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PREDICTION PROGRAMMING OF THE WATER QUALITY AND ITS APPLICATION

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Abstract: This paper predicts the total phosphorus concentration in the water in the West Lake using a model of the convection and dispersion equation. The theory of the model is presented and predictions are made using a FORTRAN 77 program in a Dell 486 micro-computer. The results of numerical simulations are also discussed. The results presented in the paper have a practicable significance in controlling the environment of the water quality.

Key words: Convection dispersion model, FORTRAN 77 program, Water quality of the West Lake.

Introduction

The West Lake is a relatively small and shallow fresh water lake. It is surrounded by mountains the three directions. The sources of the lake water is mountain streams and the surrounding surface water covering more than 20 Km^2. The resource of the water is not enough long-term. The great amount of nutritious substances such as phosphorus and nitrogen have been continuously entering the lake. The algae have been growing exceedingly so that the water color and transparancy have been influenced. In order to reveal the density change of nutritious substances in the water body, we detected the changes in the selected points of the lake so as to provide scientific basis for improving water quality.

1. The convection dispersion model

$$\frac{\ni C}{\ni t}+\left(u*\frac{\ni C}{\ni x}+v*\frac{\ni C}{\ni y}\right)=D*\left(\frac{\ni^2 C}{\ni x^2}+\frac{\ni^2 C}{\ni y^2}\right)+S \qquad (1)$$

$$C_i \mid \Gamma(t,X_i,Y_i)=0 \qquad (2)$$

$$\frac{\ni C}{\ni n}\mid \Gamma^2=0 \qquad (3)$$

$$C_j(0,X_j,Y_j)=C_j \qquad (4)$$

In the balance of quality equation (1) of quality, u and v are horizontal and vertical flow rates in the lake, respectively. D is the dispersion coefficient. The quality is the same in each direction. S refers to the total contribution of biological, chemical and physical effects to the concentration of total phosphorus in the lake water. In this case, it actually represents the net exchange quantity of pollutants in sediment. $\Gamma 1 \cup \Gamma 2$ are fixed borders for the lakes bank and islands within the West Lake. In the border condition (equation 2), C_i is the total phosphorus concentration at every entrance and the exit points (x_i , y_i) of the lake. C_j is remained constant during the calculation time period. The fixed border condition (equation 3) indicates that the gradient of total phosphorus concentration is zero in the normal direction of the lakes bank. The initial condition (equation 4) is established according to actual cinditions.

Programing method

A triangular network covering the other water surface of the lake was provided. Special points such as pollution source points was also included in the network points. The program network encompassed a total of 128 knots and 182 triangular elements.

Firstly, using the dispersed method and finite element analysis of Gajorking weighted residual integration, the equation (1) was converted into the normal differential equation group about C_j (t), shown below:

$$A_{ij}C_j'(t)+B_{ij}C_j(t)=T_i \tag{5}$$

where
$$A_{ij}=\int\Omega\int\Phi_i\Phi_j dxdy \tag{6}$$

$$B_{ij}=\int\Omega\int\left[D\left(\frac{\ni\Phi_i}{\ni x}*\frac{\ni\Phi_j}{\ni x}+\frac{\ni\Phi_i}{\ni y}*\frac{\ni\Phi_j}{\ni y}\right)+\Phi_i\left(u_j\frac{\ni\Phi_i}{\ni x}+v_j\frac{\ni\Phi_j}{\ni y}\right)\right]dxdy \tag{7}$$

and

$$T_i=\int\Omega\int(K\Phi_i/Z)dxdy \tag{8}$$

Reasoning course could be seen in our paper of the study on the water quality model of the West Lake in Hangzhou (He Jingtu and Pei Hongping, 1992).

Through integral transformations, the integration of the triangular element given in equation (6) (where A is the area and △ is the region) was then converted to the following integration:

$$\int(\Delta)\int\Phi_i\Phi_j dxdy = A/3 \qquad when \quad i=j$$
$$= A/12 \qquad when \quad i\neq j$$

Using integration by parts and Euler's integral formula, for the integral as(7), we can inference:

$D(a_i a_j+b_ib_j)A+(u_ja_j+v_jb_j)A/3$

Where $a_i=(y_j-y_k)/2A$, $b_i=(x_k-x_j)/2A$

$A_j=(y_k-y_i)/2A$, $b_j=(x_i-x_k)/2A$

The integration shown in equation (8) was then changed into:

$$\int(\Delta)\int \Phi_i \frac{K}{z_j} dxdy = \frac{K}{z_j} * \frac{A}{3}$$

Accordingly, population model matrixes were formed prior to compiling the programs. Second, The inverse matrix of A was then solved using Gauss-Jordan elimination of all pivot selections, forming the standard normal differential equation group. The above equation group was then able to be solvedusing the classical fourth-order Kunge-Kutta formula and outputting T-P concentration values at each point. The average T-P concentration values and the relevant curvilinear figure of the five lake areas was determined by shifting charting subroutine.

Calculation program

The main calculation program was written using FORTRAN 77 language and is shown below:

```
      program West Lake
      external ff
      dimension n(182,3),x(182,3),y(182,3),s(182)
      dimension b(182,3),a(182,3),v(128),u(128),z(128)
      dimension c(128,43),e(128,128),yy(128),dd(128),bb(128)
      dimension f(128,128),q(128),w(128),t(182,3),d(128,128)
      real g(3,3),l(3,3),m(3,3),p(20)
      integer r,h(20),is(128),js(128)
      open(3,file='fp2.dat',status='old')
      do 5 i=1,20
      read(3,4,end=9) h(i),p(i)
5     continue
4     format(i3, f6.3)
9      close(3)
      open(10,file='cio2.dat',status='old')
      do 24 i=1,128
      read(10,23,end=11) yy(i)
24    continue
23    format(f7.3)
11    close(10)
      open(7,file='nxy2.dat',status='old')
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```
      do 8 i=1,182
      read(7,10,end=12) n(i,1), x(i,1), y(i,1), n(i,2), x(i,2), y(i,2)
     $ n(i,3), x(i,3), y(i,3)
8     continue
4     format(3(i4,2f7.1))
12     close(7)
      open(8,file='uvz2.dat',status='old')
      do 18 i=1,128
      read(8,16,end=13) u(i), v(i),z(i),
16     format(3f6.3)
18    continue
13     close(8)
     do 40 i=1,182
     do 50 j=1,3
     x(i,j)=34.78*x(i,j)
     y(i,j)=34.78*y(i,j)
50     CONTINUE
      S(I)=((X(I,2)-X(I,1))*(Y(I,3)-Y(I,1))
     C -(Y(I,2)-Y(I,1))*(X(I,3)-X(I,1)))*0.5
      WRITE(*,*) I,S(I)
      B(I,1)=0.5*(Y(I,2)-Y(I,3))/S(I)
      B(I,2)=0.5*(Y(I,3)-Y(I,1))/S(I)
     B(I,3)=0.5*(Y(I,1)-Y(I,2))/S(I)
      A(I,1)=0.5*(X(I,3)-X(I,2))/S(I)
      A(I,2)=0.5*(X(I,1)-X(I,3))/S(I)
      A(I,3)=0.5*(X(I,2)-X(I,1))/S(I)
      DO 60 J=1,3
      DO 70 R=1,3
      NIR=N(I,R)
      L(J,R)=(A(I,J)*A(I,R)+B(I,J)*B(I,R))*S(I)
      m(j,r)=(B(i,r)*u(nir)+A(i,r)*v(nir))*s(i)/3
70     continue
      t(i,j)=s(i)/3
      g(j,j)=s(i)/3
60     continue
      g(1,2)=s(i)/12
```

```
      g(1,3)=g(1,2)
      g(2,1)=g(1,2)
      G(2,3)=G(1,2)
      G(3,1)=G(1,2)
      G(3,2)=G(1,2)
      DO 90 J=1,3
      NIJ=N(I,J)
      Q(NIJ)=Q(NIJ)+0.000008*T(I,J)/Z(NIJ)
      DO 90 R=1,3
      NIR=N(I,R)
      F(NIJ,NIR)=F(NIJ,NIR)+G(j,R)
      e(nij,nir)=e(nij,nir)+0.8*l(j,r)+m(j,r)
90    continue
40    continue
      do 100 j=1,20
      jj=h(j)
      do 110 i=1,128
      q(i)=q(i)-e(i,jj)*p(j)
      f(i,jj)=0
      f(jj,i)=0
      e(i,jj)=0
      e(jj,i)=0
110   continue
      f(jj,jj)=1
      e(jj,jj)=1
      q(jj)=p(j)
100   continue
      do 88 i=1,128
      q(i)=q(i)*0.01
      do 88 j=1,128
      f(i,j)=f(i,j)*0.01
      e(i,j)=e(i,j)*0.01
88    continue
      do 38 kk=1,128
      pp=0.0
      do 20  i=kk,128
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```
      do 20 j=kk,128
      if(abs(f(i,j)) .gt. pp) then
      pp=abs(f(i,j))
      is(kk)=i
      js(kk)=j
      endif
20    continue
      if (pp+1.0 .eq. 1.0) then
      write(*,*) kk,'     err*not inv'
      stop
      endif
      do 22 j=1,128
      tt=f(kk,j)
      f(kk,j)=f(is(kk),j)
      f(is(kk),j)=tt
22    continue
      do 27 i=1,128
      tt=f(i,kk)
      f(i,kk)=f(i,js(kk))
      f(i,js(kk))=tt
27    continue
      f(kk,kk)=1.0/f(kk,kk)
      do 26 j=1,128
      if(j.ne.kk) then
      f(kk,j)=f(kk,j)*f(kk,kk)
      endif
26    continue
      do 28 i=1,128
      if(i.ne.kk) then
      do 30 j=1,128
      if(j.ne.kk) then
      f(i,j)=f(i,j)-f(i,kk)*f(kk,j)
      endif
30    continue
      endif
28    continue
```

```
      do 32 i=1,128
      if(i.ne.kk) f(i,kk)=-f(i,kk)*f(kk,kk)
32    continue
38    continue
      do 36 kk=128,1,-1
      do 35 j=1,128
      tt=f(kk,j)
      f(kk,j)=f(js(kk),j)
      f(js(kk),j)=tt
35    continue
      do 34 i=1,128
      tt=f(i,kk)
      f(i,kk)=f(i,is(kk))
      f(i,is(kk))=tt
34    continue
36    continue
      write(*,*)
      do 200 i=1,128
      do 210 j=1,128
      d(i,j)=0.0
      do 220 r=1,128
      d(i,j)=d(i,j)+f(i,r)*e(r,j)
220   continue
210   continue
200   continue
      do 230 i=1,128
      w(i)=0.0
      do 240 j=1,128
      w(i)=w(i)+f(i,j)*q(j)
240   continue
230   continue
      ta=0.0
      HH=0.167
      MM=128
      NN=43
      CALL RKTT(TA,YY,MM,HH,NN,C,D,W,FF,DD,BB)
```

```
        WRITE(*,*)
        DO 6 I=1,NN
        tA=(I-1)*HH
        WRITE(*,202) I-1, tA
       WRITE(*,505) (j,c(J,I),j=1,mm)
        WRITE(*,*)
6       CONTINUE
202     format (1x,'T(',I2,')=',F10.5)
505     format(4(1x,'c(',i3,')=',E13.6,2x))
        END
```

Main program pattern is end.

Due to space limitations, other program blocks have not been written out in this paper. In the above program, RKTT is a subprogram for solving differential equation groups using the classical fourth-order Kunge-Kutta formula. The data files, hp2.dat and cio2.dat, nxy2.dat, are the coordinates, water rates and water depths, and initial values of T-P concentrations of all knots in the network, respectively.

Analysis of the predicted result

The 486 micro-computer calculations showed that the T-P concentrations had slowly dropped in about 50 points. Most of these points were located in the main lake area (L. Wai). This indicates that the water quality of the main lake area had improved under the normal water-drawing conditions ($3*10^5$ M^3 /day). The approximate function $C\sim-0.0083t^{4/5}+0.19$ was used to imitate the change in T-P concentration. The calculated results indicated that this is suitable for about 20 days for each water-drawing project.

T-P concentrations dropped rapidly in about 20 points. The majority of these points were located in the centre of L. Xiaonan and the exits from L. Xiaonan to L. Xili, the southend of L. Xili to L. Wai, and the northend of L. Xili to L. Yuchu. Negative values appeared in the calculation which are allowed, according to finite element analysis of fluid dynamics. Suitable values were used to replace negative values when required.

T-P concentrations increased in about 14 points, most of which were located near pollution sources. The changes in T-P concentrations were insignificant in about 33 points and T-P concentrations underwent no changes in about 14 points. These points were all located at die angles of drawing water. The water quality of such points can only be improved by increasing the rate of interception of waste, controlling pollution sources, and conducting comprehensive renovations and controls in the West Lake.

The computed results of the average T-P concentration values for each lake area during a one week period are shown in Figure 1. The simulated values were compared to observed values, shown in Table 1. The results show that the simulated values and the observed values were in close agreement. Therefore, water quality models are efficient methods for predicting the actual conditions. The calculation program compiled using FORTRAN 77 language was focussed to calculating the water quality of the West Lake only. The program could also be applied, however, to other lakes with either no changes or only slight changes required. The above mentioned program could be used to calculate the extent of pollution matter dissolved in water, thus providing a scientific basis for the environmental protection of water.

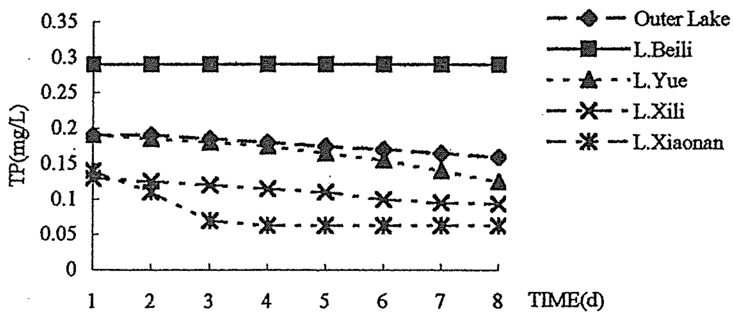

Figure 1. The average computed T-P concentration values in each lake area during a 7 day period under normal water-drawing condition.

Table 1. The comparison between observed and simulated values of TP concentration before and after water-drawing

	before water-drawing	7 day after water-drawing	
		observed values	simulated values
L. Wai	0.1900	0.1600	0.1580
L. Yue	0.1900	0.1250	0.1315
L Xili	0.1300	0.1100	0.0935
L. Xiaonan	0.1400	0.0900	0.0628
L. Beili	0.2980	0.2810	0.2945

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