Journal of Environmental Sciences Vol.16, No.2, pp.293—296, 2004

ISSN 1001—0742
CN11—2629/X

Article ID: 1001-0742(2004)02-0293-04 **CLC number**: X131.2 **Document code**: A

Numerical model of flow and pollutant transportation in non-orthogonal curvilinear coordinates

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Abstract: The planar 2D k-ε double equations' turbulence model was adopted and transformed into non-orthogonal curvilinear coordinates. The concentration convection-diffusion was introduced to planar 2D SIMPLEC algorithm of flow in non-orthogonal curvilinear coordinates. The numerical model of pollutant transportation in non-orthogonal curvilinear coordinates was constructed. The model was applied to simulate the flow and pollutant concentration fields. In the testing concentration field, two optimal operations of contamination discharging both along bank and in the centerline at the first bend of the meandering channel were adopted. Comparison with available data showed the model developed was successful, was valuable to engineering application.

Keywords: curvilinear coordinates; diffusion-transportation; SIMPLEC algorithm; concentration fields; meandering channel

Introduction

Along with the rapid development of economy, a lot of wastewater harmful to human and other lives has been discharged into natural environment without disposal, which made great harm to surface water and ground water. Natural water such as rivers, lakes and ocean has some ability of self-purification, so it is a significative project to research the environmental hydraulic engineering to utilize its ability of self-purification to save the expenses of environmental protection. It is the precondition to make clear the convection-diffusion rule and concentration distribution of pollutant in water and provide the route to settle the problem. And the hydrodynamic characteristic of rivers with flexural boundary is a basic thesis of environmental hydrodynamics. Coordinate transformation is an effective way to solve the problem, because of the flexural boundary and complicated topography of natural rivers. At present, in the computation of N-S equations in curvilinear coordinate, contravariant velocity was adopted as the calculating variable, which increases the complexity of the equations. Many researchers ignored the non-orthogonal terms of the equations and solved N-S equations in orthogonal curvilinear coordinate. Patankar and Spalding provided a remarkably successful method, the SIMPLE algorithm in 1972. Since then it has widely been used in the field of numerical simulation of incompressible flows and several variants have appeared. The SIMPLER (Patankar, 1981), SIMPLEC (Van Doormaal, 1984), SIMPLEX (Raithby, 1988) and SIMPLET (Sheng, 1998) algorithms are typically representative of variants that improve on SIMPLE algorithm in both convergence behavior and computer cost. It is noted that all of these algorithms are very successfully in handling the velocity-pressure coupling, only if the velocity field is linearly proportional to the pressure field, and all the coefficients are independent of the pressure in the discrete equations. Because of the depth-averaged shallow water model was established on the hydrostatic approximation, the problem of velocity-pressure coupling was transformed into that of water depth-velocity coupling.

In this paper, the research employed orthogonal curvilinear coordinate transformation to generate numerical grid, but depth-averaged k-ε double equations turbulence model in non-orthogonal curvilinear coordinates was adopted to calculate the velocity field, which could modify the error derived from non-orthogonal term. The contamination convective-diffusion equation is introduced into the SIMPLEC algorithm of non-orthogonal curvilinear coordinate system, and the numerical model flow and contamination transportation in non-orthogonal curvilinear coordinates is developed. The model has been applied to simulate the flow and concentration field in meandering channel of laboratory and the comparison between measured and calculated has been conducted of velocity and concentration of 4 cross sections.

1 Mathematic model

The planar 2-D flow and pollute convection-diffusion equation in Cartesian system can be written in general format as

Foundation item: the National Science Fund for Distinguished Young Scholars (No. 50125924); the National Natural Science Foundation of China (Nos. 10332050 and 50379001); the Research Fund for the Doctoral Program of Higher Education (No. 2000014112) and the Natural Science Foundation of Liaoning Province (No. 2001101073)

$$\frac{\partial}{\partial t}(H\rho\Phi)+\frac{\partial}{\partial x}(H\rho u\Phi)+\frac{\partial}{\partial y}(H\rho v\Phi)=\frac{\partial}{\partial x}\left(H\Gamma_\Phi\frac{\partial\Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(H\Gamma_\Phi\frac{\partial\Phi}{\partial y}\right)+S_\Phi^* . \quad (1)$$

Introducing a curvilinear coordinate system(ξ,η), Eq.(1) can be written as

$$\frac{\partial}{\partial t}(H\rho\Phi)+\frac{1}{J}\frac{\partial}{\partial\xi}(H\rho U\Phi)+\frac{1}{J}\frac{\partial}{\partial\eta}(H\rho V\Phi)=\frac{1}{J}\frac{\partial}{\partial\xi}\left(\frac{H\Gamma_\Phi}{J}(\alpha\Phi_\xi-\beta\Phi_\eta)\right)+\frac{1}{J}\frac{\partial}{\partial\eta}\left(\frac{H\Gamma_\Phi}{J}(-\beta\Phi_\xi+\gamma\Phi_\eta)\right)+S_\Phi(\xi,\eta), \quad (2)$$

where Φ is the depth-averaged variable in general format, U and V are the contravariant velocity along the ξ and η directions, respectively, Γ_Φ is the exchange coefficient, and S_Φ represents a source term. The values of Φ, Γ_Φ, S_Φ in each lists in Table 1.

Table 1 Exchange coefficient and source term of flux equations

Equations	Φ	Γ_Φ	S_Φ
Continuity equation	1	0	0
x-momentum equation	u	μ_{eff}	S_u
y-momentum equation	v	μ_{eff}	S_v
Transport equation of neutral concentration	C	$\frac{\mu_{eff}}{\sigma_c}$	S_c
Transport equation of turbulent kinetic energy	k	$\frac{\mu_{eff}}{\sigma_k}$	$H(G_k^0+G_{kv}-\rho\varepsilon)$
Transport equation of turbulent kinetic energy dissipation rate	ε	$\frac{\mu_{eff}}{\sigma_\varepsilon}$	$H\left[\frac{\varepsilon}{k}(C_{1\varepsilon}G_k^0-C_{2\varepsilon}\rho\varepsilon)+G_{\varepsilon v}\right]$

where $\alpha=x_\eta^2+y_\eta^2$, $\beta=x_\xi x_\eta+y_\xi y_\eta$, $\gamma=x_\xi^2+y_\xi^2$, $J=x_\xi y_\eta-x_\eta y_\xi$, $U=uy_\eta-vx_\eta$, $V=vx_\xi-uy_\xi$,

$$S_u=-\frac{1}{J}\left[\rho gH\left(y_\eta\frac{\partial z_s}{\partial\xi}-y_\xi\frac{\partial z_s}{\partial\eta}\right)\right]+\frac{1}{J}\frac{\partial}{\partial\xi}\left\{\frac{H\mu_{eff}}{J}\left[y_\eta^2\frac{\partial u}{\partial\xi}-y_\xi y_\eta\frac{\partial u}{\partial\eta}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\xi}\left\{\frac{H\mu_{eff}}{J}\left[y_\xi x_\eta\frac{\partial v}{\partial\eta}-x_\eta y_\eta\frac{\partial v}{\partial\xi}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\eta}\left\{\frac{H\mu_{eff}}{J}\left[x_\xi y_\eta\frac{\partial v}{\partial\xi}-x_\xi y_\xi\frac{\partial v}{\partial\eta}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\eta}\left\{\frac{H\mu_{eff}}{J}\left[y_\xi^2\frac{\partial u}{\partial\eta}-y_\xi y_\eta\frac{\partial u}{\partial\xi}\right]\right\}-\tau_{bx},$$

$$S_v=-\frac{1}{J}\left[\rho gH\left(x_\xi\frac{\partial z_s}{\partial\eta}-x_\eta\frac{\partial z_s}{\partial\xi}\right)\right]+\frac{1}{J}\frac{\partial}{\partial\xi}\left\{\frac{H\mu_{eff}}{J}\left[x_\eta^2\frac{\partial v}{\partial\xi}-x_\xi x_\eta\frac{\partial v}{\partial\eta}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\xi}\left\{\frac{H\mu_{eff}}{J}\left[x_\xi y_\eta\frac{\partial u}{\partial\eta}-x_\eta y_\eta\frac{\partial u}{\partial\xi}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\eta}\left\{\frac{H\mu_{eff}}{J}\left[y_\xi x_\eta\frac{\partial u}{\partial\xi}-x_\xi y_\xi\frac{\partial u}{\partial\eta}\right]\right\}+\frac{1}{J}\frac{\partial}{\partial\eta}\left\{\frac{H\mu_{eff}}{J}\left[x_\xi^2\frac{\partial v}{\partial\eta}-x_\xi x_\eta\frac{\partial v}{\partial\xi}\right]\right\}-\tau_{by},$$

$$G_k^0=2\mu_{eff}\left(\frac{\partial u}{\partial\xi}\frac{y_\eta}{J}-\frac{\partial u}{\partial\eta}\frac{y_\xi}{J}\right)^2+2\mu_{eff}\left(-\frac{\partial v}{\partial\xi}\frac{x_\eta}{J}+\frac{\partial v}{\partial\eta}\frac{x_\xi}{J}\right)^2+\mu_{eff}\left(\frac{\partial v}{\partial\xi}\frac{y_\eta}{J}-\frac{\partial v}{\partial\eta}\frac{y_\xi}{J}\right)+\left(-\frac{\partial u}{\partial\xi}\frac{x_\eta}{J}+\frac{\partial u}{\partial\eta}\frac{x_\xi}{J}\right)^2,$$

$$G_{kv}=\frac{c_k\rho U_*^3}{H},\quad G_{\varepsilon v}=\frac{c_\varepsilon\rho U_*^4}{H^2},$$

$$U_*=\sqrt{c_f(u^2+v^2)},\quad c_k=\frac{1}{c_f},\quad c_\varepsilon=\frac{3.6C_{\varepsilon_2}}{c_f^{0.75}}\sqrt{C_\mu},$$

$$\nu_t=C_\mu\frac{k^2}{\varepsilon},\quad \tau_{bx}=\frac{gn^2u\sqrt{u^2+v^2}}{H^{1/3}},$$

$$\tau_{by}=\frac{gn^2v\sqrt{u^2+v^2}}{H^{1/3}},\quad H=z_s-z_b,$$

$$\mu_{eff}=\rho(\nu+\nu_t),\quad c_f=0.003,$$

where s_c is the source term of pollution intension; u, v are the depth-averaged velocity in Cartesian coordinate system along x, y direction; k, ε are the depth-averaged turbulent kinetic energy and its dissipation rate, respectively; H is the water depth; z_s is the water level; z_b is the bed elevation; ν is the molecule viscosity coefficient; ν_t is the isotropic turbulent viscosity coefficient; μ_{eff} is the effective viscosity coefficient; τ_{bx}, τ_{by} is the bottom shear stresses; n is the bottom roughness and C_μ, C_{ε_1}, C_{ε_2}, σ_k, σ_ε and σ_c are the turbulent constants. The value of turbulent constants are listed in Table 2.

Table 2 Turbulent constant

C_μ	C_{ε_1}	C_{ε_2}	σ_k	σ_ε	σ_c
0.09	1.44	1.92	1.0	1.3	1.0

2 Equation discretization

Control volume method was adopted to discrete the equations, and for treating convection terms, the hybrid scheme was used to simplicity. Eq.(2) was discretized to the Eq.(3):

$$a_P\Phi_P=a_E\Phi_E+a_W\Phi_W+a_N\Phi_N+a_S\Phi_S+a_0, \quad (3)$$

where

$$a_E=\max\left(\left|\frac{1}{2}F_e\right|,\ D_e\right)-\frac{1}{2}F_e,$$

$$a_W=\max\left(\left|\frac{1}{2}F_w\right|,\ D_w\right)+\frac{1}{2}F_w,$$

$$a_N=\max\left(\left|\frac{1}{2}F_n\right|,\ D_n\right)-\frac{1}{2}F_n,$$

$$a_S=\max\left(\left|\frac{1}{2}F_s\right|,\ D_s\right)+\frac{1}{2}F_s,$$

$$F_e=(\rho U\Delta\eta)_e,\quad F_w=(\rho U\Delta\eta)_w,$$

$$F_n=(\rho V\Delta\xi)_n,\quad F_s=(\rho V\Delta\xi)_s,$$

$$D_e=\left(\frac{\alpha}{J}\Gamma_e\frac{\Delta\eta}{\Delta\xi}\right)_e,\quad D_w=\left(\frac{\alpha}{J}\Gamma_\Phi\frac{\Delta\eta}{\Delta\xi}\right)_w,$$

$$D_n=\left(\frac{\alpha}{J}\Gamma_\Phi\frac{\Delta\xi}{\Delta\eta}\right)_n,\quad D_s=\left(\frac{\alpha}{J}\Gamma_\Phi\frac{\Delta\xi}{\Delta\eta}\right)_s,$$

$$a_0=S_CJ\Delta\xi\Delta\eta-\left[\left(\frac{\Gamma_\Phi}{J}\beta\Phi_\eta\Delta\eta\right)_w^e+\left(\frac{\Gamma_\Phi}{J}\beta\Phi_\xi\Delta\xi\right)_s^n\right]+\frac{\Delta\xi\Delta\eta}{\Delta t}\overline{H}_P\Phi_0,$$

$$a_P = a_E + a_w + a_N + a_S - S_P + \frac{\Delta\xi\Delta\eta}{\Delta t}\overline{H}_P .$$

3 Boundary conditions

At the inlet, the known boundary values for all the dependent variables (u, v, k and ε) are prescribed either from the experimental data or analytical profiles,

$$u = u_0, \quad v = v_0, \quad k = k_0, \quad \varepsilon = \varepsilon_0 .$$

At the downstream outlet, the normal gradients of all dependent variables are set to zero, i.e., $\frac{\partial Z_s}{\partial n} = \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = \frac{\partial k}{\partial n} = \frac{\partial \varepsilon}{\partial n} = 0$.

At wall boundary, the k-ε double equations' turbulence model is the high Reynolds number model, which is only applied to the mature turbulent flow, but near the wall, viscosity plays the main effect. As the value of the variable changes quickly, it need make grid dense in order to simulate the actual flow well. So, the "wall function method" was employed, that used the solution resulting from semi-analyzing method to replace the distribution law of velocity, turbulent kinetic energy and turbulent kinetic energy dissipation rate from wall to the core area of turbulent flow approximately, and appending the impact of wall, such as wall stress, to the difference equations, besides, set the coefficient of boundary to zero.

4 SIMPLEC algorithms

The overall numerical procedure can be summarized as follows: (1) Started with guessed fields u^*, v^*, and according to the water level of the inlet and outlet, give the water level of full area and calculating the water depth H^* of every grid point; (2) calculate the coordinate changing coefficient; (3) solving the momentum equation to get u^n, v^n; (4) solving the k-ε turbulent model to get k^n, ε^n; (5) solving the water depth correction equation to get H', and modify water-depth $H = H^* + \alpha_h H'$; (6) modify velocity u, v and the effective viscosity coefficient μ_{eff}, then return to step 3 and repeat the whole procedure until convergence reached; (7) solving the concentration equation until convergence reached. Where α_h is the under-relaxation coefficient.

During solving the model, the under-relaxation method was applied in order to convergence of the non-linear equation. The ADI technique and TDMA algorithm have been employed, and the maximal error of continuity equation act as the criterion to judge convergence. In the calculation of constant flow, the maximal absolute value of velocity error among two sequential steps at each point in the calculation domain act as the criterion to judge convergence.

5 Model application

Chang (Chang, 1971) conducted a series of experiments in meandering channels measured both flow and neutral buoyant pollutant concentration. The channels had smooth beds and rectangular cross sections and uniform 90° bends in alternating directions interconnected by straight reaches. The channel with a single meander is illustrated in Fig. 1 with the water depth $H = 0.115$ m and bulk velocity $U_0 = 0.366$ m/s. The model was applied with a grid system of 167×23, the time step $\Delta t = 5$s and roughness is 0.015. The program will converge to prescriptive value 10^{-7} at 800th time step and velocity field of whole river reach is drawn as Fig. 2. In order to validate the model further, velocity of 4 cross sections with measured data is selected to compare with computing results (Fig. 3). The contamination concentration at 4 cross sections has been compared between measured and computed, which is discharged in the centerline and from bank at the entrance of the first bend, as Fig. 4 and Fig. 5.

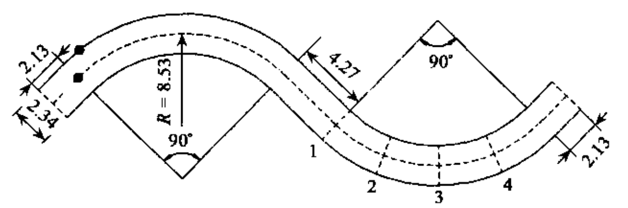

Fig. 1 Sketch of meandering channel in lab (unit: m)

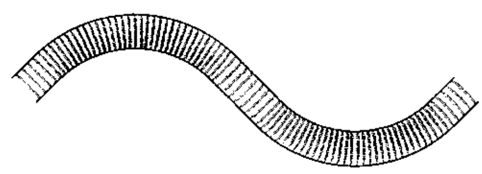

Fig. 2 Computed velocity field of meandering channel in lab

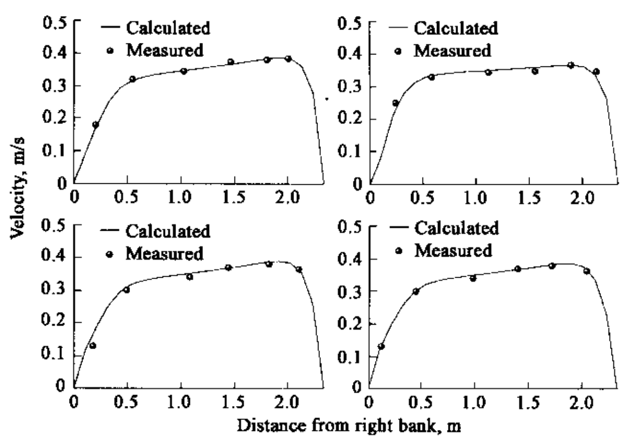

Fig. 3 Comparisons of measured and computed velocity (Section 1 to 4)

The comparison of velocity coincides very well with the experimental data, but there are some dispersion at the boundary between the calculated outcome and experimental data. First, the lateral diffusion coefficient of contaminant is difficult to make certain. Second, the schmidt number σ_c plays a very important action in the diffusion of contaminant in turbulent flow. In this paper, the value of σ_c is 1.0, but

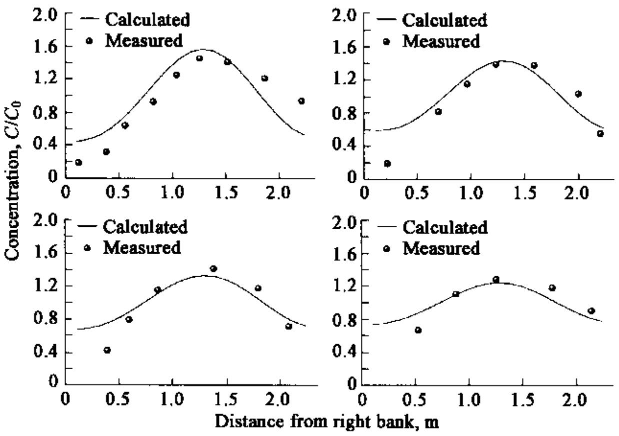

Fig.4 Comparisons of concentration discharged in centerline(Section 1 to 4)

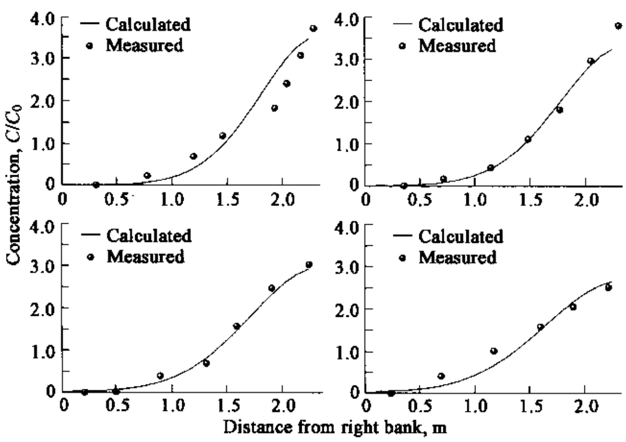

Fig. 5 Comparisons of concentration discharged from bank(Section 1 to 4)

Ye J. adopt 0.5(Ye, 1997). The finite difference scheme of convection term is another reason to impact the diffusion of contaminant. For the sake of simpleness, hybrid scheme is adopted in the discretization of the convection term, and high-order scheme such as third-order upstream, fifth-order upstream has better precision than that used in this study.

6 Conclusions

The numerical model of depth-averaged pollutant convection-diffusion in non-orthogonal curvilinear coordinates has been developed and the SIMPLEC algorithm has been adopted to solve the equations. The model has been applied to simulate the flow and concentration field. In validating concentration field, we adopt two optimal operations of contamination discharging both along bank and in the centerline at the first bend of the meandering channel in the laboratory, and the calculating results coincide well with the measured data.

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(Received for review November 18, 2002. Accepted January 20, 2003)