A THREE-DIMENSIONAL POLLUTANT TRANSPORT MODEL IN ORTHOGONAL CURVILINEAR AND SIGMA COORDINATE SYSTEM FOR PEARL RIVER ESTUARY

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Abstract: In this paper, the development of a three-dimensional numerical pollutant transport model, which is coupled with a previously developed hydrodynamic model, is delineated in details. Special features of the model include orthogonal curvilinear coordinate in the horizontal direction and sigma coordinate in the vertical direction. Besides, a simple but efficient open boundary condition of pollutant transport is adopted. It is then applied to simulate the transport of a representative water quality parameter Chemical Oxygen Demand in Manganese (COD_{Mn}) in the Pearl River estuary, which is the largest estuary in South China. It can be shown, from the simulated results, that there exists a transboundary action between Guangdong Province and Hong Kong Special Administrative Region for the pollutants in the wastewater discharged from Pearl River Delta Region have.

Keywords
Three-dimensional, pollutant transport, numerical model, boundary condition, Pearl River estuary

INTRODUCTION

In this paper, the development of a three-dimensional numerical pollutant transport model, which is coupled with a previously developed numerical hydrodynamic model (Chau and Jiang 1999), is delineated in details. Special features of the model include orthogonal curvilinear coordinate in the horizontal direction and sigma coordinate in the vertical direction. Besides, a simple but efficient open boundary condition of transport is adopted. This model is applied to the Pearl River estuary (PRE), which is the largest river system in South China. The Pearl River Delta Region (PRDR), which is one of the most quickly developing regions in China and Asia, includes eight cities, Guangzhou, Shenzhen, Zhuhai, Foshan, Zhongshan, Dongguan, Huizhou and Jiangmen. The rapid economic development has given rise to a significant impact on the local environment. In particular, the rate of untreated sewage discharge is increasing in high speed. Lots of the pollutants have been discharged into the network of Pearl River and passed through the five main outlets, ie. Hu men, Jiao men, Hongqi men,

Heng men, and Shenzhen river outlet to PRE (see Figure 1).

Under the interaction of flood tide, ebb tide and upstream runoff of the river, the pollutants in the PRDR transport from the outlets of the Pearl River system to the entrance of PRE. Hong Kong Special Administrative Region (HKSAR), whose sovereignty and administration of the territory was restored to the People's Republic of China on 1 July 1997, is located on the eastern side of the entrance. Macau, whose sovereignty and administration of the territory will be restored to the People's Republic of China on 20 December 1999, is located on the western side of the entrance. The transboundary pollutants from the inner PRE as potentially significant matters of concern have, however, added a further complicating dimension to the task of environmental protection in the HKSAR (Hills & Zhang 1998) and Macau.

Hence it is very important to estimate how much the pollutants from the PRDR impact the water quality in seawaters of HKSAR. In this paper a three-dimensional pollutant transport numerical model with advanced open boundary of transportation is developed, and it takes the COD_{Mn} as an index to assess the action of pollution transboundary.

DESCRIPTION OF THE POLLUTANT TRANSPORT MODEL

The model is based on a three-dimensional hydrodynamic numerical model (Chau & Jiang 1999) developed from the POM (the Ocean Model of Princeton University, Mellor 1996). The principal attributes of the model are as follows:

1. It contains an embedded second moment turbulence closure sub-model to provide vertical mixing coefficients.
2. The curvilinear orthogonal coordinate is used in the horizontal direction and sigma coordinate is used in the vertical direction.
3. The horizontal and vertical time differencing are treated semi-implicitly. A time-splitting method is used for the horizontal time differencing of external model and hence the allowable time step is larger than that from CFL stability criterion.
4. Complete thermodynamics have been implemented and the stratification of salinity and temperature are considered.

The hydrodynamic equations and the corresponding solving method can be referred to Mellor 1996. The equations under the orthogonal curvilinear transformation can be referred to Chau and Jin 1991. Chau and Jiang 1999 have described the hydrodynamic model of PRE coupled in the present pollutant transport study.

The Equation of Pollutant Transport

The equation of pollutant transport in this model can be written as:

$$\frac{\partial SD}{\partial t} + \frac{\partial SUD}{\partial x} + \frac{\partial SVD}{\partial y} + \frac{\partial S\omega}{\partial \sigma} = \frac{\partial}{\partial x}(A_S H \frac{\partial S}{\partial x}) + \frac{\partial}{\partial y}(A_S H \frac{\partial S}{\partial y}) + \frac{\partial}{\partial \sigma}\left[\frac{K_H}{D}\frac{\partial S}{\partial \sigma}\right] - K_S DS + S_S \tag{1}$$

where (U, V, ω) are mean fluid velocities in the (x, y, σ) direction, S is the density of

the pollutant, which in this paper being the density of COD_{Mn}; $D = \eta + H$, η is the elevation of sea surface above the undisturbed level, H is the undisturbed mean depth of the water; K_H is the vertical turbulent flux coefficient, which can be derived from the second moment $q^2 \sim q^2 l$ turbulence energy model (Mellor 1996). K_s is the decay rate of pollutant; S_s is the source of pollutant; A_s is horizontal turbulent coefficient, which can be obtained through Smagorinsky formula (Oey *et al* 1985)

$$A_s = C\Delta x \Delta y \left[\left(\frac{\partial U}{\partial x}\right)^2 + \tfrac{1}{2}\left(\frac{\partial V}{\partial x} + \frac{\partial U}{\partial y}\right)^2 + \left(\frac{\partial V}{\partial y}\right)^2 \right]^{\frac{1}{2}} \tag{2}$$

where C is constant ranged from 0.1 to 0.2. In this model, 0.12 is adopted and seems to work well.

Pollutant transport equations can be written in differencing equations depending on the "Arakawa C" grids (Figure 2) as below:

$$\delta_t (SD) + \delta_x (\overline{S}^x \overline{D}^x U) + \delta_y (\overline{S}^y \overline{D}^y V) + \delta_\sigma (\overline{S}^\sigma \omega) = \delta_x (\overline{H}^x \overline{A}_s^x \delta_x S) + \delta_y (\overline{H}^y \overline{A}_s^y \delta_y S)$$
$$+ \delta_\sigma (\overline{K}_H^\sigma \delta_\sigma S_+ / D) - K_S D S_+ + S_s$$
$$\tag{3}$$

In equation (3), for any parameter on the point x, y, σ, t , letting $F = F(x, y, \sigma, t)$,we have:

$$\delta_t F = \tfrac{1}{2\Delta t}(F(x, y, \sigma, t + \Delta t) - F(x, y, \sigma, t - \Delta t)) \tag{4}$$

$$\overline{F}^x = \tfrac{1}{2}\left[F(x + \tfrac{\Delta x}{2}, y, \sigma, t) + F(x - \tfrac{\Delta x}{2}, y, \sigma, t)\right] \tag{5}$$

$$\delta_x F = \tfrac{1}{\Delta x}\left[F(x + \tfrac{\Delta x}{2}, y, \sigma, t) - F(x - \tfrac{\Delta x}{2}, y, \sigma, t)\right] \tag{6}$$

$$S_+ = S(x, y, \sigma, t + \Delta t) \tag{7}$$

In the differencing equation (3), all the components can be obtained from the previous time steps or hydrodynamic model except unknowns $S(x, y, \sigma, t + \Delta t)$, $S(x, y, \sigma + \Delta\sigma, t + \Delta t)$, and $S(x, y, \sigma - \Delta\sigma, t + \Delta t)$ in the first term of left hand side and the third and fourth term of right hand side. So equation (3) can be written in formula below:

$$AS(x, y, \sigma - \Delta\sigma, t + \Delta t) + BS(x, y, \sigma, t + \Delta t) + CS(x, y, \sigma + \Delta\sigma, t + \Delta t) = D \tag{8}$$

where A, B, C, D are known coefficients. Hence equation (8) is a tri-diagonal matrix in the vertical direction and this equation can be solved with the method described by

Pichtmeyer and Morton 1967.

APPLICATION TO THE PEARL RIVER ESTUARY

Hydrology Condition

The study area (Figure 1) is a delta estuary with four main outlets (Hu men, Jiao men, Hongqi men, Heng men) in the north-west of PRE and Shenzhen river outlet at the Deep Bay. According to the published data (Pang and Li 1998) the multi-years averaged net discharges of the former four outlets in different seasons are listed in Table 1. The tide in PRE is semi-diurnal irregular tide and the mean tidal range is about 1.0m. At the entrance of the estuary the mean tidal range is 0.85-0.9m. The range is higher in the inner estuary and when it come to Hu men the mean range is 1.6m(Kot 1995). In the wet season (May to September) the runoff of the rivers is so strong to become the predominate hydrodynamic forcing in PRE, and in dry season (December to March) the tidal current is the main force. In order to know the transportation of pollutant, the distribution of pollutant in different seasons shall be studied.

The horizontal grid of the orthogonal curvilinear coordinate system in this model is displayed in Figure3, and the corresponding transformed grid is shown in Figure 4. The total number of horizontal grids is 3400, and there are 6 layers in the vertical direction. Each layers has the same $\delta\sigma$, and the value is *1/6*.

The Initial and Boundary Condition

In the beginning the density of pollutant in the computing domain is set to zero. After a number of computational tidal periods (in this model 100 tidal periods, which is about 50 days) the density become stable.

There are two open boundaries in the domain of this model, the eastern open boundary and the southern open boundary. The open boundary condition of transportation is usually treated simply (Leendertse & Crittion 1971). Taking grids near eastern open boundary for example (Figure 2), the method used by Leendertse 1970 is:

$$P_{i,j}^{n+1} = P_{set} \qquad\qquad U_{i-\frac{1}{2},j}^{n+1} < 0 \qquad\qquad (9)$$

$$\frac{dP}{dt} = 0 \quad that \quad is \frac{P_{i,j}^{n+1} - P_{i,j}^{n-1}}{2\Delta t} + U_{i-\frac{1}{2},j}^{n+1} \frac{P_{i,j}^{n} - P_{i-1,j}^{n}}{\Delta x} = 0 \qquad\qquad U_{i-\frac{1}{2},j}^{n+1} > 0 \qquad (10)$$

where P_{set} denotes the prescription for the along-boundary component of pollutant density. If it is a known value, the value can be used. More often it is unknown and the value, 0, has to be set. Thus the open boundary condition above is reasonable just on the occasion that the value on boundary is known or the capacity of water exchange along the open boundary is very good. When the model is applied to the PRE, no such data are available and the exchange capacity on the entrance of PRE is not so strong that $P_{set} = 0$

can be used. A simple efficient open condition of transportation is advanced in this model:

$$\frac{P_{i,j}^{n+1} - P_{i,j}^{n-1}}{2\Delta t} + U_{i-\frac{1}{2},j}^{n+1} \frac{(a-1)P_{i-1,j}^{n}}{\Delta x} = 0 \qquad\qquad U_{i-\frac{1}{2},j}^{n+1} < 0 \qquad (11)$$

$$\frac{dP}{dt} = 0 \quad that \quad is \frac{P_{i,j}^{n+1} - P_{i,j}^{n-1}}{2\Delta t} + U_{i-\frac{1}{2},j}^{n+1} \frac{P_{i,j}^{n} - P_{i-1,j}^{n}}{\Delta x} = 0 \qquad\qquad U_{i-\frac{1}{2},j}^{n+1} > 0 \qquad (12)$$

In this condition, equation (12) is the same as equation (10) at ebb tide, but when it come to flood tide equation (11) takes the place of equation (9). In equation (11) a is a constant coefficient, whose range is $0 \le a < 1$. The value of a depends on the capacity of water exchange outside the open boundary. When the exchange capacity is strong, the value of a can be set small, otherwise the value is set large. Figure 5 shows the difference of the COD_{Mn} density on the boundary corresponding to different a when the computation becomes stable. In this model of PRE, $a = 0.9$ is adopted, which seems to work well.

The Load of COD in Different Outlets

Pollutants have been discharged to PRE mainly from four outlets at the northwest of PRDR and the outlet of Shenzhen River at Deep Bay (Figure1). Because there are no direct COD data discharged from different outlets, the loading of COD at different outlets in this model is calculated through the way described below.

Table 2 shows that the domestic and industrial wastewater discharged from Guangdong Province according to Guangdong Yearbook Editorial Committee (1996). From this table a relationship between COD discharge rate and the domestic and industrial wastewater discharge rates can be achieved:

$$Q_{COD} = 0.00027Q_d + 0.000305Q_i \qquad (13)$$

Q_{COD} is the discharge rate of COD, Q_i is the industrial wastewater discharge rate, Q_d is the domestic wastewater discharge rate. Through this formula, the quantity of the COD discharged from the eight cities in PRDR can be derived from the corresponding wastewater discharges. The results of 1996 are listed in table 3.

From Table 3, the COD loadings at five outlets can be achieved, the results and net water discharges in different seasons are listed in Table 4. Because Pearl River is a river network system, the COD loading data are approximated by the COD discharge of eight cities and net water flow rates of the corresponding Pearl River system branch.

SIMULATED RESULTS

The COD Distribution of Simulation Results in Different Season

Since the COD loading of PRDR in different season is estimated, the data has been used in this numerical model to simulate the distribution of increasing COD_{Mn} caused

by these pollutant sources. Through this method, the impacts of the pollutant sources from PRDR on Hong Kong seawaters can be assessed.

Because the vertical mixing is quite well, the difference of vertical averaged COD_{Mn} densities in different layers can be omitted. Figure 6 shows the distribution of COD_{Mn} in different seasons during the ebb tide. It is indicated from this figure that the influence of COD from the five outlets is significant up to the northern part of the Lantau Island, and its effect is lesser to the other areas of Hong Kong seawaters. The maximum increasing density of COD_{Mn} caused by the loadings of the five outlets is about 0.75 mg/L in former area. In the wet season, the COD_{Mn} is transporting most widely, and it affects the quality of Hong Kong seawaters more notably. During the wet season the density change of COD_{Mn} in inner estuary is not so high as other seasons. The reason is that the conveyance capacity is highest with the largest net discharge. On the contrary, in the dry season, density of COD_{Mn} is very high in inner PRE. But at the entrance of PRE, especially at Hong Kong seawaters, COD_{Mn} is more dilute than in the wet season.

It is also shown that the pollutants from the Humen outlet and Shenzhen river outlet impact the PRE and Hong Kong seawaters more than other outlets. The reason is that the former has the largest pollutant loading, and the hydrodynamic transportation capacity of the latter is limited because of its location and little net water discharge of Shenzhen River.

CONCLUSIONS

A three-dimensional numerical model based on orthogonal curvilinear grid in the horizontal direction and sigma coordinate in the vertical direction for the prediction of water quality constituents is developed, and a simple efficient open boundary condition of transportation is advanced in this model. This model is applied to the typical estuary domain, PRE, to assess the transbounday pollution between Guangdong and Hong Kong.

The pollutant load data at five main outlets in PRE is not directly available, so the COD_{Mn} discharge rate of different outlets is estimated and adopted as the pollutant sources into the water quality model. The simulated results show that the pollutants from the PRDR influent the Hong Kong seawaters notably, especially in wet season with large net water discharge from upstream. It is also indicated that the pollutants discharged from Humen outlet and Shenzhen outlet impact the water quality in PRE and Hong Kong seawaters more than other outlets of PRE.

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Table 1. The discharge of four northwestern outlets in different seasons (Wet season month: May to September; Mean season month: April, October and November; Dry season month: December to March) (unit: $10^8 m^3/season$)

Hu men			Jiao men			Hongqi men			Heng men		
Wet	Mean	Dry	Wet	Mean	Dry	Wet	Mean	Dry	Wet	Mean	Dry
312.9	140.6	81.2	299.2	129.7	70.2	116.1	45.7	20.7	196.3	80.3	44.9

Table 2. Summary statistics of wastewater and COD discharge from Guangdong Province (unit: 10,000 ton)

Source	1990	1991	1992	1993	1994	1995	1996
Domestic	111012	105847	131049	149291	198131	212369	212222
Industrial	140250	139224	141939	139762	131531	160979	150874
Total wastewater	251262	251090	280103	295990	337207	381657	371405
COD	69.5	71.71	78.	79.67	94.46	112.36	106.30

Source: Guangdong Province Yearbook Editorial Committee (1996)

Table 3. The quantity of COD discharges from eight cities in 1996 according to equation 13.

(unit:10,000 ton)

Source in 1996	Guangzhou	Shenzhen	Zhuhai	Huizhou	Dongguan	Zhongshang	Jiangmen	Foshan
Domestic	78990	11645	7113	16701	4170	5866	6895	22627
Industrial	32325	5501	3054	1926	10778	9645	11126	16911
Total wastewater	111315	17146	10167	18627	14948	15511	18021	39538
COD	31.2	4.8	2.9	5.1	4.4	4.5	5.3	11.3

Source: Guangdong Province Yearbook Editorial Committee (1996)

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Table 4. Net water discharge and COD load of five river outlerts in different season

	Hu men	Jiao men	Hongqi men	Heng men	Shengzhen
Wet(10^8m^3/day)	2.09	1.99	0.77	1.31	0.06*
Mean(10^8m^3/day)	1.56	1.44	0.51	0.89	0.06
Dry(10^8m^3/day)	0.68	0.59	0.17	0.37	0.06
COD(kg/day)	1115068	309000	70285	12300	89877

* Accurate data are not available, estimated data are made from the annual rainfall