TẠP CHÍ KHOA HỌC ĐHQGHN, KHTN, t.XV, n^{0}3 - 1999

ĐIỀU TRA CÁC PROTEIN ỨC CHẾ PROTEINAZ (PPI) Ở HẠT MỘT SỐ CÂY THUỘC HỌ MORACEAE VÀ MỘT VÀI HỌ KHÁC.

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Đại học KH Tự nhiên - ĐHQG Hà Nội

Chúng tôi đã tiến hành điều tra sơ bộ PPI của 17 mẫu hạt thuộc các họ Dâu tằm, Bông, Sim, Bồ hòn, Thị và Na. Trong đó 4 mẫu hạt Mít mật, Mít dai, Roi, Đậu bắp có chứa cả chất ức chế tripxin và kimotripxin. Năm mẫu hạt khác: Chay, Mít tố nữ, Hồng đỏ, Na có chứa TI hoặc KI. Từ các kết quả trên cúng tôi đã chọn hạt Mít mật và Mít dai để nghiên cứu tiếp. Kết quả điện di dịch chiết hạt 2 mẫu Mít mật và Mít dai cho thấy phổ điện di protein 2 mẫu này khá giống nhau, trừ băng protein có Rm = 0.39 (Mít dai không có băng protein này). Phải chăng băng protein trên qui định sự sai khác giữa Mít mật và Mít dai. Sắc ký qua cột Sephadex G75 cũng cho thấy phổ sắc kí 2 mẫu này khá giống nhau gồm 2 đỉnh protein chính, trong đó đỉnh thứ nhất có cả KIA và TIA nhưng ở mức độ thấp hơn. TI và KI từ hạt mít khá bền với nhiệt, sau khi sử lý ở 100^0C trong 15 phút, hoạt độ kìm hãm chỉ còn lại khoảng 30 % so với hoạt độ ban đầu.

BUILDING SYSTEM FOR SIMULATION OF DYNAMICS AND POLLUTION TRANSPORT IN SHALLOW BASINS*

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Abstract. *The two-dimension models for the dynamical processes and conservative substance transport in the sea based on the systems of differential equations of long wave propagation in shallow water and diffusion equation integrated over the depth are summarized. In order to apply these models to the shallow basins of real complex shape and bathymetry the equations were solved numerically using a simple explicit scheme. All the processes of computation of the water dynamic parameters and substance concentrations are integrated into a computer program that allows undertake calculations for arbitrary domains in coastal zone. The experiments with different geographical objects point out that in conditions of restricted initial data or full lack of them the simple two-dimension models lead to the some interesting features and quantitative characteristics in dynamic and pollutant distribution regime of basins that are sufficient to different decisions both in level of investigation and in designs.*

Nowadays many technical activities relate to the coastal regions and near-shore basins and the need for environment protection in these domains rapidly increases. This all makes engineers and designers in their works must learn much about the dynamic characteristics and processes of pollution transport there. At the same time for almost regions along our sea shore the observed data is general not available and the works for obtaining them are very expensive. The numerical realization of mathematical models of these processes is a cheap way to get some initial information for different designing decisions. This paper presents some experiences on the application of mathematical models of long wave induced circulation and the model of pollutant transport for different shallow basins. The purpose of our work was to build a system of computer programs to facilitate the calculation of current field or, simultaneously, of the current field and field of pollutant concentration in a coastal basin with its complex real coastline and bathymetry. The results of experiments with different regions of interest confirm the efficiency of the system both at diagnostic and prognostic level.

The circulation in coastal areas is commonly generated and sustained by various factors such as the tide, the wind or atmospheric pressure acting on the water surface and

*) This work is a result of the theme 7.8.11 "The system of currents in the west of South-china sea and its impact on the natural conditions of Vietnam coastal" (Basic Research Program, The Earth Sciences 1998-1999).

by the variation of water density in space of the considered domain. The mathematical models for these types of circulation well developed in coastal engineering (see [2,3,4]) and experience of practical use of these models can be found in our country [1,5]. Various numerical schemes for the solution may be found in literature. To yield the current field used when calculating the concentration field of a pollutant we applied two models: model of long wave induced circulation (tidal model) and model of wind generated circulation.

1. Two - dimension circulation models

The circulation generating factor is a periodic perturbation of the free surface elevation arriving from the open sea. So the circulation in this case is called tide- induced circulation. The integration of Reinolds equations of movement and equation of continuity over the depth, the approximation of the non-linear convective terms by their depth mean values and using the quadratic form for the bed friction result in a following simple two-dimension horizontal tidal flow model [3]:

$$\frac{\partial U}{\partial t}+U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial y}-fV=-g\frac{\partial}{\partial x}\xi-\frac{gU}{(H+\xi)C^2}\sqrt{U^2+V^2}+\nu_h\nabla_h^2 U, \tag{1}$$

$$\frac{\partial V}{\partial t}+U\frac{\partial V}{\partial x}+V\frac{\partial V}{\partial y}+fU=-g\frac{\partial}{\partial y}\xi-\frac{gV}{(H+xi)C^2}\sqrt{U^2+V^2}+\nu_h\nabla_h^2 V, \tag{2}$$

$$\frac{\partial \xi}{\partial t}=\frac{\partial (H+\xi)U}{\partial x}-\frac{\partial (H+\xi)V}{\partial x}, \tag{3}$$

where U, V depth-averaged current components along axes $x, y; \xi$ - elevation (tide head); H - sea depth; C -Chezy bed friction coefficient; ρ - water density; t - time; f- Coriolis parameter, $f=2\omega sin\varphi$ (ω - angle speed of the Earth rotation, φ - mean latitude of the computed domain).

If the wind-generated current is considered, the vertical distribution of velocity must be taken in the parabolic form

$$u(z)=\Big(\frac{3}{4}a-\frac{3}{2}U\Big)\Big[\Big(\frac{z}{H}\Big)^2-1\Big]+a\Big(\frac{z}{H}+1\Big), \tag{4}$$

where $a=\frac{\tau_s H}{\rho\nu}$, ν - eddy viscosity, τ_s - wind stress at the water surface.

With this vertical distribution of velocity the equations of movement with depth-averaged velocities have the forms

$$\frac{\partial U}{\partial t}+U\frac{\partial U}{\partial x}+V\frac{\partial U}{\partial y}+\Big(0,2U+\frac{a_x}{40}\Big)\frac{\partial U}{\partial x}+\Big(0,2V+\frac{a_y}{40}\Big)\frac{\partial U}{\partial y}=$$
$$-g\frac{\partial \xi}{\partial x}+fV+\frac{\tau_{sx}}{\rho H}-\Big(0,18\frac{U}{H}\sqrt{\frac{\tau_s}{\rho}}-0,5\frac{\tau_{sy}}{\rho H}\Big), \tag{5}$$

$$\frac{\partial V}{\partial t}+U\frac{\partial V}{\partial x}+V\frac{\partial V}{\partial y}+\Big(0,2U+\frac{a_x}{40}\Big)\frac{\partial V}{\partial x}+\Big(0,2V+\frac{a_y}{40}\Big)\frac{\partial V}{\partial y}=$$
$$-g\frac{\partial \xi}{\partial y}-fU+\frac{\tau_{sy}}{\rho H}-\Big(0,18\frac{V}{H}\sqrt{\frac{\tau_s}{\rho}}-0,5\frac{\tau_{sy}}{\rho H}, \tag{6}$$

and the equation of continuity in this case has the same form (3). If the free surface velocity is required for subsequent use in pollutant model its components can be computed from the equation (4)

$$u_{z=\xi} = 1,5U + \frac{a_x}{4},$$
$$\nu_{z=\xi} = 1,5V + \frac{a_y}{4}. \qquad (7)$$

2. The initial and boundary conditions

- Initial condition:

$$\xi_{t=0} = U_{t=0} = V_{t=0} = 0. \qquad (8)$$

- At land boundaries G_1 (sea shore or river bank) normal velocity equals to zero:

$$Ucos\alpha + Vsin\alpha|_{G_1} = 0, \qquad (9)$$

where α - the angle between current direction and shoreline orthogonal.

- For the open boundaries G_2 one of the following conditions is applied:

a) The heights of sea level are given by observed values

$$\xi\Big|_{G_2} = \xi(x, y, t). \qquad (10)$$

b) The elevation is given by the harmonic constants of tide constituents:

$$\xi\Big|_{G_2} = \sum_{i=1}^{n} f_i H_i cos\Big[q_i t + (V_0 + u)_i - g_i\Big]. \qquad (11)$$

c) No level changes at boundary during the calculation period:

$$\xi\Big|_{G_2} = 0. \qquad (12)$$

d) The long wave is freely radiated from the computation domain:

$$Ucos\alpha + Vsin\alpha\Big|_{G_2} = \xi\sqrt{g(H+\xi)}. \qquad (13)$$

e) No level orthogonal gradient at open boundary:

$$\frac{\partial\xi}{\partial n}\Big|_{G_2} = 0. \qquad (14)$$

3. Finite difference schemes

To solve numerically the governing equations of the above dynamic models one can use schemes based on the finite difference or finite element methods [2,3]. We chose the explicit finite difference scheme for the sake of simplicity.

The flow domain is discretised by an orthogonal horizontal grid with mesh $\Delta x, \Delta y$. The boundaries are approximated by mesh sides paralleled to the axes Ox or Oy. The unknown functions U, V, ξ are computed on characteristic locations in a staggered way. If the depth is given at the intersection of mesh sides then the U, V values refer to the center of the mesh sides paralleled to Oy and Ox respectively and the ξ value refer to the mesh center (Figure 1).

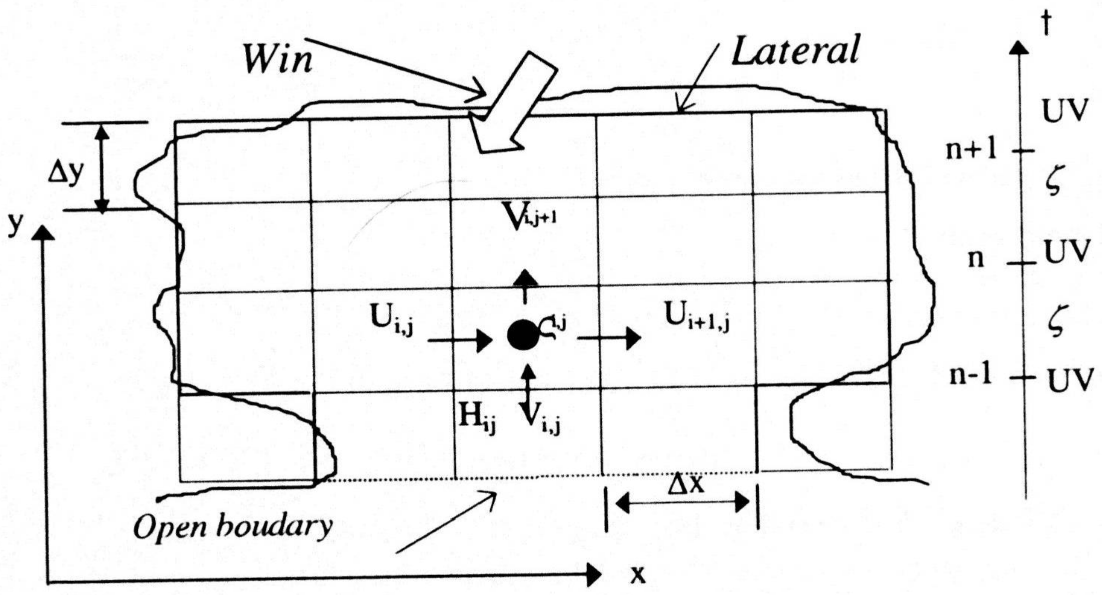

Figure 1: Orthogonal grid for spatial and time discretisation

In this case the finite difference analogs of the equations (1) (3) for example have the forms

$$U_{ij}^{n+1} = U_{ij}^{n} - \frac{\Delta t}{8\Delta x}\left[\left(U_{i+1j}^{n} + U_{ij}^{n}\right)^2 - \left(U_{i+1j}^{n} + U_{ij}^{n}\right)^2\right] - \frac{\Delta t}{2\Delta y}\tilde{V}_{ij}^{n}\left(U_{ij+1}^{n} - U_{ij-1}^{n}\right)$$

$$- \frac{g\Delta t}{\Delta x}\left(\xi_{ij}^{n+1/2} - \xi_{i-1j}^{n+1/2}\right) - \frac{2gU_{ij}^{n}\sqrt{\left((U_{ij}^{n})^2 + (\tilde{V}_{ij}^{n})^2\right)}}{C^2\left(H_{ij} + H_{i-1j}\right)} + f\tilde{V}_{ij}^{n}\,; \tag{15}$$

$$V_{ij}^{n+1} = V_{ij}^{n} - \frac{\Delta t}{8\Delta y}\left[\left(V_{jj}^{n} + V_{ij+1}^{n}\right)^2 - \left(V_{ij}^{n} + U_{ij-1}^{n}\right)^2\right] - \frac{\Delta t}{2\Delta x}\tilde{U}_{ij}^{n}\left(V_{i-1j}^{n} - U_{i-1j}^{n}\right)$$

$$- \frac{g\Delta t}{\Delta y}\left(\xi_{ij}^{n+1/2} - \xi_{ij-1}^{n+1/2}\right) - \frac{2gV_{ij}^{n}\sqrt{\left((\tilde{U}_{ij}^{n})^2 + (V_{ij}^{n})^2\right)}}{C^2\left(H_{ij} + H_{ij-1}\right)} - f\tilde{U}_{ij}^{n}\,; \tag{16}$$

$$\xi_{ij}^{n+3/2} = \xi_{ij}^{n+1/2} - \frac{\Delta t}{2\Delta x}\left[U_{i+1j}^{n+1}\left(H_{ij} + H_{i+1j}\right) - U_{ij}^{n+1}\left(H_{ij} + H_{(i-1)j}\right)\right]$$

$$- \frac{\Delta t}{2\Delta y}\left[V_{ij+1}^{n+1}\left(H_{ij} + H_{(i+1)j}\right) - V_{ij}^{n+1}\left(H_{ij} + H_{ij-1}\right)\right] + q_{ij}\Delta t\,; \tag{17}$$

$$\tilde{V}_{ij}^{n} = \frac{V_{ij}^{n} + V_{i-1j}^{n} + V_{ij+1}^{n} + V_{i-1j+1}}{4}, \qquad \tilde{U}_{ij}^{n} = \frac{U_{ij}^{n} + U_{ij-1}^{n} + U_{i+1j}^{n} + U_{i+1j-1}^{n}}{4},$$

with the CFL criteria of stability $\frac{\sqrt{g}H_{max}\Delta t}{\sqrt{(\Delta x)^2+(\Delta y)^2<1}}$, here H_{max} - maximum depth in the computed domain.

4. Two - dimension model for pollutant transport

$$\frac{\partial C}{\partial t} = -\frac{\partial (CU)}{\partial x} - \frac{\partial (CV}{\partial y} + \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) - \lambda C, \tag{18}$$

where C - pollutant depth-mean concentration; D_x, D_y- diffusion coefficients on axes O_x, O_y; λ - decay coefficient; U, V- depth- averaged components of current in directions O_x, O_y computing from the system (1) - (3) and/or (5) - (6), (3). This equation is completed by the following appropriate boundary conditions

a) At solid boundary normal flux is equal to zero:

$$\frac{\partial C}{\partial n} = 0 \text{ at } G_1. \tag{19}$$

b) At open boundary

- Concentration is given as a function of coordinates and time (in the problem of salt intrusion):

$$C_s = S(t, x, y) \text{ at } G_2. \tag{20}$$

- Or free transmission boundary (pollutant trap) (in the problem of pollutant transport):

$$\frac{\partial}{\partial}\left(D_n \frac{\partial C}{\partial n}\right) = 0. \tag{21}$$

c) At the pollution sources the concentration is known and prefixed

$$C\Big|_{x,y,t} = C_s(x, y, t). \tag{22}$$

5. The above mentioned models had been realized by a computer program which access flow domain with arbitrary coastal geometry. Bellow are presented some results of experiments to show the performance of the build program.

a) *Experiment 1*: Predicting level oscillations at river mouths along the shoreline of Red river delta after the tidal oscillations at open boundaries given (Figure 2). The results showed the increase of the phase of sea level oscillations southward. That is closed to the theoretical picture of tidal propagation in Tonkin gulf. The comparison of level predicted by the model and that due to the tidal table is shown in Figure 3.

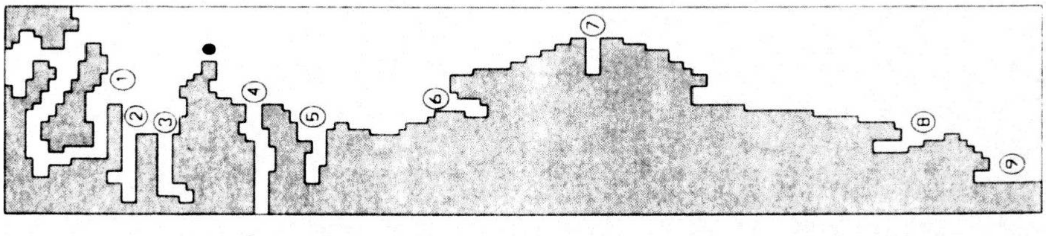

Figure 2: Coastal zone of West Tonkin gulf (shown tide gauge Hondau (•) and nine river mouths:
1. Nam Trieu, 2. Cua Cam, 3. Kien An, 4. Van Uc, 5. Thai Binh
6. Tra Ly, 7. Ba Lat, 8. Phu Le, 9. Nhu Tan)

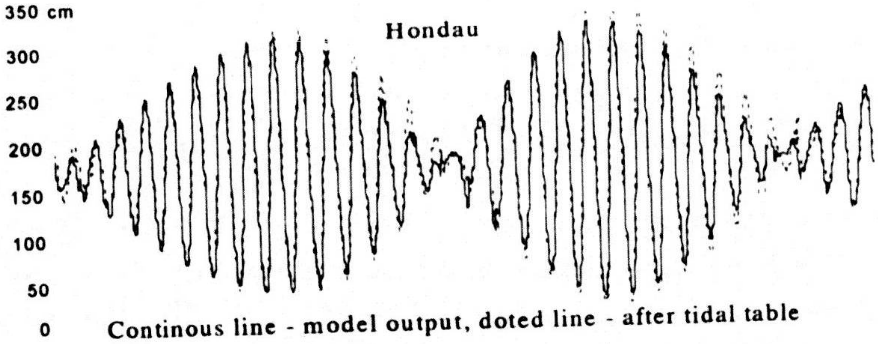

Figure 3: Tide gauge Hondau:
Camparison of levels predicted by model with the tide table

b) *Experiment 2*: Computing tide and tidal circulation in lagoon Tra O (Central Vietnam). The purpose of the calculation was to predict the oscillation regime of water level and current in the lagoon when a channel connecting it with the South- china sea built. As a sequence of this dynamic regime the intrusion of salt from the South-china sea into the lagoon waters had been investigated by the pollutant transport model. The input was tidal oscillation of water level (with the magnitude of 0.5m) and prefix salinity 35 ‰at the seaward end of the connecting channel. At the beginning of the simulation the water in the lagoon was supposed to be fresh.

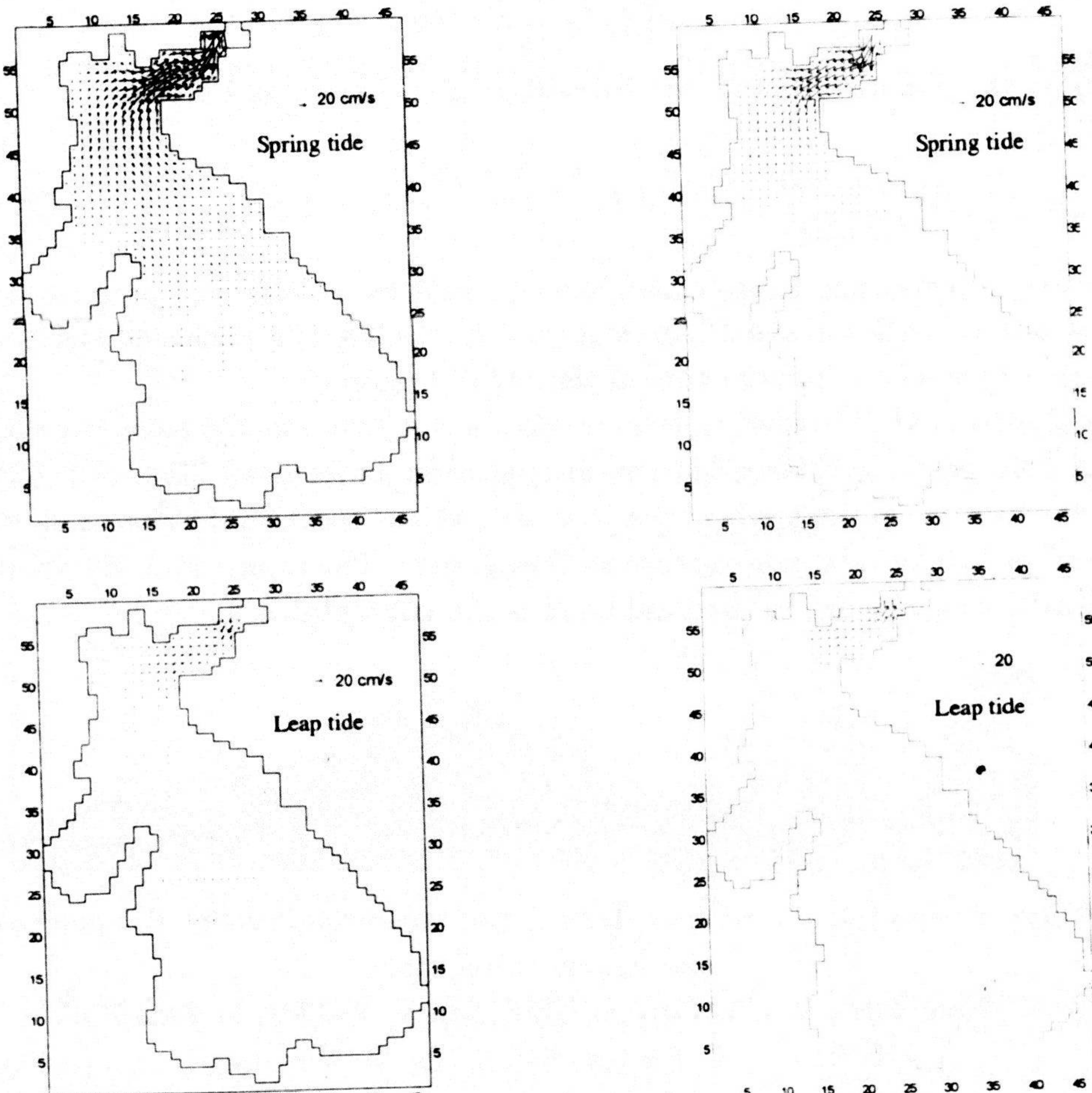

Figure 4: Tidal current patterns in Tra O lagoon

Due to results of the simulation the tidal current of diurnal period with maximum velocity up to 30-50 cm/s had developed in spring tide in the north part of the lagoon near the connecting channel (Figure 4). The tidal oscillation of water level in the lagoon was of standing wave type, the level oscillations in different locations in the lagoon were in the same phase (Figure 5). The tidal currents strengthened the process of intrusion of salty water from the sea into the lagoon. Thus after simulation for one day of variable t, the water in a half of lagoon area had become salty or brackish. After two days of the water exchange with the sea the lagoon had almost become a marine basin (Figure 6).

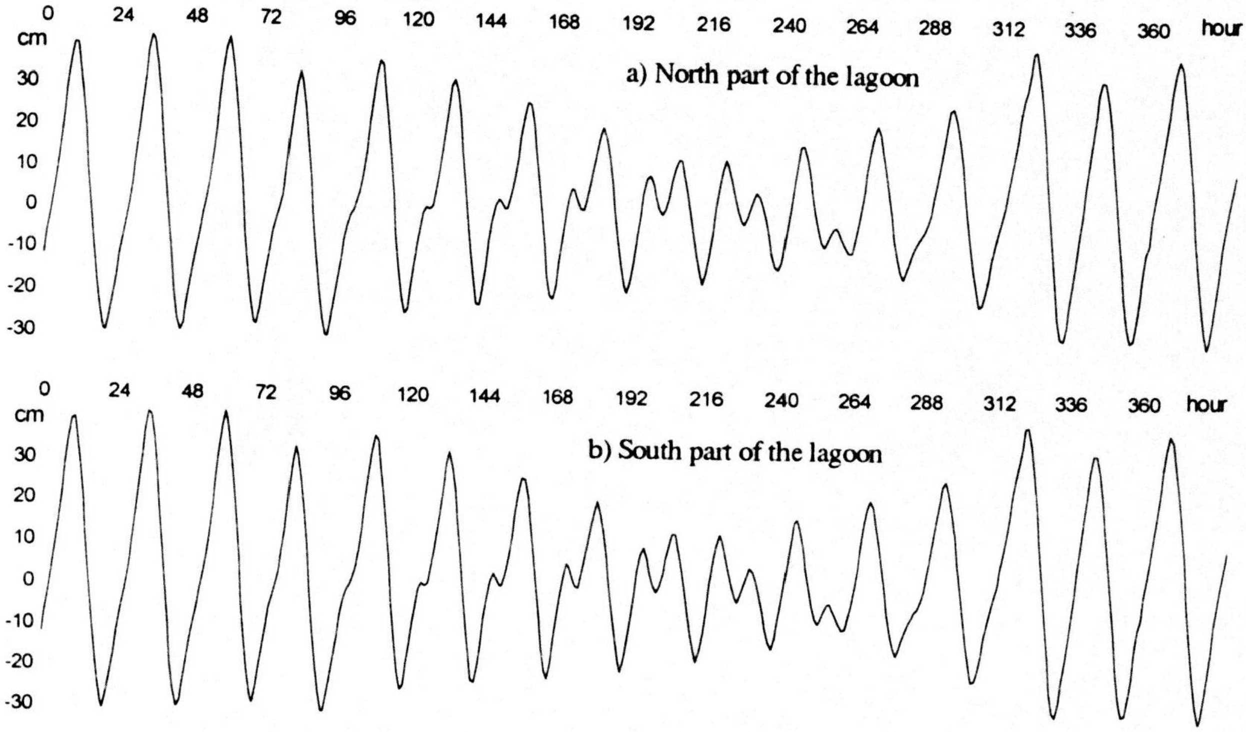

Figure 5: Tidal oscillation of water level in different parts of the lagoon

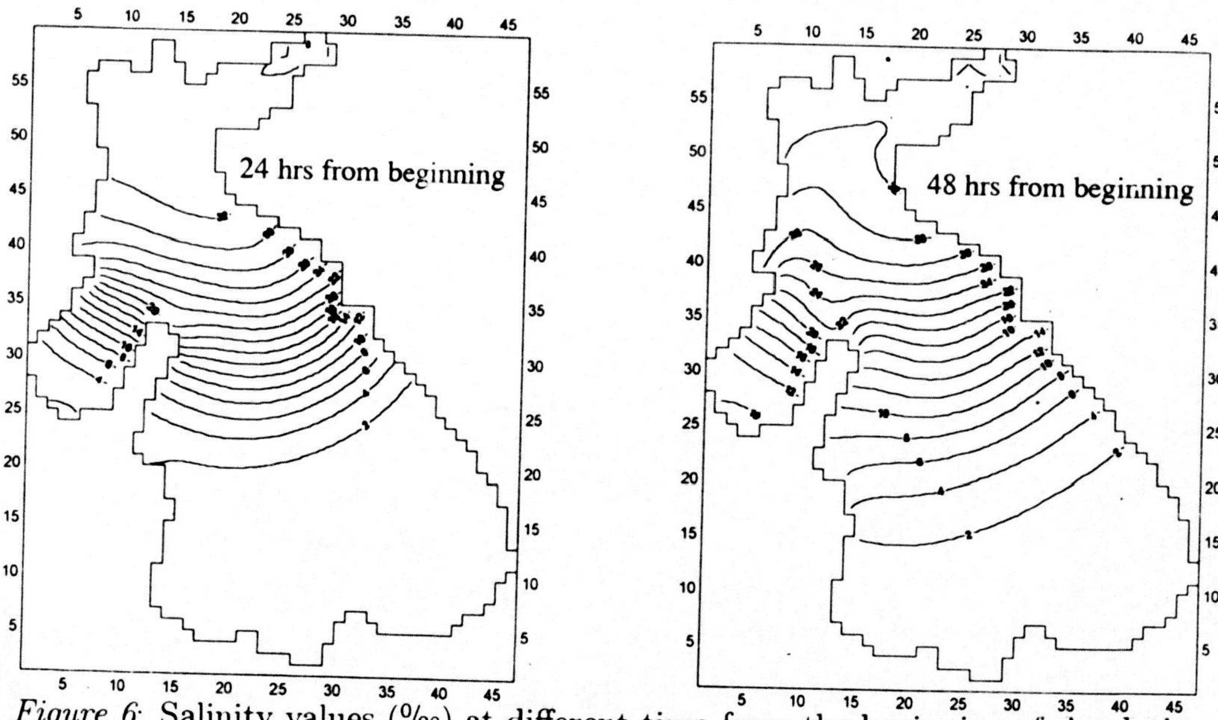

Figure 6: Salinity values (‰) at different time from the beginning of simulation

c) *Experiment 3*: Computing oil spills propagation in Ha Long Bay. The author had used two-dimension model to get dynamic picture of this basin before [1]. The starting place of oil slicks was near the Cai Lan port. Oil spills became to spread under the tide-induced and wind-generated circulation computed by model (1)-(3) and (5)-(7). The tidal levels were given both at Quang Ninh entrance and Hai Phong entrance of the Ha Long Bay. Results of the simulation showed that for one tidal circle the oil spills do not spread far (Figure 7). It is seen that the oil spills tended to the southeast from their starting place.

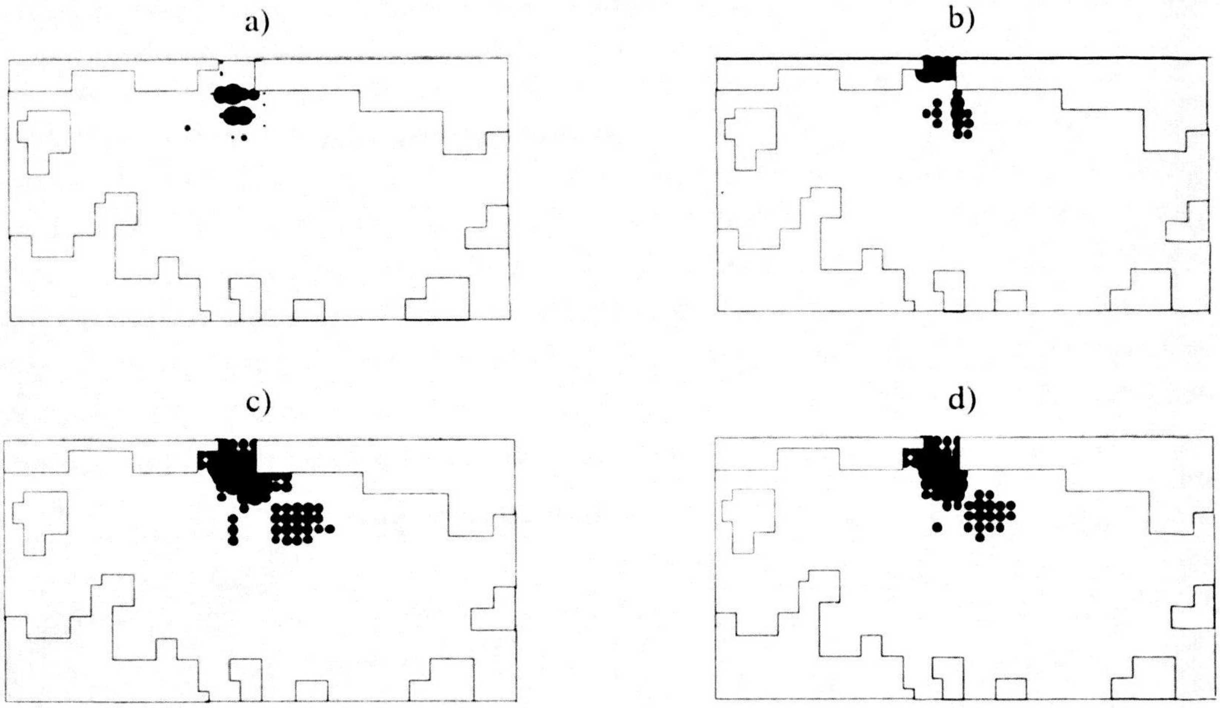

Figure 7: The position of oil spills after 6h (a), 12h (b), 18h(c) and 24h(d) from the beginning of simulation (starting oil slick near Cai Lan port)

All the above mentioned experiments show that two-dimension models appear to be useful in simulation of dynamics and transport processes in near-shore shallow basins and coastal zone. In conditions of restricted initial data or full lack of them these simple models lead to the some interesting features and quantitative characteristics in dynamic regime of basins that are sufficient to different decisions both in level of investigation and in designs.

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XÂY DỰNG HỆ THỐNG MÔ PHỎNG ĐỘNG LỰC VÀ LAN TRUYỀN Ô NHIỄM TRONG CÁC THỦY VỰC VEN BIỂN

Phạm Văn Huấn

Khoa Khí tượng Thủy văn & Hải dương học

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Giới thiệu tổng quan các mô hình hai chiều về các quá trình động lực và vận chuyển chất thụ động dựa trên các phương trình truyền sóng dài trong nước nông và phương trình khuếch tán vật chất tích phân theo độ sâu vùng tính. Đã hiện thực hoá các mô hình này bằng một chương trình máy tính thống nhất cho phép đồng thời tính các tham số động lực của môi trường và phân bố nồng độ muối, chất ô nhiễm... tiện áp dụng cho thủy vực ven biển với hình dạng và địa hình đáy bất kỳ. Kết quả thí nghiệm cho các vùng địa lý khác nhau cho thấy rằng việc ứng dụng các mô hình hai chiều đơn giản khá hiệu quả: Trong điều kiện số liệu ban đầu hạn chế hoặc hoàn toàn thiếu, những mô hình vẫn dẫn tới một số đặc điểm lý thú và những đặc trưng định lượng về chế độ động lực và quá trình trao đổi trong nước cần thiết cho những quyết định trong nghiên cứu hay thiết kế.