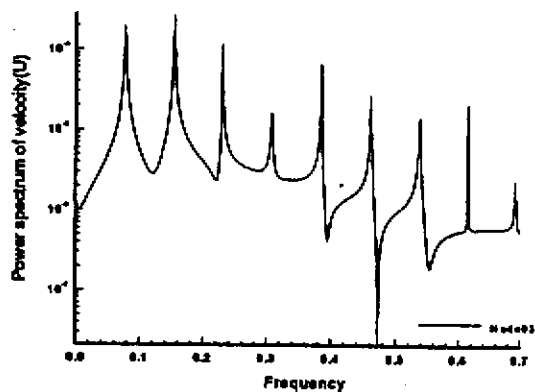
圖 3: 二維穴室流場在 $Re=1$ 於節點 03 之 u 速度場特性



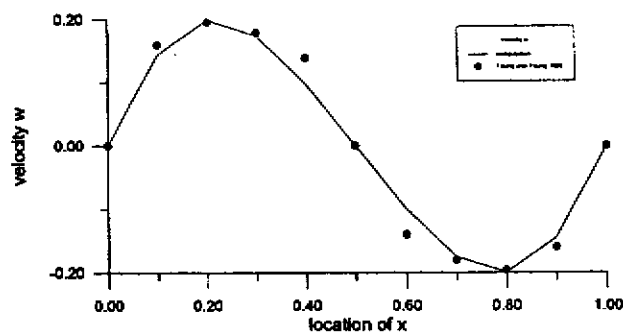
(4) Phase plane of velocity(U) and velocity difference



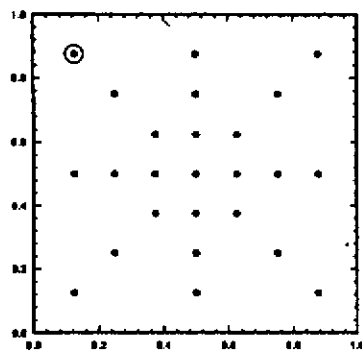
(1) u-velocity distribution at the plane of $x=0.5 \cap y=0.5$



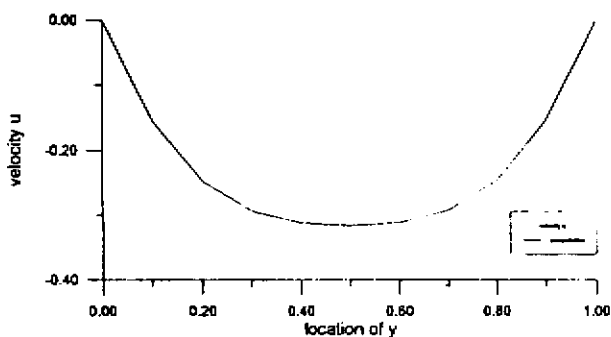
(5) Power spectrum of velocity(U)



(2) w-velocity distribution at the plane of $y=0.5 \cap z=0.5$



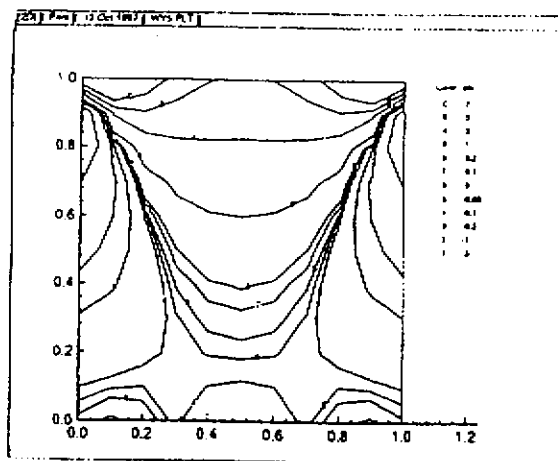
(6) Location of the present node



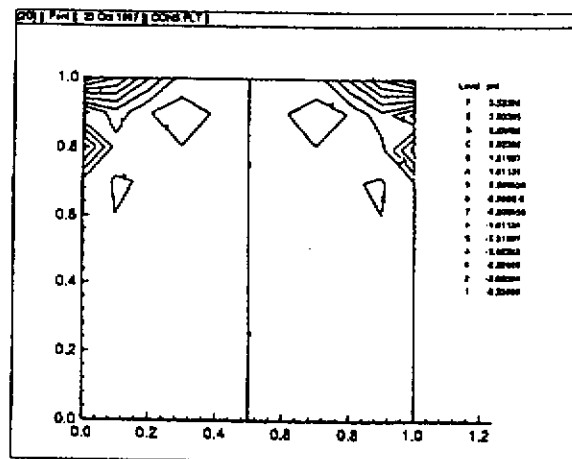
(3) u-velocity distribution at the plane of $x=0.5 \cap z=0.5$

圖 4:二維穴室流場在 $Re=10$ 於節點 03 之 u 速度場特性

最後對於三維流場之 Stokes 流場，圖 5 顯示水平速度 u ，垂直速度 w 及水平速度 v ， y 方向渦度之分佈圖及連續方程式之收斂分佈圖。



(4) η -velocity distribution at the plane of $y=0.5$



(5) Convergence for 3D Stokes flow

圖 5: 三維 Stokes 穴室流場之物理特性

四、結論

本研究希望藉由速度渦度方法之觀念，經由邊界元素法及歐拉-拉格蘭吉邊界元素法 (ELBEM) 求解非線性三維河口污染物擴散之機制，以其提昇基礎研究之數值模擬能力，探討物理現象，提供實際工程設計規畫與污染物之控制與管理。達成保護台灣地區河口海域及近岸海域之環境保護。

經由速度-渦度列式，速度場為線性，且為簡單之勢能 Poisson 方程式流場，而非線性則僅存在於渦度方程式。如此一來，如果渦度亂成一

團，有混沌現象，成為紊流，則速度場將隨之混亂。吾人已由低雷諾數之二維 Navier-Stokes 方程式求得驗證。本研究已證明速度-渦度可以精確地求解到非線性之 Navier-stokes 方程式，至少二維是可行的。目前已進行三維之演算，線性之 Stokes 方程式已有初步之結果。目前為了改善計算效率，正積極從事其他較為省時或更具效率但仍不失精度的 RUNGE-KUTTA FEM 方法，以比較目前發展之 ELBEM 法之效率及精確度。

誌謝

本論文依國科會專題研究計畫「非線性三維河口污染物擴散模式之研究 (一)」(編號 NSC86-2611-E-002-026) 之研究成果，楊德良等 (1997)。承蒙國科會經費之贊助使本研究得以完成，僅敘感謝之意。

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利用速度-渦度法解析三維黏性不可壓縮流場

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摘要

本文利用速度(Velocity)-渦度(Vorticity)法搭配有限元素法(Finite element method)，邊界元素法(Boundary element method)及二階朗吉庫特法(Runge-Kutta method)求解三維慣性座標和非慣性座標不可壓縮黏性流場，文中以簡單之三維箱型穴室流(cavity flow)作為驗證程式的依據。在驗證過程中，發現速度-渦度法對於流場物理特性的掌握，相較於傳統的速度-壓力法，有其獨特的一面。

關鍵詞：三維，速度-渦度法，有限元素法，邊界元素法，二階朗吉庫特法，穴室流

一、前言

本研究希望以Navier-Stokes方程式為基礎，加入流體不可壓縮的假設，以速度-渦度法配合有限元素法(Finite element method)(Reddy, 1993; 張仁德, 1995)、邊界元素法(Boundary element method)(Liggett and Liu, 1983)及有限差分法(Finite difference method)(Dennis et al., 1979; 廖清標等, 1997)等數值方法，希望探討出三維流場的奧秘，進而期能應用在實際的問題上，以發展出三維流場應用及分析的模式，並求模式的突破與改進。

本研究中以速度(Velocity)及渦度(Vorticity)為主軸(楊適良與楊勝凱, 1996)，配合邊界積分法、有限元素法及有限差分，求解三維穩態不可壓縮史徒克斯(Stokes)流場及三維不可壓縮流場和非慣性座標之流場。文中驗證三維箱型穴室流(Cavity flow)之簡單例子，其邊界條件為在 $z=1.0$ 的表面邊界，其速度 $u=1$ ，其餘表面邊界均為無滑動邊界(No-slip boundary)，而其主要的物理現象是角渦的產生。計算上的困難在上方四邊的速度不連續處而引起奇異渦度之處理。在本研究中，對於速度 $u=1$ 和速度 $u=0$ 之交界處以 $u=0.5$ 將邊界速度不連續處平滑化。初步驗證結果與二維穴室流相較，有些差異，顯示出三維效應。而在其他的驗證，發現與前人作品的結果有些許誤差，因為計算量較為龐大，程式之驗證，仍有待更進一步之探討。

二、理論推導及控制方程式

三維黏性不可壓縮流場的控制方程式為Navier-Stokes方程式和連續方程式。若將Navier-Stokes方程式寫成無因次形式則為(Batchelor, 1967)

$$\frac{\partial \bar{u}}{\partial \bar{t}} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{Re} \nabla^2 \bar{u} \quad (1)$$

其中

Re表雷諾茲數，在本研究中之特性長度為穴室流之邊長，特性速度為上方之拖曳速度； $\bar{u}$ 表流場速度； p 表動壓力。對(1)式作叉積(curl)計算，可得無因次之渦度方程式

$$\frac{\partial \bar{\omega}}{\partial \bar{t}} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{Re} \nabla^2 \bar{\omega} \quad (2)$$

其中

$\bar{\omega}$ 表渦度

若利用不可壓縮流中，速度需滿足連續方程式(3)式及速度和渦度的關係(4)式，即

$$\nabla \cdot \bar{u} = 0 \quad (3)$$

$$\bar{\omega} = \nabla \times \bar{u} \quad (4)$$

可得

$$\nabla^2 \bar{u} = -\nabla \times \bar{\omega} \quad (5)$$

若改寫成直角座標的純量式，則為

$$\nabla^2 u = -\frac{\partial \xi}{\partial y} + \frac{\partial \eta}{\partial z} \quad (6)$$

$$\nabla^2 v = \frac{\partial \xi}{\partial x} - \frac{\partial \xi}{\partial z} \quad (7)$$

$$\nabla^2 w = -\frac{\partial \eta}{\partial x} + \frac{\partial \xi}{\partial y} \quad (8)$$

其中 (u, v, w) 為速度 $\bar{u}$ 之分量， (ξ, η, ζ) 為渦度 $\bar{\omega}$ 之分量。若將(2)式表示成直角座標的純量式

$$\begin{aligned} \frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} = \\ \xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z} + \frac{1}{\text{Re}} \nabla^2 \xi \end{aligned} \quad (9)$$

$$\begin{aligned} \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + v \frac{\partial \eta}{\partial y} + w \frac{\partial \eta}{\partial z} = \\ \xi \frac{\partial v}{\partial x} + \eta \frac{\partial v}{\partial y} + \zeta \frac{\partial v}{\partial z} + \frac{1}{\text{Re}} \nabla^2 \eta \end{aligned} \quad (10)$$

$$\begin{aligned} \frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} + w \frac{\partial \zeta}{\partial z} = \\ \xi \frac{\partial w}{\partial x} + \eta \frac{\partial w}{\partial y} + \zeta \frac{\partial w}{\partial z} + \frac{1}{\text{Re}} \nabla^2 \zeta \end{aligned} \quad (11)$$

在加入適當速度邊界條件後，由(6)、(7)、(8)、(9)、(10)、(11)式來解速度值及渦度值，這就是速度-渦度法解三維不可壓縮流場的主要原理。

速度-渦度法的運算過程如下：

第一步：先假設 $(\xi, \eta, \zeta) = (0, 0, 0)$ ，再加上合適的速度邊界條件，則(6)、(7)、(8)可解出 (u, v, w) 。

第二步：利用(4)式，將 (ξ, η, ζ) 在邊界上的值算出並作為邊界條件，故(9)、(10)、(11)可解 (ξ, η, ζ) 。

第三步：而後用第二步所得之 (ξ, η, ζ) 計算(6)、(7)、(8)式右邊的source項，再去推算速度 (u, v, w) 。如此相互迭代求解，直到兩者均為之收斂，這就是速度-渦度法的運算法則。

由上可知，速度-渦度法之計算原理，與流體流動之物理機制完全相符，此用物理觀念出發的計算方法，是計算流場中最自然而有效的方法。再者，因為速度場為線性，且為向量方程式，可引進平行計算法則，渦度場亦然。再者，因為渦度之基本方程式，可以逐項增加其source term，所以在計算方法中，可以使用疊加原理，由簡而繁，依序漸進。例如有科氏力及密度層變之外力，均可輕而易舉的加入計算程式中，達成通用(general-purpose)的程式設計。

在非慣性座標中運動方程式需加入向心力 $\bar{\Omega} \times (\bar{\Omega} \times \bar{r})$ 及科氏力 $\bar{\Omega} \times \bar{u}$ ，則(1)式變為

$$\begin{aligned} \frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\nabla p + \frac{1}{\text{Re}} \nabla^2 \bar{u} \\ - \frac{\bar{\Omega}^2 L^2}{U^2} (\bar{\Omega} \times (\bar{\Omega} \times \bar{r})) - \frac{2\bar{\Omega} L}{U} (\bar{\Omega} \times \bar{u}) \end{aligned} \quad (12)$$

其中

$\bar{\Omega}$ 為旋轉之特性值， U 為速度之特性值， L 為長度之特性值

一般在非慣性座標中的轉動 $\bar{\Omega}$ 值是沿某一方向的固定值，因此向心力為一軸向應力，可視為一保守力，因而可以改寫成為一勢能場，對於渦度值的改變並沒有影響。故渦度方程式在非慣性座標中為

$$\begin{aligned} \frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{\text{Re}} \nabla^2 \bar{\omega} \\ - \frac{2\bar{\Omega} L}{U} \nabla \times (\bar{\Omega} \times \bar{u}) \end{aligned} \quad (13)$$

因為

$$\begin{aligned} \nabla \times (\bar{\Omega} \times \bar{u}) = -\bar{\Omega} \cdot \nabla \bar{u} + \bar{u} \cdot \nabla \bar{\Omega} \\ - \bar{u} (\nabla \cdot \bar{\Omega}) + \bar{\Omega} (\nabla \cdot \bar{u}) \end{aligned}$$

再加入連續方程式的條件，又因 $\bar{\Omega}$ 為固定值的假設，所以(13)式可簡化為

$$\begin{aligned} \frac{\partial \bar{\omega}}{\partial t} + \bar{u} \cdot \nabla \bar{\omega} = \bar{\omega} \cdot \nabla \bar{u} + \frac{1}{\text{Re}} \nabla^2 \bar{\omega} \\ + \frac{2}{\text{Ro}} \bar{\Omega} \cdot \nabla \bar{u} \end{aligned} \quad (14)$$

其中

$$\text{Ro} = \frac{U}{\bar{\Omega} L} \quad \text{表Rossby數}$$

三、計算方法

本文中，速度滿足Poisson方程式，若以 Φ 來代表各個方向的速度 u, v, w ，則速度方程式可寫成通式為

$$\nabla^2 \Phi(\bar{x}) = b(\bar{x}) \quad (15)$$

在配合Dirichlet邊界條件，且利用Green's second identity推導(15)式在三維的通式為(Kytbe, 1995)

$$\begin{aligned} \alpha \Phi(\bar{p}) = \iint_s \frac{\partial \Phi}{\partial n} \frac{1}{4\pi r} dA(\bar{x}) + \iint_s \Phi_0 \frac{\eta}{4\pi r^3} dA(\bar{x}) \\ - \iiint_v \frac{b}{4\pi r} dV(\bar{x}) \end{aligned} \quad (16)$$

其中

$$\alpha = \frac{\theta}{2\pi}, \quad \theta \text{ 為內域角}, \quad \lambda \text{ 為P至積分平面的}$$

距離， r 為P至積分平面上任一點之距離

而渦度方程式可由method of weighted Residuals中的Galerkin criterion可將(9)式((10)式、(11)式相同)變為

$$\begin{aligned} 0 = \iiint_v N_i \left(\frac{\partial \xi}{\partial t} + u \frac{\partial \xi}{\partial x} + v \frac{\partial \xi}{\partial y} + w \frac{\partial \xi}{\partial z} \right. \\ \left. - \xi \frac{\partial u}{\partial x} - \eta \frac{\partial u}{\partial y} - \zeta \frac{\partial u}{\partial z} \right) \end{aligned}$$

$$-\frac{1}{\text{Re}}\left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} + \frac{\partial^2 \xi}{\partial z^2}\right)dV \quad (17)$$

令 $\xi = \xi(x, y, z, t) = \sum N_i(x, y, z) \bar{\xi}_i(t)$ ， $\bar{\xi}(t)$ 為 ξ 在時間 t 之節點值，將上式做分部積分，則

$$\begin{aligned} 0 = & \sum \int_V N_i N_j \bar{\xi}_j dV \\ & + \sum \int_V (u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z}) \bar{\xi}_j dV \\ & - \sum \int_V N_i (\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z}) dV \\ & - \sum \int_S q_n N_i dA \\ & + \frac{1}{\text{Re}} \sum \int_V (\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z}) \bar{\xi}_j dV \end{aligned} \quad (18)$$

其中

$N_i = N_i(x, y, z)$ 為 shape function

$$q_n = \frac{\partial \Phi}{\partial x} n_x + \frac{\partial \Phi}{\partial y} n_y + \frac{\partial \Phi}{\partial z} n_z$$

V^* 為離散化後各小元素的區域

故(18)可寫成矩陣式

$$\begin{aligned} \sum [M^*] \bar{\xi} + [L^*] \bar{\xi} - [R^*] - [Q^*] \\ + \frac{1}{\text{Re}} [K^*] \bar{\xi} = 0 \end{aligned} \quad (19)$$

其中

$$M_v^* = \sum \int_V N_i N_j dV \quad (20)$$

$$L_v^* = \sum \int_V (u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z}) dV \quad (21)$$

$$R_v^* = \sum \int_V (\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z}) N_i dV \quad (22)$$

$$K_v^* = \sum \int_V (\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z}) dV \quad (23)$$

$$Q_v^* = \sum \int_S q_n N_i dA \quad (24)$$

本文使用二階朗吉庫特法解渦度方程式之初始值問題，其原理是利用顯式法先求出下一時刻的值作為預測值，再將本時刻的值與預測值做平均後，用平均值去推估下一時刻的值。方法如下，

$$\text{由(19)式，令 } \bar{\xi} = \frac{\bar{\xi}_{n+1} - \bar{\xi}_n}{\Delta t}, \quad \bar{\xi} = \bar{\xi}_n$$

其中

$\bar{\xi}_n$ 為 ξ 在時間 $t = n$ 之節點值

$\bar{\xi}_{n+1}$ 為 ξ 在時間 $t = n+1$ 之節點值

Δt 為時間 $t = n$ 至 $t = n+1$ 之時間差

所以(19)式變為

$$[M^*] \bar{\xi}_{n+1} - [M^*] \bar{\xi}_n + \Delta t [L^*] \bar{\xi}_n - \Delta t [R^*]$$

$$- \Delta t [Q^*] + \frac{\Delta t}{\text{Re}} [K^*] \bar{\xi}_n = 0 \quad (25)$$

$$\begin{aligned} \therefore [M^*] \bar{\xi}_{n+1} &= [M^*] \bar{\xi}_n - \Delta t [L^*] \bar{\xi}_n \\ &+ \Delta t [R^*] + \Delta t [Q^*] - \frac{\Delta t}{\text{Re}} [K^*] \bar{\xi}_n \end{aligned} \quad (26)$$

令 $\bar{\xi}_p = \bar{\xi}_{n+1}$ 代入上式

$$\begin{aligned} \therefore [M^*] \bar{\xi}_p &= [M^*] \bar{\xi}_n - \Delta t [L^*] \bar{\xi}_n \\ &+ \Delta t [R^*] + \Delta t [Q^*] - \frac{\Delta t}{\text{Re}} [K^*] \bar{\xi}_n \end{aligned} \quad (27)$$

其中

$\bar{\xi}_p$ 為 ξ 在時間 $t = n+1$ 之預測節點值

令 $\bar{\xi}_n = \frac{\bar{\xi}_p + \bar{\xi}_n}{2}$ 代入(26)式

$$\begin{aligned} \therefore [M^*] \bar{\xi}_{n+1} &= [M^*] \frac{\bar{\xi}_p + \bar{\xi}_n}{2} \\ &- \Delta t [L^*] \frac{\bar{\xi}_p + \bar{\xi}_n}{2} + \Delta t [R^*] + \Delta t [Q^*] \\ &- \frac{\Delta t}{\text{Re}} [K^*] \frac{\bar{\xi}_p + \bar{\xi}_n}{2} \end{aligned} \quad (28)$$

其中

$$M_v^* = \sum \int_V N_i N_j dV \quad (29)$$

$$L_v^* = \sum \int_V (u N_i \frac{\partial N_j}{\partial x} + v N_i \frac{\partial N_j}{\partial y} + w N_i \frac{\partial N_j}{\partial z}) dV \quad (30)$$

$$R_v^* = \sum \int_V (\xi \frac{\partial u}{\partial x} + \eta \frac{\partial u}{\partial y} + \zeta \frac{\partial u}{\partial z}) N_i dV \quad (31)$$

$$K_v^* = \sum \int_V (\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z}) dV \quad (32)$$

$$Q_v^* = \sum \int_S q_n N_i dA \quad (33)$$

其中

u_n, v_n, w_n 是其在時間 $t = n$ 下元素中之平均

值， $\xi_n, \eta_n, \zeta_n, \frac{\partial u_n}{\partial x}, \frac{\partial v_n}{\partial y}, \frac{\partial w_n}{\partial z}$ 也是其在時間 $t = n$ 下元素中之平均值

四、數值結果與分析

雷諾茲數100之速度 u 及速度 w 的比較圖中，即圖1和圖2，可看出速度 u 及 w 因 $z=1.0$ 移動邊界所造成的拖曳力效應，三維的比較弱。圖1中和Ku et al. (1986) 及Goda (1979) 速度 u 的比較中發現在 $z=0.8$ 至 $z=0.4$ 中，本模式計算的速度 u 較小，應是網格不夠細造成彼此的誤差，因為Ku et al. (1986) 的網格為 $25 \times 13 \times 25$ 而Goda (1979) 的網格為 $20 \times 10 \times 20$ 。和Ku et al. (1986) 相比其絕對誤差值為0.036，而和Goda (1979) 相比為0.035。圖2中和Ku et al. (1986) 速度 w 比較來看，差異較小，

其絕對誤差值為0.011。因此從比較中可知，在低雷諾茲數的流場中，速度u的計算誤差較大。

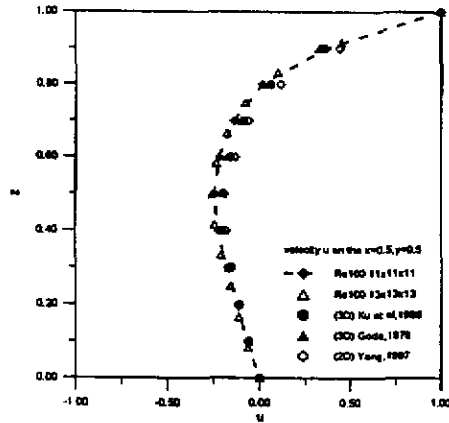


圖1:雷諾茲數100在 $x=0.5$ ， $y=0.5$ 之速度分佈比較圖

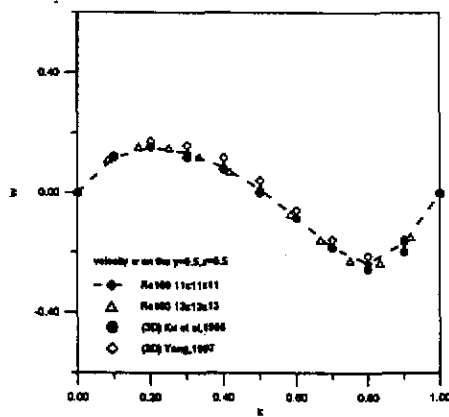


圖2:雷諾茲數100在 $y=0.5$ ， $z=0.5$ 之速度分佈比較圖

雷諾茲數400在圖3速度u比較圖中，誤差較大的地方在 $z=0.2$ 附近。此時Ku et al.(1986)的網格為 $25 \times 13 \times 25$ 而Goda(1979)的網格為 $20 \times 10 \times 20$ 。速度u和Ku et al.(1986)相比，絕對誤差值為0.043，和Goda(1979)相比則為0.018。圖4速度w比較圖中，誤差較大的地方在 $x=0.9$ 附近。速度w和Ku et al.(1986)相比，絕對誤差值為0.036。造成這些誤差的原因，在於慣性圈和粘性圈交會處，速度變化較大，計算精度比較差。

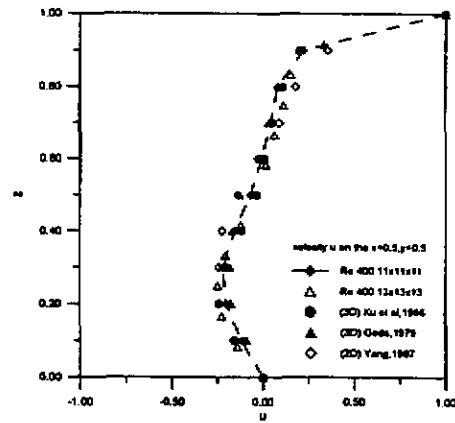


圖3:雷諾茲數400在 $x=0.5$ ， $y=0.5$ 之速度分佈比較圖

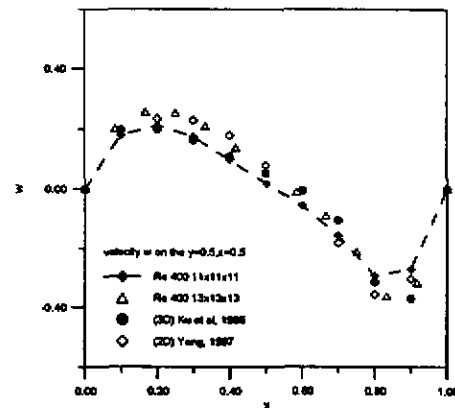


圖4:雷諾茲數400在 $y=0.5$ ， $z=0.5$ 之速度分佈比較圖

雷諾茲數1000，由速度u分佈比較圖中，即圖5發現上邊界的邊界層厚度大至在 $z=1.0$ 至 $z=0.9$ ，而下邊界層厚度會驅近 $z=0.0$ 至 $z=0.1$ ，而速度w分佈比較圖中，即圖6，左邊界的邊界層厚度大至在 $x=0.0$ 至 $x=0.1$ ，而右邊界層厚度會驅近 $x=0.9$ 至 $x=1.0$ 。此時Ku et al.(1986)的網格為 $31 \times 16 \times 31$ ，速度u和Ku et al.(1986)相比，絕對誤差平均值為0.034，而速度w和Ku et al.(1986)相比，絕對誤差值為0.056。

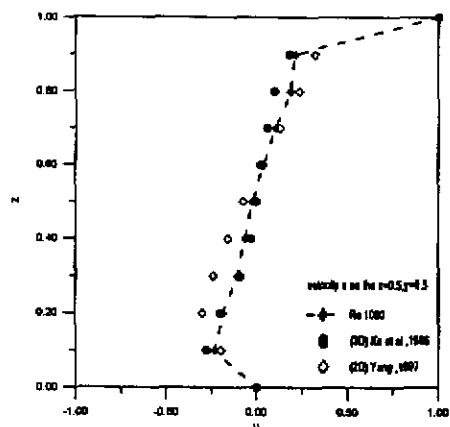


圖5:雷諾茲數1000在 $x=0.5$, $y=0.5$ 之速度分佈比較圖

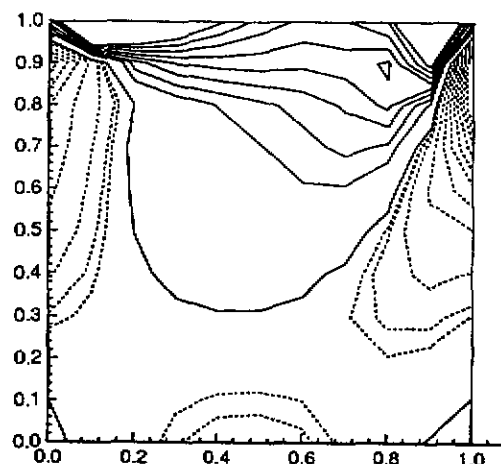


圖7:雷諾茲數100在 $y=0.5$ 之渦度場 η 分佈圖

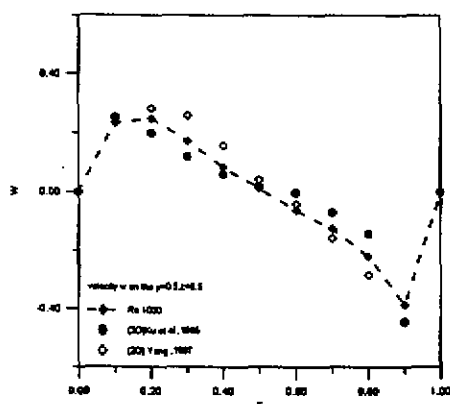


圖6:雷諾茲數1000在 $y=0.5$, $z=0.5$ 之速度分佈比較圖

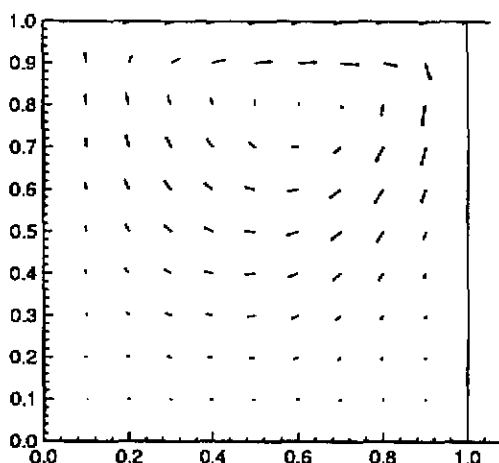


圖8:雷諾茲數100在 $y=0.5$ 之速度場 u 和 w 分佈圖

圖7及圖8分別是雷諾茲數100，在 $y=0.5$ 的渦度及速度分佈圖，可看出渦心已往右偏移。圖9及圖10分別是雷諾茲數400，在 $z=0.5$ 的速度及渦度分佈圖。圖11及圖12分別是雷諾茲數1000，在 $x=0.5$ 的速度及渦度分佈圖，可看出流場有明顯的漩渦產生。

在非慣性座標的流場，先假設向心力沒有影響，而流場的邊界條件和先前一樣，只是方程式中因沿負 z 軸旋轉， $\vec{\Omega} = -\vec{k}$ ，造成科氏力影響渦度的變化。若和無科氏力影響的流場比較，整個流場是做一螺旋轉動。平面 $z=0.5$ 之渦度 ζ 和速度場，即圖13和圖14，可明顯看出此平面受科氏力的影響。因為此平面之速度場原是往負 x 軸方向前進，因受科氏力的影響，使得速度場轉向負 y 軸方向前進。

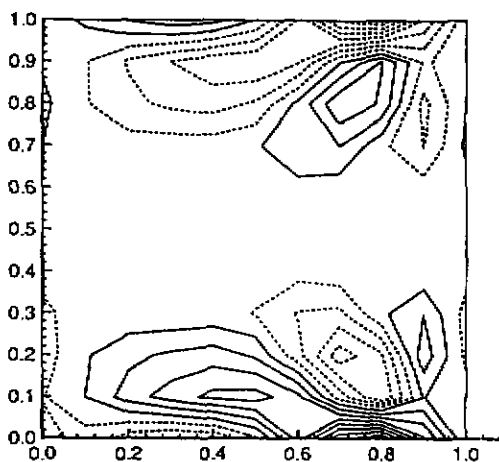


圖9:雷諾茲數400在 $z=0.5$ 之渦度場 ζ 分佈圖

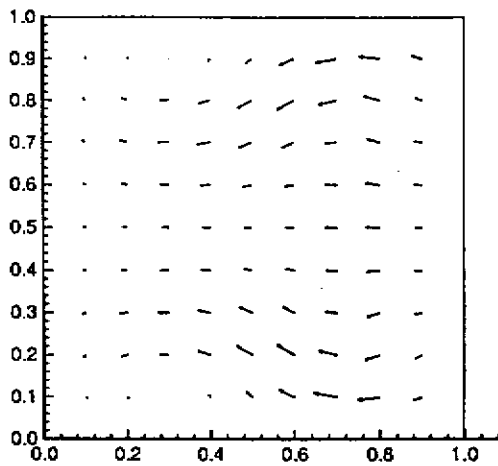


圖10: 雷諾數400在 $z=0.5$ 之速度場 u 和 v 分佈圖

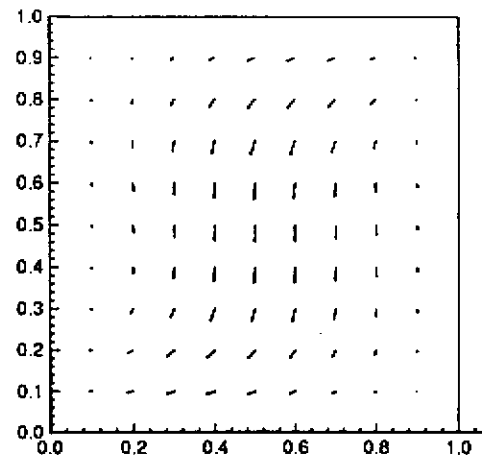


圖13: 雷諾數10, Rossby數為0.1在 $z=0.5$ 之速度場 u 和 v 分佈圖

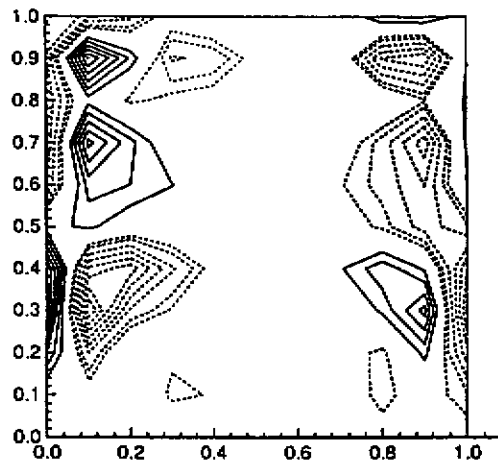


圖11: 雷諾數1000在 $x=0.5$ 之渦度場 ξ 分佈圖

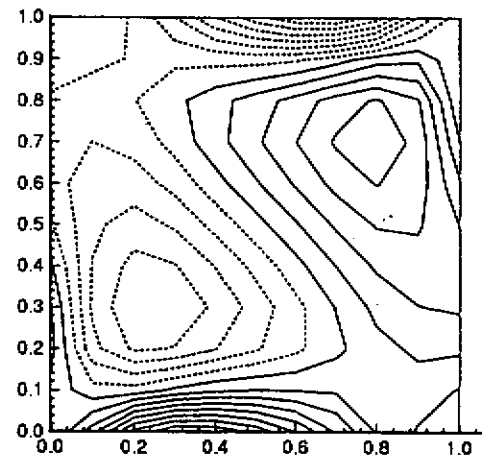


圖14: 雷諾數10, Rossby數為0.1在 $z=0.5$ 之渦度場 ξ 分佈圖

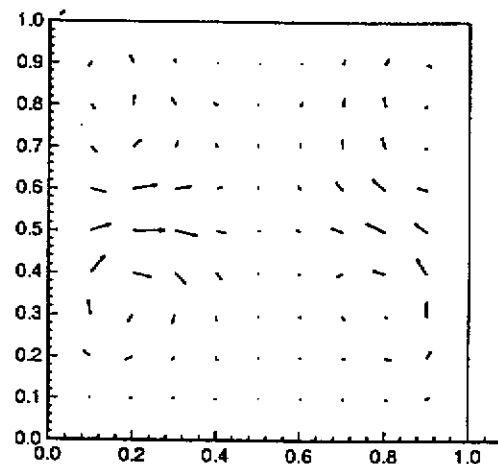


圖12: 雷諾數1000在 $x=0.5$ 之速度場 v 和 w 分佈圖

五、結論

1. 各種雷諾茲數之流場的討論，已在第四節中說明，儘管本研究的網格不夠細，造成各節點之函數值有誤差，但在各種流況中，主要的流場特性均有涉及。可見速度-渦度法配合採用之數值方法，十分恰當。尤其是以BEM決定渦度方程式之邊界條件，既避開複雜的差分方法，也增加了精度。
2. 本模式雖為速度-渦度法，實則主要在估算渦度方程式，速度只是扮演一校正疊代的角色，在疊代過程中順便將速度求出。因此只要渦度估算正確，儘管網格不夠細，速度場的準確度也會不錯，主要原因在於渦度是速度的一次微分。當渦度估算不錯時，代表速度變化可算的準，因此速度也就算的很準。這和以速度-壓力

作為主要變數的數值方法不同，因其主要是估算運動方程式，以壓力為輔，而壓力的邊界條件較渦度的邊界條件更難以處理，造成在疊代時，容易引進誤差。

誌謝

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Velocity-Vorticity Method For The Three-Dimensional Incompressible Viscous Flows

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Abstract

In this study, we use the velocity-vorticity method, in combination with finite element method, boundary element method and Runge-Kutta method to solve the 3D incompressible Navier-Stokes equations. The correctness of the model is verified by a simple driven cavity flow by comparing with existing literature. By the process of verification, the velocity-vorticity method has shown much better control in the physics of the flows and also the accuracy in the process of computation than the velocity-pressure method.

Keywords: three-dimension, velocity-vorticity method, finite element method, boundary element method, 2nd-order Runge-Kutta method, cavity flow

- B3. Young, D.L., Her, B.C., and Wang, Y.F., 1998, "Three-dimensional Mathematical Modeling of Pollutant Transport in Stratified Estuaries", Proceedings of the 2nd. International Symposium on Environmental Hydraulics, Hong Kong, 16-18 December 1998, pp.93-97.

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Three-dimensional mathematical modeling of pollutant transport in stratified estuaries

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ABSTRACT: This study, in the flow computation, uses a three-dimensional shallow water BEM(Boundary Element Method) model. However, to investigate the temperature distribution, we adopt a three-dimensional advection-diffusion ELBEM(Eulerian-Lagrangian Boundary Element Method) model. The advection part of ELBEM model is treated by the concept of Eulerian-Lagrangian scheme, which overcomes the limitation of traditional BEM scheme which is incapable to deal with the arbitrary velocity field. The linkage of three-dimensional shallow water BEM model and advection-diffusion ELBEM model enables us to deal with the fluctuation of free surface and density stratification in a stratified estuary. The simulation results are satisfactory through the comparison with analytical solutions and the results from other numerical schemes. Furthermore, this model is applied to simulate conditions which flow field is effected under different boundary conditions such as surface wind shear or heat flux. The simulation results, as comparing with those of homogeneous flow field, show the phenomenon of overturn under the condition of unstable density stratification. As far as stably stratified flow fields are concerned, the phenomena of multiple circulating gyres and the thermocline are also captured.

1. INTRODUCTION

With the advent of computer technology, such as the efficient computation of parallel computing and high-performance computers of main frames, work stations or even PC, the numerical modelling of large scale three-dimensional flow fields becomes more feasible nowadays. The purpose of this study is to establish a three-dimensional boundary element model to analyze the pollutant transport in the stratified estuaries, bays, or coastal waters. Under the assumption of shallow water theory, an Ekman boundary layer model is developed with the consideration of density stratification due to temperature and salinity or even the pollutant concentrations. The wind shear effect will also be taken into account as far as flow mixing mechanism is concerned.

We have successfully developed a 3-D boundary element model to investigate the pollutant transport in a homogeneous (non-stratified) estuary, Young and Wang (1995a), Young and Wang (1995b), Young and Wang (1995c). With the framework of the previous studies, we are able to extend the homogeneous bodies of water into the more complex and realistic stratified basins. However, with the consideration of stratified effects, the phenomena of circulating gyres and the associated formation, maintenance of thermocline in a stably stratified environment, as well as the overturn and the hydrodynamic instability in a unstably stratified estuary will highly enhance the degree of difficulty of numerical simulations.

2. GOVERNING EQUATIONS

Under the assumptions of (1) shallow water approximation, that is, the vertical scale is much less than the horizontal scale, and hydrostatic pressure distribution in vertical direction, (2) small Rossby number, (3) ignoring the horizontal diffusion in the momentum equations, (4) constant eddy viscosity and eddy diffusivity, (5) constant Coriolis parameter, and (6) Boussinesq approximation, we obtain the following governing equations

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1)$$

$$\frac{\partial u}{\partial t} - fv = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} - \frac{1}{\rho_0} \frac{\partial p'}{\partial x} + \nu \frac{\partial^2 u}{\partial z^2} \quad (2)$$

$$\frac{\partial v}{\partial t} + fu = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} - \frac{1}{\rho_0} \frac{\partial p'}{\partial y} + \nu \frac{\partial^2 v}{\partial z^2} \quad (3)$$

$$0 = -\frac{1}{\rho} \left(\frac{\partial p}{\partial z} + \frac{\partial p'}{\partial z} \right) - g \quad (4)$$

$$\rho = \rho_0 + \rho', \rho' \ll \rho \quad (5)$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} = \frac{\partial}{\partial x} (K_x^T \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (K_y^T \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (K_z^T \frac{\partial T}{\partial z}) + S^T(x, y, z, t) \quad (6)$$

$$\rho = \rho_0 \{1 - [7(T - T_0)^2 - 750\phi] \times 10^{-6}\} \quad (7)$$

Herein, ν =eddy viscosity, $f=2\omega \sin \theta$ =Coriolis parameter, ω =angular speed of earth rotation, θ =the latitude, g =gravitational acceleration, ρ =density, ρ' =density deviation from the standard water density, ρ_0 =water density at $4^\circ\text{C}=999.972 \text{ Kg/m}^3$, T =temperature in degree Celsius, p' =pressure variation due to ρ' , ϕ =salinity, in parts per thousand, K_x^T, K_y^T, K_z^T =eddy diffusivity for temperature.

3. NUMERICAL MODEL

After the non-dimensional procedure, and the discretization of difference scheme in time, together with the boundary element method, we obtain the following boundary integral equation for the hydrodynamic equations for the flow field.

$$\begin{aligned} u^{n+1}(\vec{x}) = & \int_{\Omega_0} \left\{ \hat{u}_x \left[-\left(\frac{\partial \eta}{\partial x} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Su^n \right] + \hat{v}_x \left[-\left(\frac{\partial \eta}{\partial y} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Sv^n \right] \right\} d\Omega_0 \\ & - \int_{\Gamma_0} \left\{ u^{n+1} \left[E_k \frac{\partial \hat{u}_k}{\partial z} \vec{k} \right] \cdot \vec{n} + v^{n+1} \left[E_k \frac{\partial \hat{v}_k}{\partial z} \vec{k} \right] \cdot \vec{n} \right\} d\Gamma_0 + \int_{\Gamma_0} \left\{ \hat{u}_x \left[E_k \frac{\partial u^{n+1}}{\partial z} \vec{k} \right] \cdot \vec{n} + \hat{v}_x \left[E_k \frac{\partial v^{n+1}}{\partial z} \vec{k} \right] \cdot \vec{n} \right\} d\Gamma_0 \end{aligned} \quad (8)$$

$$\begin{aligned} v^{n+1}(\vec{x}) = & \int_{\Omega_0} \left\{ \hat{u}_y \left[-\left(\frac{\partial \eta}{\partial x} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Su^n \right] + \hat{v}_y \left[-\left(\frac{\partial \eta}{\partial y} \right)^{n+1} - \left(\frac{\partial p'}{\partial x} \right)^{n+1} + Sv^n \right] \right\} d\Omega_0 \\ & - \int_{\Omega_0} \left\{ u^{n+1} \left[E_k \frac{\partial \hat{u}_k}{\partial z} \vec{k} \right] \cdot \vec{n} + v^{n+1} \left[E_k \frac{\partial \hat{v}_k}{\partial z} \vec{k} \right] \cdot \vec{n} \right\} d\Gamma_0 + \int_{\Gamma_0} \left\{ \hat{u}_y \left[E_k \frac{\partial u^{n+1}}{\partial z} \vec{k} \right] \cdot \vec{n} + \hat{v}_y \left[E_k \frac{\partial v^{n+1}}{\partial z} \vec{k} \right] \cdot \vec{n} \right\} d\Gamma_0 \end{aligned} \quad (9)$$

where

$$p' = \int_z^{\eta} \rho^* dz \quad , \quad \rho^* = \frac{\rho'}{\rho_0}$$

After the introduction of Eulerian-Lagrangian boundary element method (ELBEM), the corresponding non-dimensional-diffusion equation for temperature is written as follows:

$$\alpha(\bar{x}, t^{n+1})T(\bar{x}, t^{n+1}) = \int_{\Omega_E} \hat{T}(\bar{x}, t^{n+1}; \bar{x}, t^n)T(\bar{x}, t^n)d\Omega_E - \int_{t^n}^{t^{n+1}} \int_{\Gamma_E} \hat{T}(\bar{x}, t^n; \bar{x}, t)q(\bar{x}, t)d\Gamma_E dt + \int_{t^n}^{t^{n+1}} \int_{\Gamma_E} \hat{q}(\bar{x}, t^n; \bar{x}, t)T(\bar{x}, t)d\Gamma_E dt \quad (10)$$

Furthermore, we use the constant element to deal with the temperature domain, and obtain the following equation

$$\alpha(\bar{x}, t^{n+1})T(\bar{x}, t^{n+1}) = \int_{\Omega_E} \hat{T}(\bar{x}, t^{n+1}; \bar{x}, t^n)T(\bar{x}, t^n)d\Omega_E - \int_{\Gamma_E} \hat{T}(\bar{x}, t^{n+1}; \bar{x}, t^n)q(\bar{x}, t^n)d\Gamma_E + \int_{\Gamma_E} \hat{q}(\bar{x}, t^{n+1}; \bar{x}, t^n)T(\bar{x}, t^n)d\Gamma_E \quad (11)$$

where,

$$\hat{T}^* = \frac{1}{[4\pi Kr]} \operatorname{erfc}(\eta^*) \quad (12)$$

$$\hat{q}^* = \frac{1}{[4\pi r^2]} \frac{\partial r}{\partial n} \left[-\frac{2\eta^*}{\sqrt{\pi}} \exp(-\eta^{*2}) - \operatorname{erfc}(\eta^*) \right] \quad (13)$$

$$\eta^* = \frac{r}{2\sqrt{K(t^{n+1} - t^n)}} \quad (14)$$

The boundary element methods will not be presented here due to the limitation of space, and the previous papers of the writers are recommended for the details.

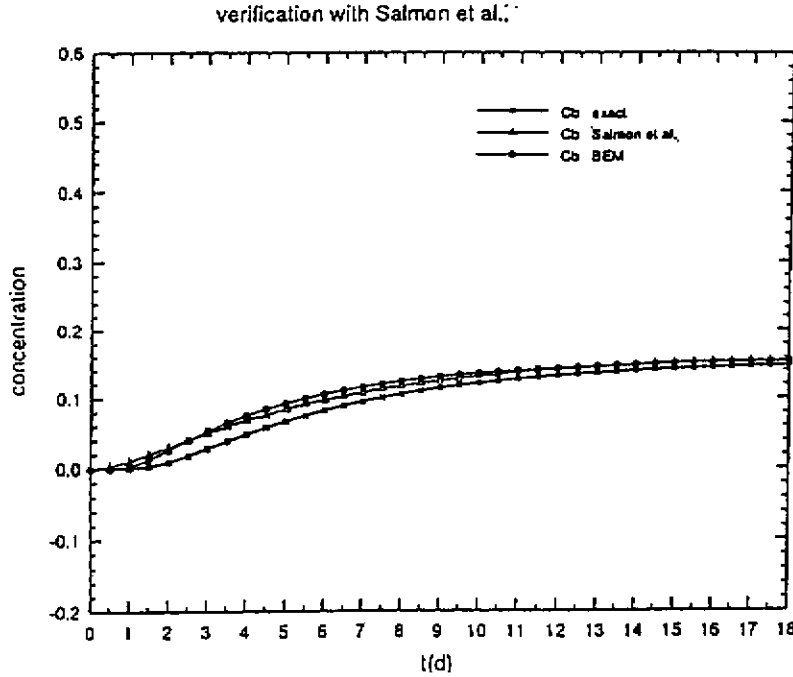


Fig.1: Comparison of Concentration evolution of exact, Salmon et al and present study (BEM)

4. NUMERICAL RESULTS

We first calibrate a simple large and shallow lake to test the performance of the numerical models. A square lake with the geometric sizes of $62.5\text{km} \times 62.5\text{km} \times 80\text{m}$ is undertaken. The horizontal and vertical eddy diffusivities are $20\text{m}^2/\text{s}$ and $0.02\text{m}^2/\text{s}$ respectively. For the concentration of pollutant at the position of $(45.9\text{km} \times 32.3\text{km} \times 80\text{m})$, the comparison of the exact solution, Salmon et al (1980) and present model is shown in Fig.1. The three results are all very agreeable.

We now consider another case study as performed by Davies (1983). This is a rectangular shallow basin with the dimensions of $400\text{km} \times 400\text{km} \times 65\text{m}$. The following physical parameters are chosen: $\nu = 650\text{cm}^2/\text{s}$, $f = 0.00012222\text{ rad/s}$, $\tau_{yx} = -14.6341463\text{cm}^2/\text{s}$ = shear stress in the y-direction, $\Delta t = 409.1\text{s}$. As far as the boundary conditions are concerned, except there is heat transfer on the air-sea interface, the other sides are all insulated. For the non-stratified (homogeneous) lake, the velocity distributions at the profiles of $x=0.4, y=1.0$ and $z=-0.5$ are depicted at Fig.2a for the time-step of 50. The corresponding figures for the time-step of 100 is also described in Fig.2b. it is concluded from the numerical results that for the homogeneous lake, there is only one circulating gyre in the whole water body after the long action of wind shear stress. The flow field is very simple. However, where there are both wind shear and heat transfer on the water surface, the flow and temperature fields are more complicated, as shown in Fig.3. This graph reveals the distribution of density and flow at the time-step of 100. The density stratification as well as the multiple circulating gyres in the lake are very dominant. We can see very clearly there are two circulating gyres and also the phenomenon of overturn the physics of the stratified basin in general is more interesting and more challenging in the modeling of bodies of water. Since the present model is able to treat the constant eddy viscosity and diffusivity only, a quantitative and vigorous comparison of Davies model (1983) is not possible. However, the qualitative features of both models all render fundamental fluid dynamics for the homogeneous and stratified basins.

5. CONCLUSION

We draw the following conclusions:

- (1) A three-dimensional pollutant transport model in the stratied bodies of water is established after the

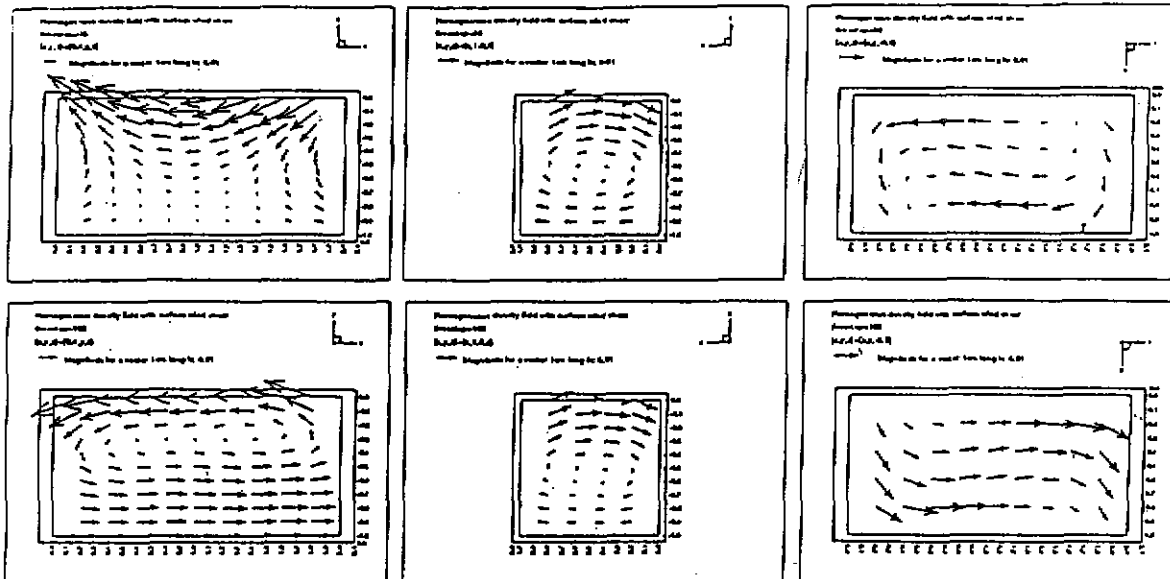


Fig.2:(a)Flow field at the profiles of $x=0.4, y=1.0, z=-0.5$ at time-step 50

(b)Same as (a) at time-step 100

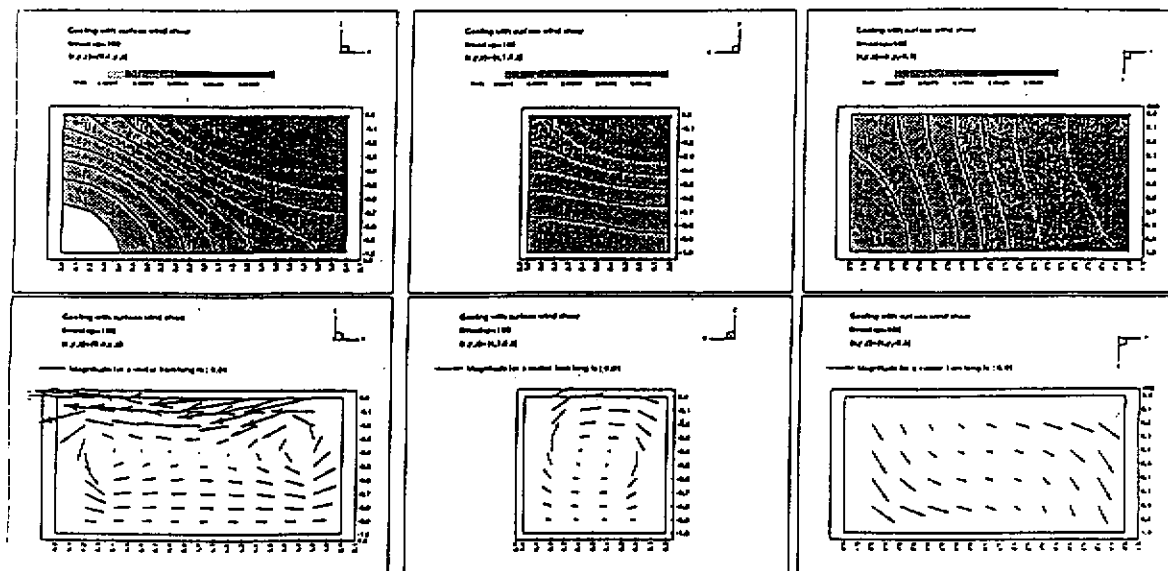


Fig.3: Density (top) and flow (bottom) fields at the profiles of $x=0.4$, $y=1.0$, $z=-0.5$ at time-step 100

calibration and verification of the existing literature. The model consists of two submodels: the flow equation is solved by the three-dimensional shallow water theory using the boundary element method, while the density, temperature, or pollutant concentrations are solved by the three-dimensional advection-diffusion equation using the Eulerian-Lagrangian boundary element method. The overall performance of the present model is satisfactory and comparable to the other numerical models.

- (2) The present model is able to handle both the homogeneous and stratified environments under the air-sea interaction at the water surface to consider the mass, momentum and heat transfers. The homogeneous circulation of water is the simplest case, however, we have obtained the physical characteristics of thermocline for stably stratified basins and overturn for the unstably stratified environments.

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1.3 Jets and plumes – I

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