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THREE-DIMENSIONAL POLLUTANT TRANSPORT MODEL FOR THE PEARL RIVER ESTUARY

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Abstract: In this paper, the development and implementation of a three-dimensional, numerical pollutant transport model, which is based on an orthogonal curvilinear coordinate system in the horizontal direction and a sigma coordinate system in the vertical direction, is delineated. An efficient as well as simple open boundary condition is employed for pollutant transport in this mathematical model. It is then applied to model the distribution and transport of Chemical Oxygen Demand (COD) in the Pearl River Estuary (PRE). The results from the numerical simulations illustrate that the transboundary or inter-boundary effects of pollutants, between the Guangdong Province and the Hong Kong Special Administrative Region due to the wastewater discharged from the Pearl River Delta Region, are quite strong.

Keywords
COD concentration, numerical model, Pearl River estuary, pollutant transport, three-dimensional model

Short title
Pollutant model for Pearl River Estuary

INTRODUCTION

In this paper, the development and implementation of a three-dimensional, numerical pollutant transport model, which is coupled with the orthogonal curvilinear and sigma coordinate system numerical hydrodynamic model (Chau and Jiang 2001), is delineated. Besides, an efficient and simple open boundary condition of transport is employed. Application of this model is then made to the largest river system in South China, namely, the Pearl River Estuary (PRE). The Pearl River Delta Region (PRDR), covering eight large cities,namely, Dongguan, Foshan, Guangzhou, Huizhou, Jiangmen, Shenzhen, Zhongshan and Zhuhai, is one of the rapidly developing regions in China as well as in Asia. As a result of this rapid economic development and prosperous activities within the area, an adverse impact on the ambient environment has become inevitable. Amongst various types of pollution, the rate of untreated sewage discharge is escalating at a exceedingly fast rate. During the last decade, an enormous amount of the pollutants has been discharged into the Pearl River Estuary, which are originated from five main outlets, namely, Hu men, Jiao men, Hongqi men, Heng men, and Shenzhen River (see Figure 1).

The pollutants in the PRDR are transported from the outlets of the Pearl River system to the entrance of the PRE subjected to the coupled physical interaction of the upstream river runoff as well as the tidal effect. Macau is located on the western side of the PRE entrance whereas the Hong Kong Special Administrative Region (HKSAR) is located on the eastern side of the PRE entrance. Whilst nowadays the environment protection issues within the HKSAR and Macau themselves are already a significant matter of concern, the transboundary pollutants from the inner PRE have contributed an additional dimension and complication to their tasks. (Hills et al. 1998)

As such, there is a strong need to determine the impact of pollutants from the PRDR to the water quality in the surrounding coastal waters of the HKSAR. A three-dimensional pollutant transport numerical model with an advanced open boundary transport condition is developed in this paper. In order to assess the transboundary action of pollutants, the COD is employed as an indicative index to mimic the pollutant transport and distribution pattern in PRE. Another feature, which is quite different from other usual procedure, is that, during the determination of the COD to measure the amount of oxygen required for chemical oxidation of organic matter, instead of employing the more commonly used dichromate solution, permanganate solution is employed in this study. It is because dichromate solution is more appropriate for freshwater such as in the river, whilst permanganate solution is more suitable in a seawater environment, such as in this situation.

COD of wastewater is the measured amount of oxygen needed to chemically oxidize the organic present whilst biochemical oxygen demand (BOD) is the measured amount of oxygen required by acclimated microorganisms to biologically degrade the organic matter in the wastewater. Owing to the relatively simple laboratory procedure, BOD is commonly used in water quality modeling. However, in this case, since the composition of the wastewater from the sources shows that it is mainly constituted by industrial wastewater, it may contain higher proportion of chemical materials, which are not easily degradable biologically. It is thus worthwhile to study the transport effect on COD to truly characterize the organic strength as well as the pollution scenario. Besides, it has been reported that BOD is of limited value in measuring the actual oxygen demand of surface waters since the laboratory environment cannot easily reproduce the ambient physical, chemical and biological condition. (Hammer and Hammer 1996)

POLLUTANT TRANSPORT MODEL DESCRIPTION

The 3D Hydrodynamic Model

The pollutant transport model is based on a three-dimensional, hydrodynamic numerical model (Chau and Jiang 2001) developed from the Ocean Model of Princeton

University POM (Mellor 1996). The principal attributes of this model are as follows:

1. The curvilinear, orthogonal coordinate system is used in the horizontal direction and the sigma coordinate system is used in the vertical direction.
2. The horizontal and vertical time differencing are treated semi-implicitly (Casulli and Cheng 1992). In time integration of the governing equation, all terms in the equation are treated explicitly except for the vertical flux term and the decay term that are treated implicitly. A time-splitting method is used for the horizontal time differencing of external mode and, hence, the allowable time step is larger than that from Courant-Friendrichs-Lewy (CFL) stability criterion, which requires the condition: $dt < dx \big/ \sqrt{2gh} + U_{MAX} / \sqrt{2}$.
3. Complete thermodynamics are implemented and the thermal structure of the estuary, including the density and salinity stratification as a function of temperature variation in both horizontal and vertical direction, is considered.
4. It contains an embedded, second moment, turbulence closure sub-model to provide vertical mixing coefficients.

The hydrodynamic equations and the corresponding solution method are detailed in Mellor (1996) and the equations for the orthogonal curvilinear transformation are detailed in Chau and Jin (1995). Chau and Jiang (2001) have described in detail the hydrodynamic model of the PRE used in the present pollutant transport study. In the hydrodynamic model, the density structure of the transporting seawater is calculated as a spatial and temporal function through fulfilling the momentum equations, and the temperature as well as salinity transport equations subjected to the appropriate boundary conditions. Details about the level of confidence, accuracy, previous calibrations and usage of the POM can be found in Quamrul and Blumberg (1999) and Blumberg and Mellor (1987).

The most significant difference between this model and the POM is in the second attribute. In the POM, the horizontal time differencing is entirely explicit, with the time step based on the CFL condition, but in this model the horizontal time differencing is semi-implicit with the use of a time-splitting method. The allowable time step of this model is much larger than that in the POM. This attribute can fit the application to some domains in which there are complex flow patterns and large currents caused by tide and river discharges, such as Pearl River estuary.

Pollutant Transport Equation

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

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

where U, V, ω are the mean fluid velocities in the x, y, σ directions; S is the pollutant concentration as a function of x, y, σ, t, which in this study is the concentration of the

COD; $D = \eta + H$, where η is the elevation of the sea surface above the mean water level, H is the mean water depth; and K_H is the vertical turbulent flux coefficient, which can be derived from the second moment *(q^2~ $q^2\ell$)* turbulence energy model (Mellor 1996). The term $q^2/2$ is the turbulent kinetic energy and ℓ is the turbulence length scale. In this type of model, one equation is written for q^2, representing turbulent kinetic energy, and another equation is written for $q^2\ell$, representing turbulent dissipation. K_s is the decay rate of the pollutant and S_s is the source of the pollutant. A_s is the horizontal turbulence coefficient, which can be obtained from the Smagorinsky formula (Oey *et. al.* 1985):

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

where C is a constant ranging from 0.1 to 0.2. In this application, a constant of 0.12 is adopted and seems to work well based on calibration against standard idealized tests used to verify the accuracy of this model.

The pollutant transport equations can be written in differencing equations using the "Arakawa C" grids (Figure 2) as follows:

$$\delta_t(SD) + \delta_x(\overline{S}^x\overline{D}^xU) + \delta_y(\overline{S}^y\overline{D}^yV) + \delta_\sigma(\overline{S}^\sigma\omega) = \delta_x(\overline{H}^x\overline{A}_s^x\delta_xS) + \delta_y(\overline{H}^y\overline{A}_s^y\delta_yS)$$
$$+ \delta_\sigma(\overline{K}_H^\sigma\delta_\sigma S_+/D) - K_SDS_+ + S_s \quad (3)$$

In equation (3), for any parameter as a function of x, y, σ, t and, letting

$F = F(x, y, \sigma, t)$, results in:

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

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

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

$$S_+ = S(x, y, \sigma, t+\Delta t) \quad (7)$$

In the differencing equation (3), all of the components can be obtained from the previous time step of the hydrodynamic model except for the 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 the left hand side and the third and fourth term of the right hand side. Therefore, equation (3) can be re-written as follows:

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

where A,B,C,D are known coefficients. Hence, equation (8) is a tri-diagonal matrix in the vertical direction and can be solved with the method described by Richtmeyer and Morton (1967).

The veracity of this model has been established by performing several tests involving idealized geometries and forcing functions, which have also been previously applied to the POM. They range from simple tests, on checking the ability of the model to conserve its various constituents, to more rigorous tests involving both barotropic and baroclinic responses of an idealized coastal basin with or without topography to evolve different large scale oceanographic phenomena (Blumberg and Mellor 1987). It has been demonstrated that the model reproduces the expected physics and produces identical results to those from the well-tested POM (Chau and Jiang 2001). They provide a high degree of confidence that the numerical accuracy of the scheme is consistently high and that the level of numerical diffusion is not larger than the physical diffusion calculated in the model.

APPLICATION TO THE PEARL RIVER ESTUARY

Hydrology Conditions

The study area (Figure 1) is a delta estuary with four main river outlets (Hu men, Jiao men, Hongqi men, Heng men) in the north-west of the PRE and the Shenzhen River outlet into the Deep Bay. According to published data (Pang and Li 1998), the average, net discharges of the former four outlets during the mean season years between 1985 and 1995 are 1788, 1650, 581 and 1021, m^3/s respectively. The tide in the PRE is a semi-diurnal, irregular tide with a mean tidal range of approximately 1.0 m. At the entrance to the estuary, the mean tidal range is 0.85-0.9 m and increases into the inner estuary to 1.6 m at the Hu men River mouth (Kot and Hu 1995). During the wet season (May to September), the river runoff is high and dominates the hydrodynamic circulation in the PRE. During the dry season (December to March), the tidal current is the main driving force for circulation in the PRE. In order to examine pollutant transport in the PRE, the distribution of pollutants during different seasons will be studied.

The rectilinear transformed grid for this model is shown in Figure 3. The total number of horizontal model segments is 3,400 with 6 layers in the vertical direction, with each layer having equal $\delta\sigma$ values.

Initial and Boundary Conditions

The initial pollutant concentration of COD in the model domain was set to a fixed value of 1.8 mg/L, also referred to as background data. After a number of computational tidal periods (in this model 100 tidal periods, which is about 50 days), a steady state concentration gradient is achieved.

There are two open boundaries in the model domain, the eastern open boundary (Lei Yu Mun) and the southern open boundary (South China Sea). The open boundary condition for pollutant transport is usually treated simply (Leendertse and Crittion 1971). For example, using the method of Leendertse and Crittion (1971) and using grids near the eastern open boundary, the following equations are developed:

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

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

where P_{set} denotes the prescribed along-boundary component of pollutant concentration. Equation (9) is for flood tide while Equation (10) applies during the ebb tide condition. The value P_{set} can be used if it is a known value but more often it is unknown and an assumed value must be used based on the best available data. Thus, the open boundary condition above is reasonable if the boundary condition is known or the level of water exchange/flushing outside of the model domain is strong so that internal pollutant built up will not occur at the open boundary. COD data are not available in the PRE and the exchange capacity at the entrance of the PRE is not strong enough that the P_{set}=0 approach can be used. A simple and efficient open boundary condition for pollutant transport for flood condition is used in this model:

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

For this approach, the same equation (10) is used at ebb tide, but when at flood tide equation (11) is used instead of equation (9). While Equation (10) means that there is no spatial gradient in concentration, Equation (11) represents the proportion of pollutant concentration brought back by the flood tide. The constant coefficient, *a*, in equation (11) ranges from 0 to 1. The value of *a* depends on the level of water exchange/ flushing outside of the model domain. When the level of flushing is strong, the value of *a* is small, otherwise the value approaches 1. Figure 4 shows the COD concentration at the boundary corresponding to different *a* values after the computation becomes stable. An additional lower limit is also imposed on the boundary condition in Equation (11), i.e., $P_{i,j} = 0$ if $P_{i,j} < 0$. As shown in Figure 5, this condition occurred during some of the tidal periods at small *a* values. In this model, $a = 0.9$ is adopted, which seems to work well based on the internal COD calibration. Moreover, based on the COD initial background condition, if the COD concentration at the boundary is less than 1.8 mg/L, it is set equal to 1.8 mg/L.

COD Load in Different River Outlets

Four main river outlets discharge pollutants to the PRE that are located in the northwest PRDR and also from the Shenzhen River near Deep Bay (Figure 1). Because there are no direct COD data from the different river outlets, the loading of COD at different river outlets in this model is calculated from the following method.

The domestic and industrial wastewater flow generated in the Guangdong Province are obtained according to the Guangdong Yearbook Editorial Committee (1996). From this data, a relationship between the COD loading rate and the domestic and industrial wastewater flow rates is developed:

$$W_{COD} = 0.00027Q_d + 0.000305Q_i \qquad (12)$$

where W_{COD} is the loading rate of COD, Qi is the industrial wastewater flow rate, and Q_d is the domestic wastewater flow rate. Based on this formula, the COD loading rate from eight cities around the PRDR can be derived from the corresponding wastewater flows.

The net average water discharge rates during different seasons are presented in Table 2. Because the Pearl River is a river network system, the COD loading data at different main river outlets are approximated from the COD loading of the eight cities. From the above, the daily COD loading at the five main river outlets (Hu men, Jiao men, Hongqi men, Heng men, Shenzhen) are 671307, 479390, 123661, 210365 and 89877 kg/day, respectively.

The COD loading data from sewage outfalls A, B, C, D and E in the HKSAR are 84237, 55200, 114452, 131675 and 242101 kg/day, respectively. The data are estimated from the Hong Kong strategic sewage disposal plan (Sin et al. 1995). The positions of these sewage outfalls or discharges are shown in Figure 1.

All of the estimated COD loadings are treated as point sources discharged continuously at the corresponding locations. There is no sink term (loss rate of COD) in this application.

SIMULATED RESULTS AND DISCUSSIONS

The estimated COD loadings from the PRDR and the HKSAR during different seasons has been used in this numerical model to simulate the distribution of COD caused by these pollutant sources and also from background sources. Furthermore, the impact of the pollutant sources from the PRDR on Hong Kong seawaters is assessed through a sensitivity analysis.

Figure 5 shows the computed salinity contours of the surface layer, middle layer and bottom layer during the wet season from the hydrodynamic model calibrations, which demonstrate very slight vertical density stratification. Because the vertical mixing is strong, the top to bottom difference of COD concentrations is negligible and, therefore, a vertically averaged value is used. Figure 6 shows the average distribution of COD during different seasons at the ebb tide. It is shown in this figure that the concentration of COD in the western PRE varies with the season. In the wet season, the COD concentration in northwestern PRE is lower than the dry season because of the higher dilution associated with the larger average discharge flow. Alternatively, the wet season concentration in southwestern PRE is higher than the dry season due to the higher conveyance in the wet season. In the eastern PRE, the COD concentration variation with season is not as variable because the tidal current dominates the hydrodynamic forcing and the boundary condition does not change with the season.

Model calibration was completed at two sections, the longitudinal section A_1-A_8 and the latitudinal section C_1-C_7 (Figure 1). The observed data was monitored by Wen et al. (1994). Figure 7 presents the computed and measured COD data for these two sections at different seasons. It can be noticed that, in general, the model results tend to over-compute when compared with the actual measured data, except at the western side of the estuary. However, given the lack of actual COD loading data from different river outlets, the result shows that the accuracy of this model is satisfactory. A possible means to improve the accuracy of the results is the acquisition of the actual COD loading from all the river outlets.

In order to estimate the impact of sewage pollutants, such as COD, discharged from the PRDR on water quality in the seawaters of HKSAR, a model sensitivity analysis was completed. This was accomplished by only including the COD sewage loading from the PRDR and setting the background COD value to 0 mg/L. The results from the wet season are displayed in Figure 8 because the pollutant transport is the greatest at this time.

It is indicated from this figure that the influence of COD from the five river outlets in the PRDR is significant up to the northwestern part of Lantau Island, and its effect on other areas of Hong Kong seawaters is less. The COD concentration increase caused by the loadings of the five outlets is greater than 0.25 mg/L near Lantau Island. During the wet season, the COD is transported over a wide area since the flow is greatest during this period, and affects the water quality of Hong Kong seawaters more.

CONCLUSIONS

A three-dimensional, numerical model based on an orthogonal curvilinear grid system in the horizontal direction and a sigma coordinate system in the vertical direction for the prediction of water quality constituents is developed, and a simple and efficient open boundary condition for pollutant transport is used in this model. The model is applied to a typical estuary domain, the PRE, to simulate the distribution of COD in the PRE and to assess the transbounday pollution between Guangdong and Hong Kong. This region is the most quickly developing in China, with Hong Kong and Macau at its entrance.

In this model, the horizontal time differencing is semi-implicit with the use of a time-splitting method. As such, the allowable time step is larger than POM and less computational time is needed to keep the computation stable. This attribute is shown to be particularly useful in domains with complex flow patterns and large currents caused by tide river discharges, such as in Pearl River estuary.

The pollutant load data at the five main river outlets to the PRE is not directly available, so the COD loading rate is estimated and adopted from the pollutant sources in the water quality model. The simulated results show that the pollutants from the PRDR have certain impact on the Hong Kong seawaters, especially during the wet season when large water discharge occurs upstream.

Above all, a complicated and efficient three-dimensional pollutant transport has been developed and applied. It works well when applied to the Pearl River estuary.

ACKNOWLEDGMENTS

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Table 1. Summary statistics of wastewater flow and COD load from Guangdong Province (unit: million ton)

Source	1990	1991	1992	1993	1994	1995	1996
Domestic	1110.12	1058.47	1310.49	1492.91	1981.31	2123.69	2122.22
Industrial	1402.5	1392.24	1419.39	1397.62	1315.31	1609.79	1508.74
Total wastewater	2512.62	2510.9	2801.03	2959.9	3372.07	3816.57	3714.05
COD	0.69	0.72	0.78	0.8	0.94	1.12	1.06

Source: Guangdong Province Yearbook Editorial Committee (1996)

Table 2. Average water discharge rates for the five main river outlets during different seasons

	Hu men	Jiao men	Hongqi men	Heng men	Shenzhen
Wet($10^8 m^3$/day)	2.09	1.99	0.77	1.31	0.06*
Mean($10^8 m^3$/day)	1.56	1.44	0.51	0.89	0.06*
Dry($10^8 m^3$/day)	0.68	0.59	0.17	0.37	0.06*

* Accurate flow data is not available and therefore an estimate is made from local flow gauge and drainage area ratio

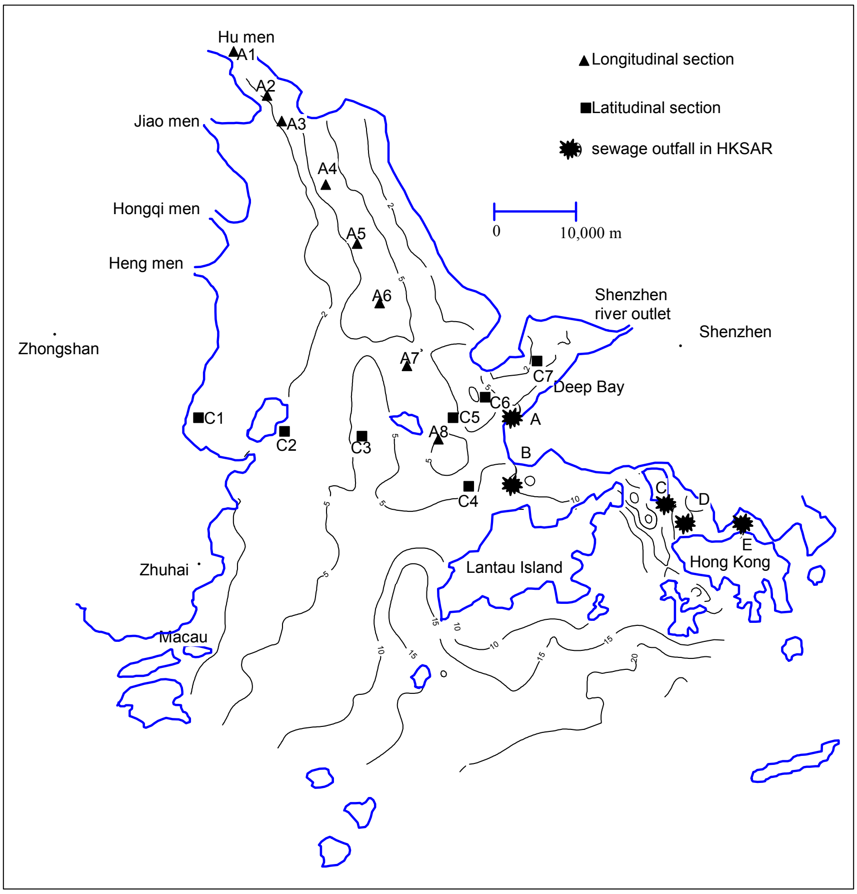

Fig. 1. Topographic map of study area

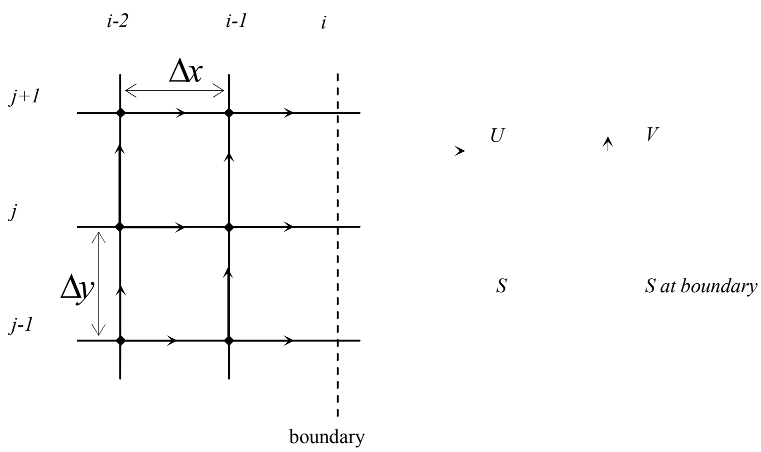

Fig. 2. Arakawa C grids with eastern open boundary

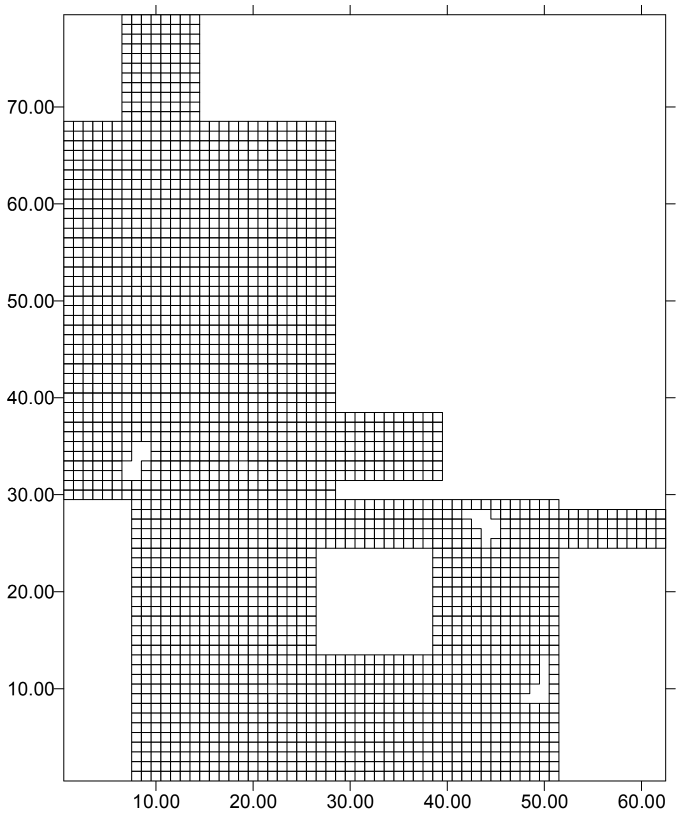

Fig. 3. The transformed plane

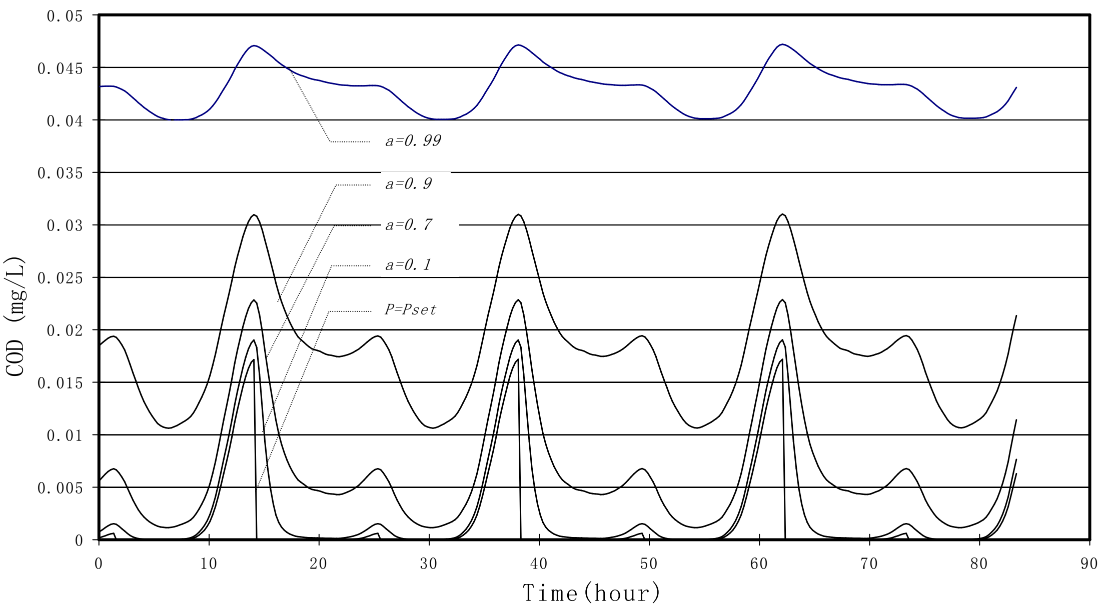

Fig. 4. COD concentration at the eastern open boundary corresponding to different *a* values

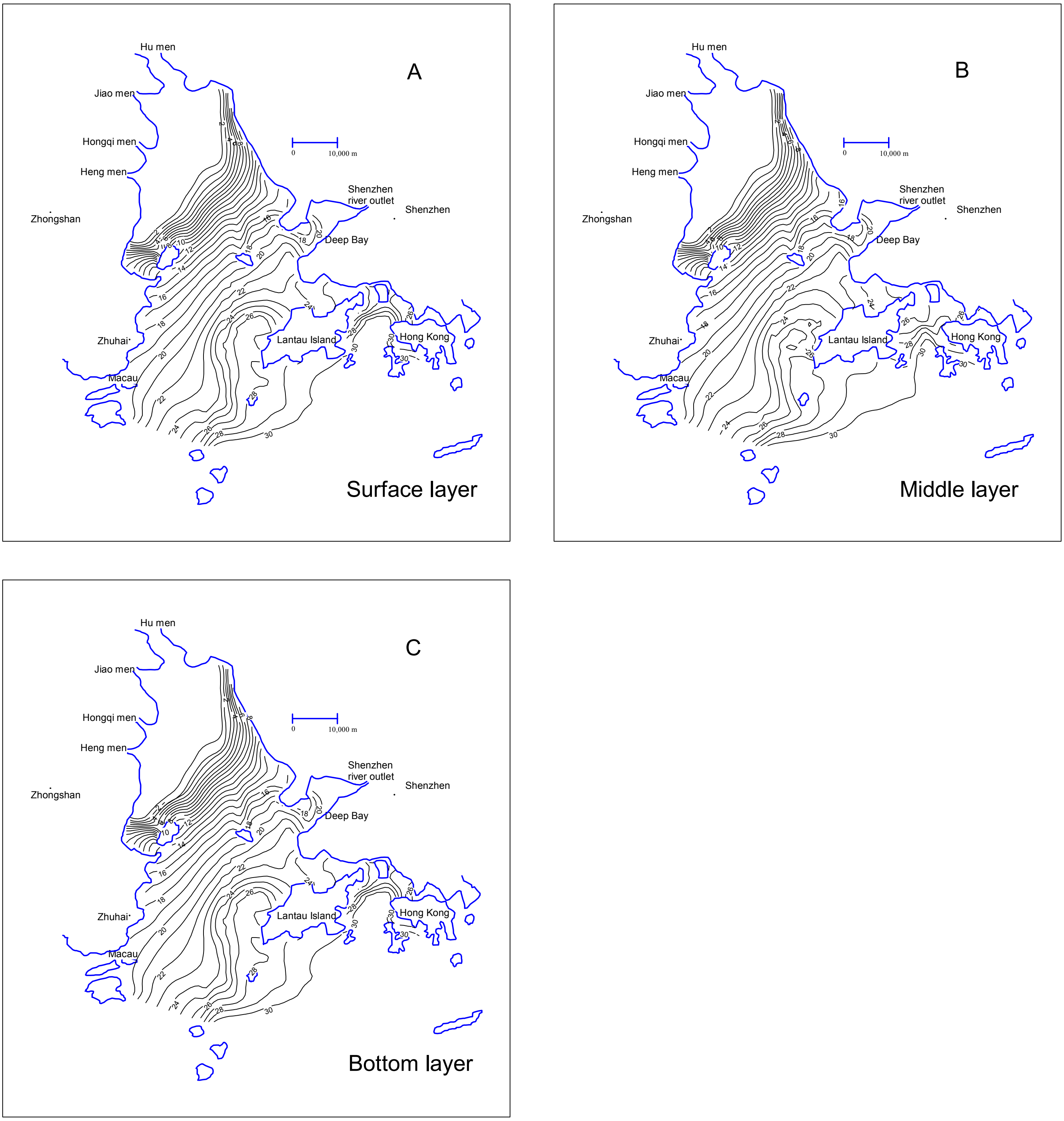

Fig. 5. The computed salinity contour of three layers in wet season
A-surface B-middle C-bottom

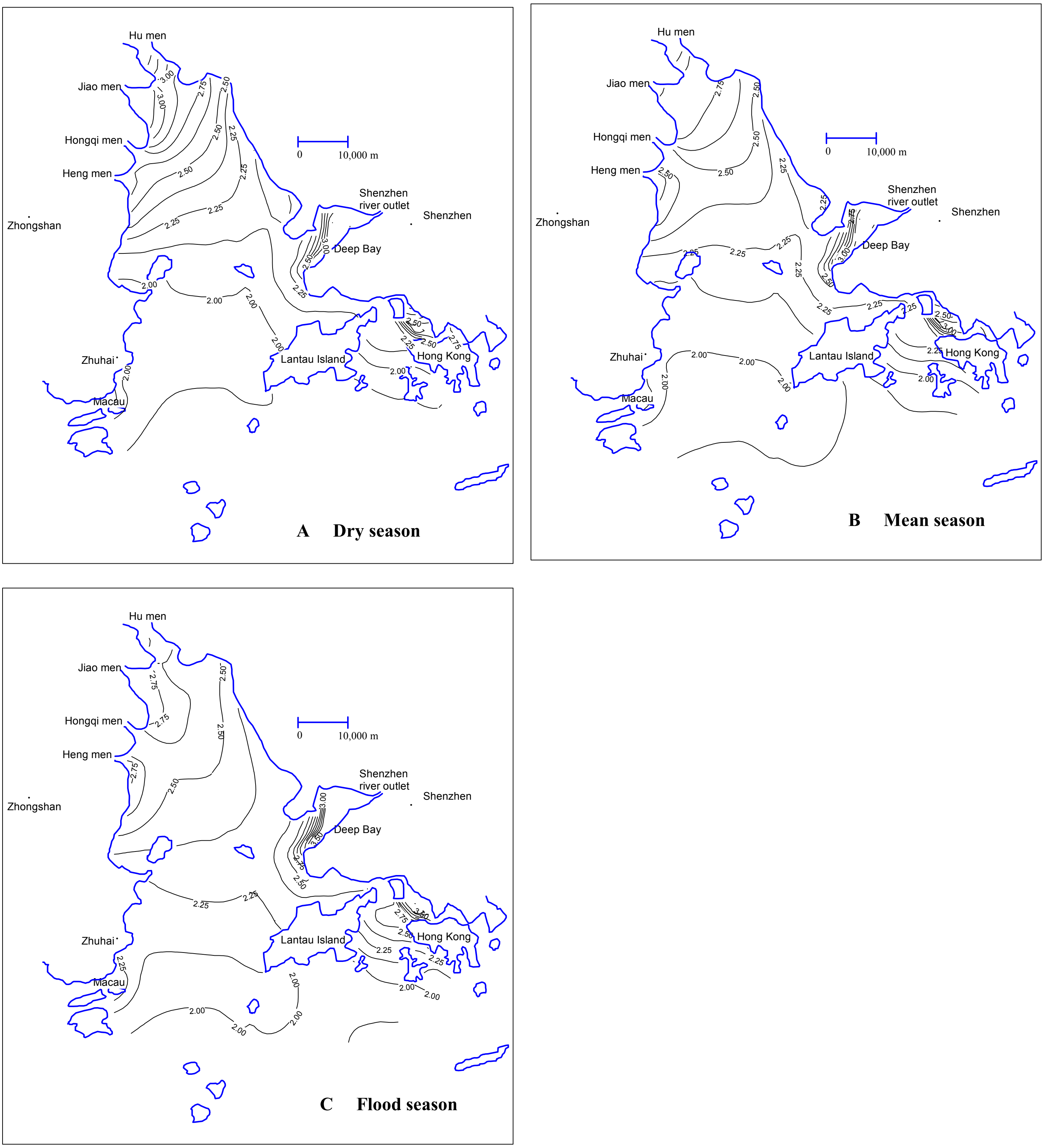

Fig. 6. The average COD distribution (in mg/L) during different seasons
A-dry season, B-mean season, C-wet season

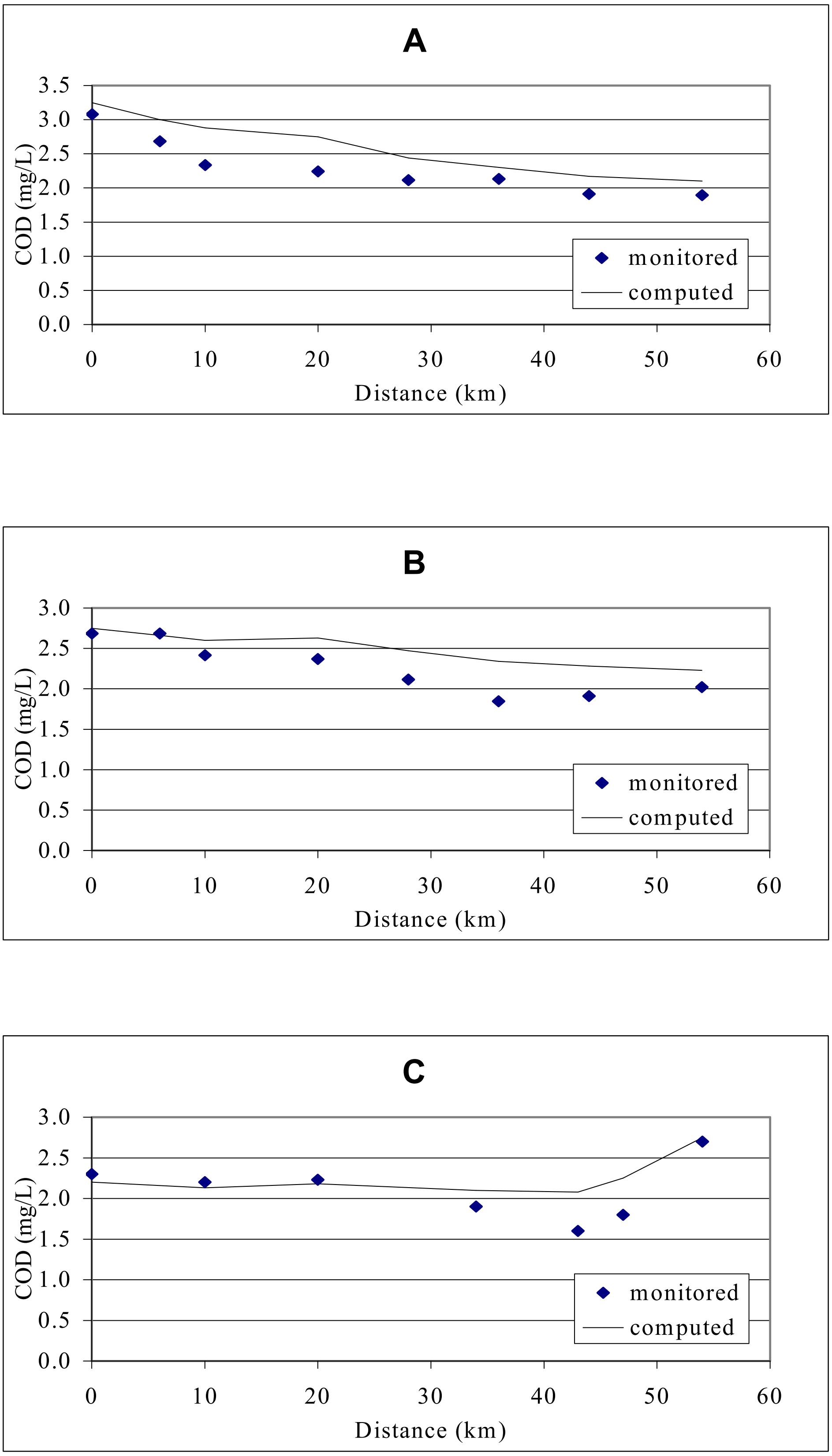

Fig. 7. Model verification of the COD concentration

A- the longitudinal section in dry season
B- the longitudinal section in wet season
C- the latitudinal section in mean season

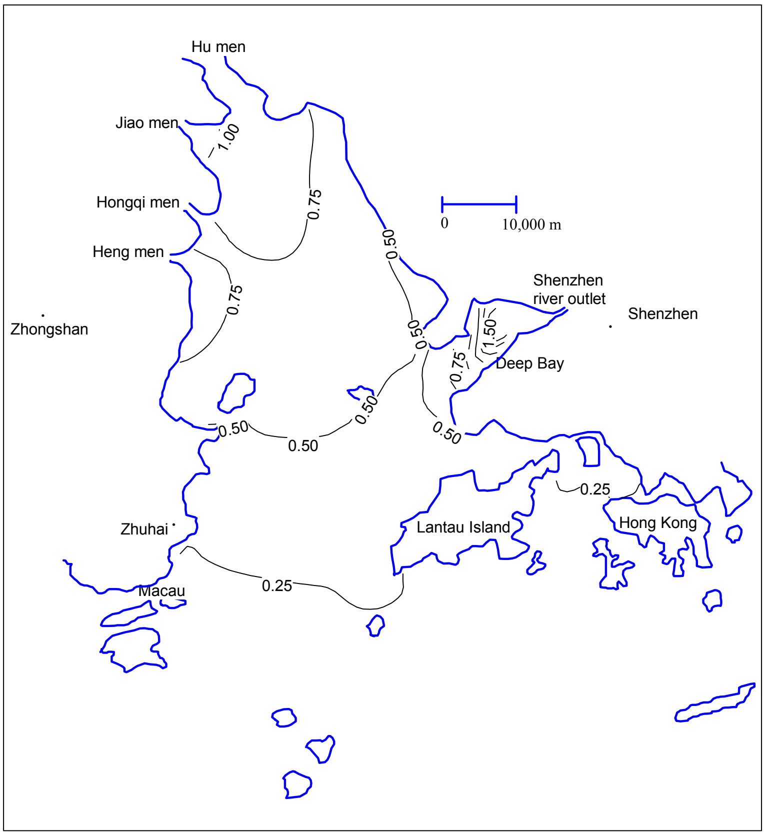

Fig. 8. Increased COD distribution (mg/L) over background due to sewage loading from the PRDR during wet season

A-dry season B-mean season C-wet season