

Chapter I

The Mathematical Model

by

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Foreword

This chapter is a synopsis of the mathematical model which has been the framework of the theoretical and experimental research conducted in the last three years in the scope of the Belgian National Program on the Environment - Sea Project¹.

The successive steps in the construction of the Model have been described in several progress reports and published papers and the details are not reproduced here. A list of references is attached.

A detailed description of the modern concepts and techniques of marine modelling can be found in *Modelling of Marine Systems*, edited by Jacques C. J. Nihoul, Elsevier Publ. Amsterdam, 1974.

The ordering of this chapter closely follows that of the book and the same notations are used.

1. Sponsored by the Ministry for Science Policy, Belgium.

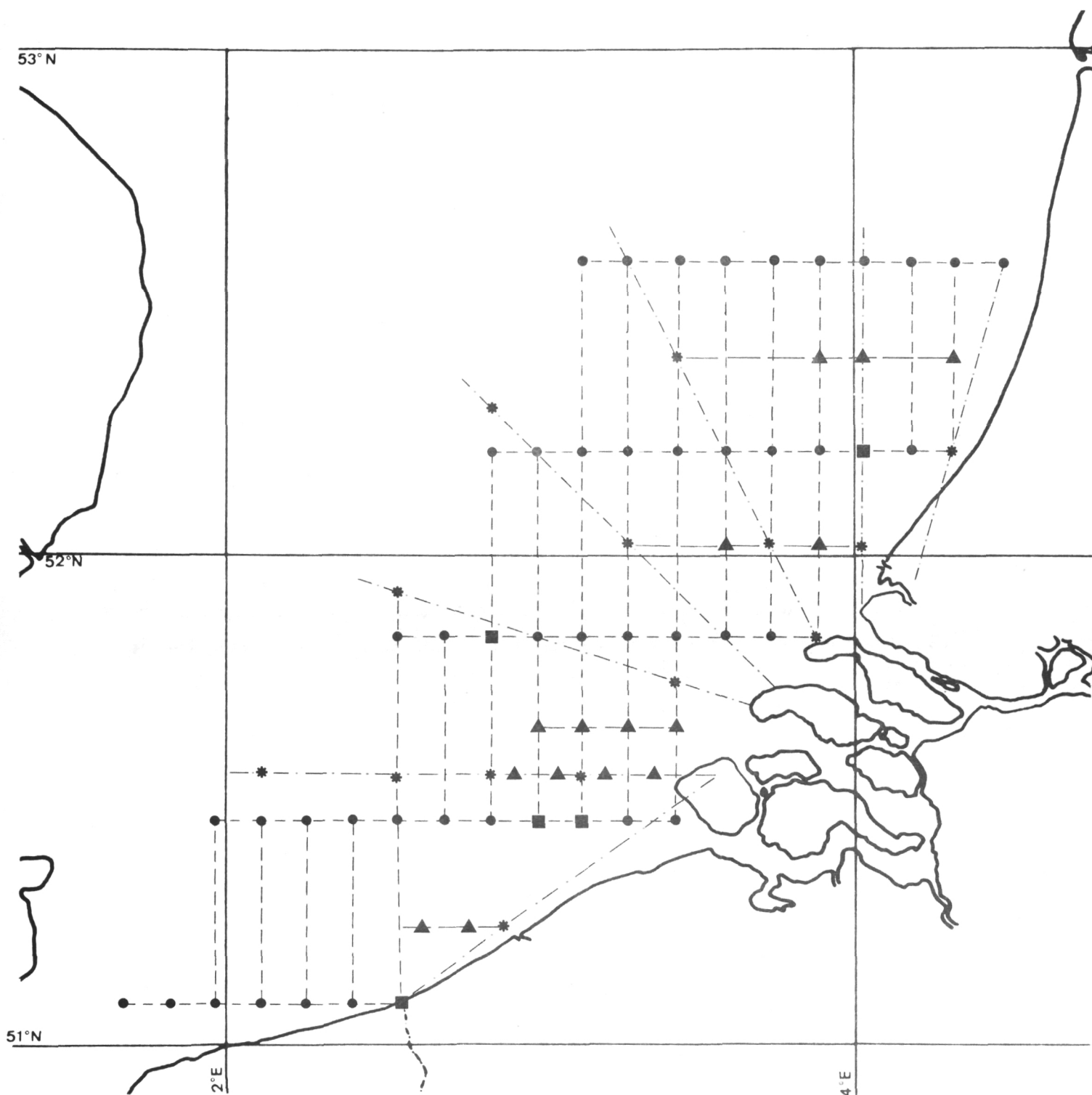


fig. 1.1.

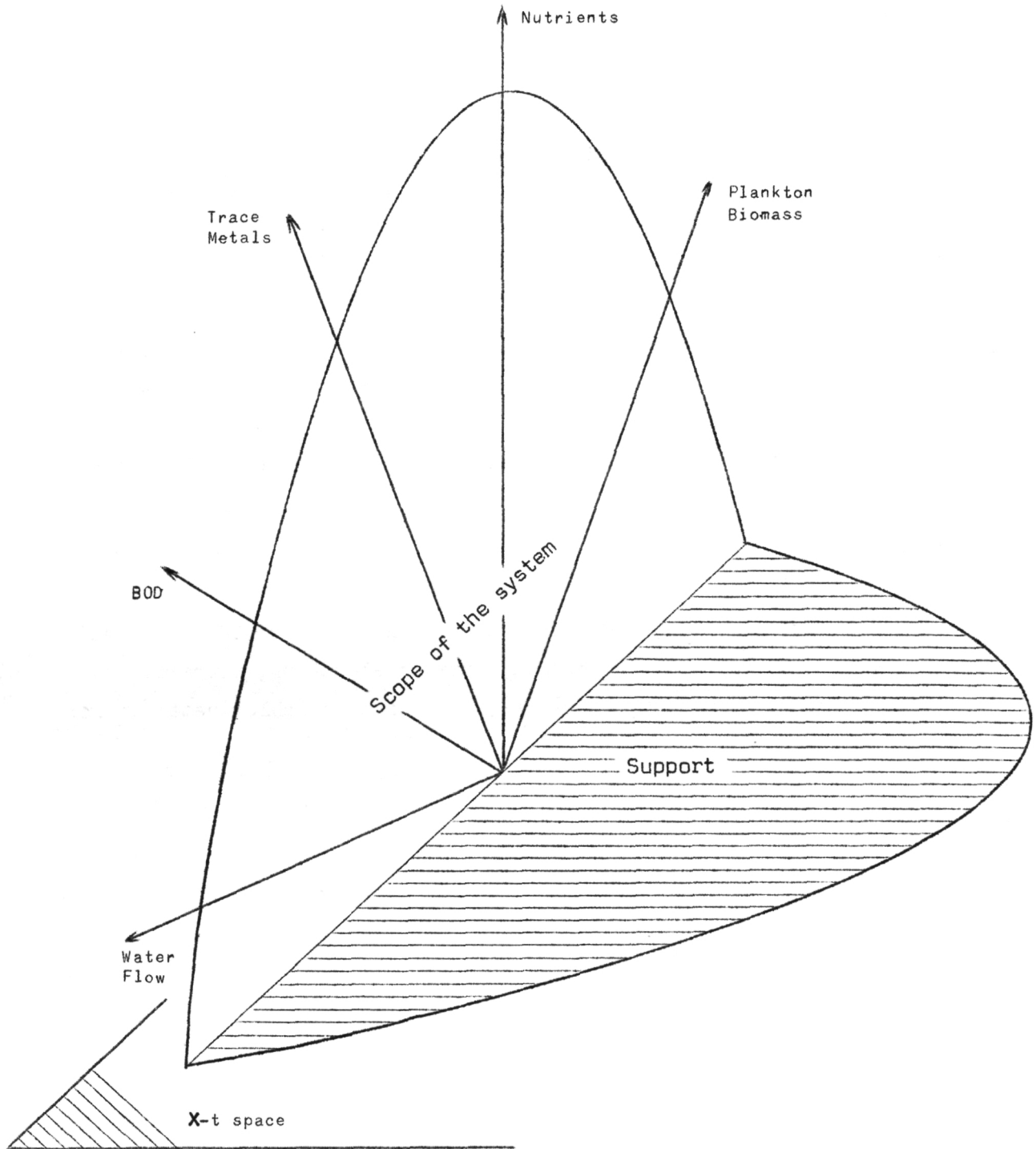


fig. 1.2.

- vii) macro- and meio-benthos,
- viii) bacteria - faecal,
 - marine heterotrophic,
 - benthic.

The state variables include the specific mass¹ of each compartment and the aggregate concentrations of the selected chemicals in compartments (i) to (vi).

Selected nutrients : P , N , Si .

Selected heavy metals : Zn , Cd , Pb , Cn , Fe , Mn , Mg .

Selected chlorinated hydrocarbons : pp' DDT , DDD , DDE , aldrine, dieldrin, endrin, lindane, heptachlore, epoxid heptachlore, PCB .

It must be emphasized here that, although the mathematical model covers all these variables, not every one of them is actually analysed experimentally. In the present state, experimental data are not always available on all chemical concentrations in all compartments at all sampling stations. This may be due to technical difficulties but it is, in most cases, a consequence of the necessity of accepting a hierarchy of priorities in the experimental work and focusing attention to what is most urgently needed (see chapter 2).

The specific masses of compartments (i) and (ii) may be called "salinity" and "turbidity" respectively; the distinction between salinity and turbidity being, in a sense, arbitrary as the experimentalist will call *dissolved* everything which goes through a filter of pre-decided fineness. This must be borne in mind also while interpreting the budgets of nutrients and pollutants in the two compartments.

Reduction of support - Space averaging

All over the support except in the Scheldt Estuary the turbulent mixing ensures a uniform density.

While separate three-dimensional and combined depth-averaged and width averaged two-dimensional models are being developed for the Scheldt Estuary, the model for the Southern Bight is further simplified by assuming constant mass density and considering only average properties over the total depth.

1. Mass per unit volume.

The mechanical variables are then reduced to the two horizontal components of the depth-averaged velocity vector and the surface elevation.

For the study of specific chemical and ecological interactions, the support may be divided in a limited number of *niches* where similar conditions prevail. In a first approach, one may study the dynamics of the aggregate properties of the niche obtained by further integrating (averaging) over the horizontal dimensions of the niche. Niche (or box) models of this sort have been developed and tested against the experimental observations made in the Ostend "*Bassin de Chasse*", a closed sea basin at the coast which has been extensively studied in the past.

2.- State variables and control parameters

The state variables are defined by the scope of the system as stated above.

As a result of turbulence and other erratic or rapidly oscillating motions of the sea, each variable shows fluctuations around a mean value. Only these mean values are significant for the model.

The evolution equations are written for the mean variables and only the general effect of the fluctuations (through non-linear terms in the basic equations) is taken into account.

The mean variables, *i.e.* the smooth running functions of space and time, obtained by filtering out the fluctuations are denoted by special symbols. A bar over the symbol indicates the average over depth of the mean variable.

In addition to the mechanical variables and temperature, the other state variables represent essentially specific masses or concentrations. (The specific biomass of phytoplankton, the specific mass of copper in solution, suspension or plankton, etc.) These "concentration" variables are noted $\bar{\rho}_a$ (smooth running part \bar{r}_a). For convenience $\bar{\rho}_a$ (\bar{r}_a) will be referred to as the specific mass of "constituent α "; the word constituent being used in a conventional sense as it may denote a whole aggregate (all dissolved substances ...) or the aggregate content of a

compartment in a specific chemical (concentration of mercury in pelagic fish ...).

The mean (smooth running) variables are noted as follows :

		depth-averaged
Velocity vector	u	\bar{u}
	(three dimensional)	(two dimensional)
Flow rate vector		$U = H \bar{u}$
Surface elevation		ζ
Total height of water (where h is the depth)		$H = h + \zeta$
Temperature	θ	$\bar{\theta}$
Specific mass of α	r_α	\bar{r}_α

"In addition to the state variables, different kinds of parameters appear inevitably in the mathematical description of the system. These may be called *control parameters* as they influence the evolution of the system (hence appear in the evolution equations) but are not predicted by the model itself (no specific evolution equation is written for them).

The first kind of control parameters one thinks of are the *guidance parameters* which are at the disposal of man to manage the marine system according to some optimal design.

Most of the parameters, however, which control the evolution of the system cannot be chosen to conform with man's concern. They are imposed by Nature. These parameters arise from the initial demarcation of the system, the necessity of restricting the state variables and formulating the laws of their evolution in a simple and tractable way. They reflect all the aspects of the natural system of which the model does not take charge; usually because the additional equations required for their prediction would jeopardize the simulation by their difficulty, their dubiousness or simply by increasing the size of the system beyond the computer's ability.

Although they are rarely known beforehand and must be, in most cases, determined approximately by separate models, experimental data or sideways theoretical reflection, the control parameters which result

from the closure of the system must be regarded, in the language of the theory of control, as *fixed* and distinct, therefore, from the guidance parameters mentioned above.

The separation between state variables and control parameters is, of course, more or less arbitrary and function of the model's capability and ambition.

For instance, all models of primary productivity (state variables : nutrients and plankton) are controlled by the incident light. In a first stage, the incident light may be taken as a fixed control parameter and be given an empirical value. The model can be refined and give the incident light at every depth as a function of the intensity of light at the sea surface, using the transparency of water as a new control parameter. In an even more perfect version of the model, the transparency of water can be included in the state variables and inferred from the turbidity which itself can be predicted by the model.

The chemical reaction rates may be regarded as control parameters hopefully determined by chemical kinetics, *i.e.* by laboratory experiments or by some fundamental molecular theory conducted in parallel with the model but not part of it.

The dynamics of *translocations* (transfer of a chemical element from one compartment to another) must be given appropriate mathematical form. This cannot be done in general without introducing several control parameters the values of which can only be ascertained experimentally."¹

To ascertain the value of the control parameters and determine the laws of interaction, complementary variables are measured or calculated. These include, for instance, transparency of water, primary production, diversity and stability indexes, antibiotic effects, etc.

1. The text between quotation marks is reproduced from Modelling of Marine Systems, edited by Jacques C.J. Nihoul, Amsterdam, Elsevier Publ., 1974.

3.- Evolution equations

The assumption of uniform sea water density which is justified by experiment (apart from the Scheldt Estuary where slightly different models are being developed) allows a decoupling between the mechanical variables and the others. The hydrodynamic equations can be solved independently of the other evolution equations and the values of the flow velocity determined by the former substituted in the latter which in turn can be solved knowing the interactions between the constituents.

The *hydrodynamic models* which one can develop in this way differ whether one is interested in unsteady sea motions produced by tides and storm surges or in the residual - "steady" - circulation which results from the average of the actual flow over a time sufficiently long to cancel out tidal oscillations and transitory wind currents.

The evolution equations for the state variables r_a are coupled through the terms expressing the interactions of the constituent α with other constituents β , γ , ... They also depend on the water motion determined by the hydrodynamic models.

In a first approach, it is rewarding to separate the two effects and study first the dispersion (by currents, sedimentation and turbulence) of a "passive" constituent *i.e.* one which does not have significant interactions with others. Then, to investigate the interactions (*e.g.* the path of a pollutant in the food chain), one can develop *niche models* concerned with mean concentrations over some reasonably homogeneous regions of space. Niche models are not affected by the detailed hydrodynamics of the sea, only its effects on inputs and outputs at the niche's frontiers remain to be known.

Although *passive dispersion models* can only give conservative estimates of the distribution of chemicals and species in the sea and *niche models* can only give an average knowledge of the interactions, they provide nevertheless a first valuable insight into the mechanisms of the marine system.

Of course, the model can combine dispersion and interactions and provide the detailed prediction of the state of the system at all points and time.

However the gigantic amount of computer work which is required to solve large systems of coupled partial differential equations commends that the full scale simulation be restricted to dramatic cases where estimates are insufficient or to special problems (like the dumpings) where, in the area of interest, only a limited number of constituents are involved in a significant way.

The general dispersion-interaction model is described in [Nihoul (1973a)] and subsequent papers. Different simplified forms of this model, pertinent to special studies, are given in the following and illustrated by examples of application.

4.- Tides and storm surges model

i) State variables

Mean depth-averaged horizontal velocity vector \bar{u}

Water height H

(The surface elevation ζ is given by $H = h + \zeta$ where h is the water depth.)

ii) External forces per unit mass of sea water

Tide-generating force ξ

Gradient of atmospheric pressure $\nabla\left(\frac{p_a}{\rho}\right)$

Wind stress τ_s

Relation of wind stress to wind velocity v at reference height $\tau_s = \frac{C}{H} v \|v\|$

iii) Evolution equations

$$\frac{\partial H}{\partial t} + \nabla \cdot (H \bar{u}) = 0$$

$$\frac{\partial \bar{u}}{\partial t} + u \cdot \nabla u + f e_3 \wedge u = \xi - \nabla\left(\frac{p_a}{\rho} + g\zeta\right) + a \nabla^2 u$$

$$- \frac{D}{H} u \|u\| + \frac{C}{H} v \|v\|$$

where the e_1 and e_2 axes are horizontal, the e_3 -axis vertical and where

$$\nabla = e_1 \frac{\partial}{\partial x_1} + e_2 \frac{\partial}{\partial x_2} .$$

iv) Control parameters

- f : Coriolis parameter (twice the vertical component of the angular velocity of the earth)
- ρ : specific mass of the sea water
- a : horizontal effective viscosity
- D : bottom friction coefficient
- C : atmospheric drag coefficient
- h : depth

v) Interpretation of the evolution equations

The time variation of the velocity vector \bar{u} is the result of

- α : advection $\bar{u} \cdot \nabla \bar{u}$
- β : rotation $f e_3 \wedge \bar{u}$ produced by the Coriolis effect in axes fixed on the rotating earth
- γ : mixing by shear effect and turbulence $a \nabla^2 \bar{u}$
- δ : friction on the bottom $-\frac{D}{H} \bar{u} \|\bar{u}\|$
- ϵ : acceleration by agents of three different types
 - $\epsilon.1$: the wind stress on the sea surface $\frac{C}{H} v \|v\|$ related to the wind velocity v at some reference height
 - $\epsilon.2$: the gradient of the atmospheric pressure and of the surface elevation $-\nabla\left(\frac{p_a}{\rho} + g\zeta\right)$
 - $\epsilon.3$: the external force ξ . The type of external force one has in mind here is essentially the tide-generating force which is generally assumed to derive from a potential. (i.e. $\nabla \wedge \xi = 0$). ξ can then be combined with the pressure and surface elevation gradients.

5.- Model of residual circulation

i) State variables

Stream function

ψ

The two components of the residual flow rate vector U_0 are given by

$$U_{0,1} = - \frac{\partial \psi}{\partial x_2}$$

$$U_{0,2} = \frac{\partial \psi}{\partial x_1} .$$

ii) External forces per unit mass of sea water

Residual stress

Θ

$$\Theta = (\tau_s)_0 + (\tau_t)_0$$

where $(\tau_s)_0$ is the residual wind stress and $(\tau_t)_0$ the residual tidal stress [Nihoul (1974)]

$$(\tau_t)_0 = [g\zeta_1 \nabla \zeta_1 + \nabla \cdot (H^{-1} \mathbf{U} \mathbf{U})]_0$$

where ζ_1 denotes the surface elevation produced by tides and transitory wind forces.

iii) Steady state residual equation

$$\begin{aligned} \kappa \nabla^2 \psi - \frac{\partial \psi}{\partial x_1} \left(f \frac{\partial h}{\partial x_2} + \frac{2\kappa}{h} \frac{\partial H}{\partial x_1} \right) + \frac{\partial \psi}{\partial x_2} \left(f \frac{\partial h}{\partial x_1} - \frac{2\kappa}{h} \frac{\partial h}{\partial x_2} \right) \\ = h \omega_3 + \frac{\partial h}{\partial x_2} \vartheta_1 - \frac{\partial h}{\partial x_1} \vartheta_2 \end{aligned}$$

where ϑ_1 and ϑ_2 are the two horizontal components of Θ and where ω_3 is the vertical component of $\nabla \wedge \Theta$.

iv) Control parameters

κ : bottom friction coefficient for residual flow

f : Coriolis parameter

h : depth.

v) Interpretation of the residual circulation equation

The space distribution of the stream function ψ is the result of

α : combination of bottom slope and Coriolis effects

$$f \left[\frac{\partial \psi}{\partial x_2} \frac{\partial h}{\partial x_1} - \frac{\partial \psi}{\partial x_1} \frac{\partial h}{\partial x_2} \right]$$

β : combination of bottom slope and bottom friction effects

$$- \frac{2\kappa}{h} \left[\frac{\partial \psi}{\partial x_1} \frac{\partial h}{\partial x_1} + \frac{\partial \psi}{\partial x_2} \frac{\partial h}{\partial x_2} \right]$$

γ : combination of bottom slope and residual stress effects

$$\vartheta_1 \frac{\partial h}{\partial x_2} - \vartheta_2 \frac{\partial h}{\partial x_1}$$

δ : residual stress forcing

$$h \omega_3 .$$

6.- Passive dispersion models

i) State variables

Depth-averaged concentration of any passive constituent α
or depth-averaged temperature \bar{c}
($\bar{c} = \bar{r}_\alpha$ or $\bar{c} = \bar{\theta}$)

Depth-averaged horizontal velocity vector \bar{u}
(given by separate hydrodynamic model)

Water height H
(given by separate hydrodynamic model)

ii) Inputs - Outputs

Total input in a water column of unit base HA
(including volume sources, surface and bottom
fluxes. If these result in a net output, A
is negative.)

iii) Evolution equation [Nihoul (1973b)]

$$\frac{\partial \bar{c}}{\partial t} + \bar{u} \cdot \nabla \bar{c} + H^{-1} \nabla \cdot \left(\gamma_2 \frac{H \sigma_3}{\bar{u}} \bar{c} \bar{u} \right) = \Lambda + H^{-1} \nabla \cdot \left[\gamma_1 \frac{H^2}{\bar{u}} \bar{u} (\bar{u} \cdot \nabla \bar{c}) \right] + \nabla \cdot \tilde{\kappa} \nabla \bar{c}$$

iv) Control parameters

- σ_3 : migration (sedimentation or ascension) velocity
 $\sigma_3 = 0$ for temperature and neutrally buoyant constituents
- $\tilde{\kappa}$: horizontal eddy diffusivity
- γ_1, γ_2 : shear effects coefficients [Nihoul (1971), (1972), (1973b), (1974)].

v) Interpretation of the evolution equation

The evolution in time of the depth-averaged variable \bar{c} is the result of

- α : advection by the depth-averaged velocity $\bar{u} \cdot \nabla \bar{c}$
- β : shear effect correction to the advection taking into account that, as a result of migration, the maximum of \bar{c} may occur in a region of the water column where the actual horizontal velocity is significantly different from \bar{u} [Nihoul (1973b), (1974)]

$$H^{-1} \nabla \cdot \left(\gamma_2 \frac{H \sigma_3}{\bar{u}} \bar{c} \bar{u} \right)$$

- γ : shear effect dispersion [Nihoul (1971), (1972), (1973b), (1974)]

$$H^{-1} \nabla \cdot \left[\gamma_1 \frac{H^2}{\bar{u}} \bar{u} (\bar{u} \cdot \nabla \bar{c}) \right]$$

- δ : turbulent dispersion $\nabla \cdot \tilde{\kappa} \nabla \bar{c}$
- ϵ : external inputs (or outputs) Λ

7.- Niche interactions model

i) State variables

Averages over the whole niche's space of all interacting chemical and ecological state variables r_a or θ

s_a

ii) Inputs - Outputs

Total input (output if negative) in the niche (including volume sources and fluxes or flows in and out of the niche at the boundaries)

s_a

iii) Evolution equations

$$\frac{ds_a}{dt} = S_a + I_a(t, s_1, s_2, \dots, s_n)$$

I_a represents the rate of production (or destruction) of s_a by chemical, biochemical or ecological interactions. In general I_a is a function of time and all interacting variables s_β . I_a depends on the particular interactions involved. In many cases, it can be simply approximated by combinations (in sums and products) of simple laws such that

- | | | |
|----|-------------------------------------|--------------------------|
| a. | k_a | (constant) |
| b. | $k_{a\beta} s_\beta$ | (linear) |
| c. | $k_{a\beta\gamma} s_\beta s_\gamma$ | (bilinear) |
| d. | $k_1 s_a - k_2 s_a^2$ | (logistic) |
| e. | $k_1 \frac{s_\beta}{k_2 + s_\beta}$ | (Michaelis-Menten-Monod) |

where the k_a , $k_{a\beta}$ and $k_{a\beta\gamma}$ are functions of time and control parameters.

iv) Control parameters

Several control parameters influence the interaction laws and appear in particular in the expressions of the coefficients k_a , $k_{a\beta}$, ...

In some cases, it is simpler to consider these coefficients as resulting control parameters to be determined experimentally.

v) Interpretation of the evolution equation

The niche-averaged value of the state variables r_a or θ changes in time as a result of

α	: input or outputs in or out of the niche	S_a
β	: chemical, biochemical or ecological interactions	I_a .

8.- Examples of applications

8.1.- Tides and storm surges model

The model has been applied with success by Ronday (1973) to the calculation of tides in the North Sea and in the Southern Bight.

Figures 1.3 and 1.4 show a comparison between lines of equal phases and amplitudes according to observation and according to simulation.

8.2.- Residual circulation model

The model has been applied with success by Ronday (1972), Runfola and Adam (1972), Nihoul and Ronday (1974) to the calculation of the residual circulation in the North Sea and in the Southern Bight.

Figure 1.5 shows the residual flows of water masses in the North Sea estimated from observation.

Figure 1.6 shows the calculated stream lines in the North Sea with the assumption of constant depth.

Figure 1.7 shows the calculated stream lines in the North Sea taking the depth variations into account and demonstrating the influence of the bottom slope on the residual circulation.

Figure 1.8 shows the calculated stream lines in the Southern Bight when the tidal stress is neglected.

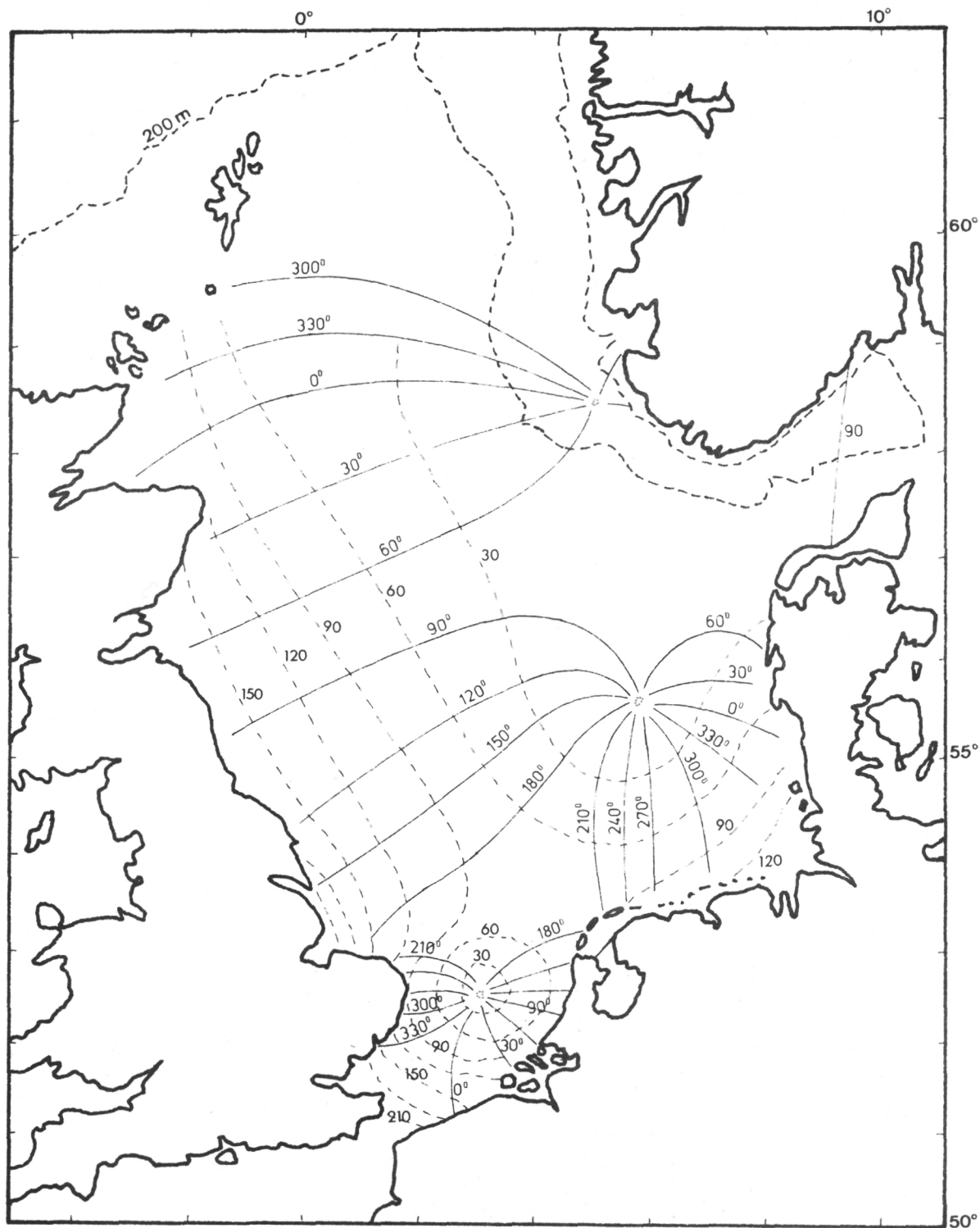


fig. 1.3.- Lines of equal tidal phases and amplitudes in the North Sea according to observations (after Proudman and Doodson, 1924).

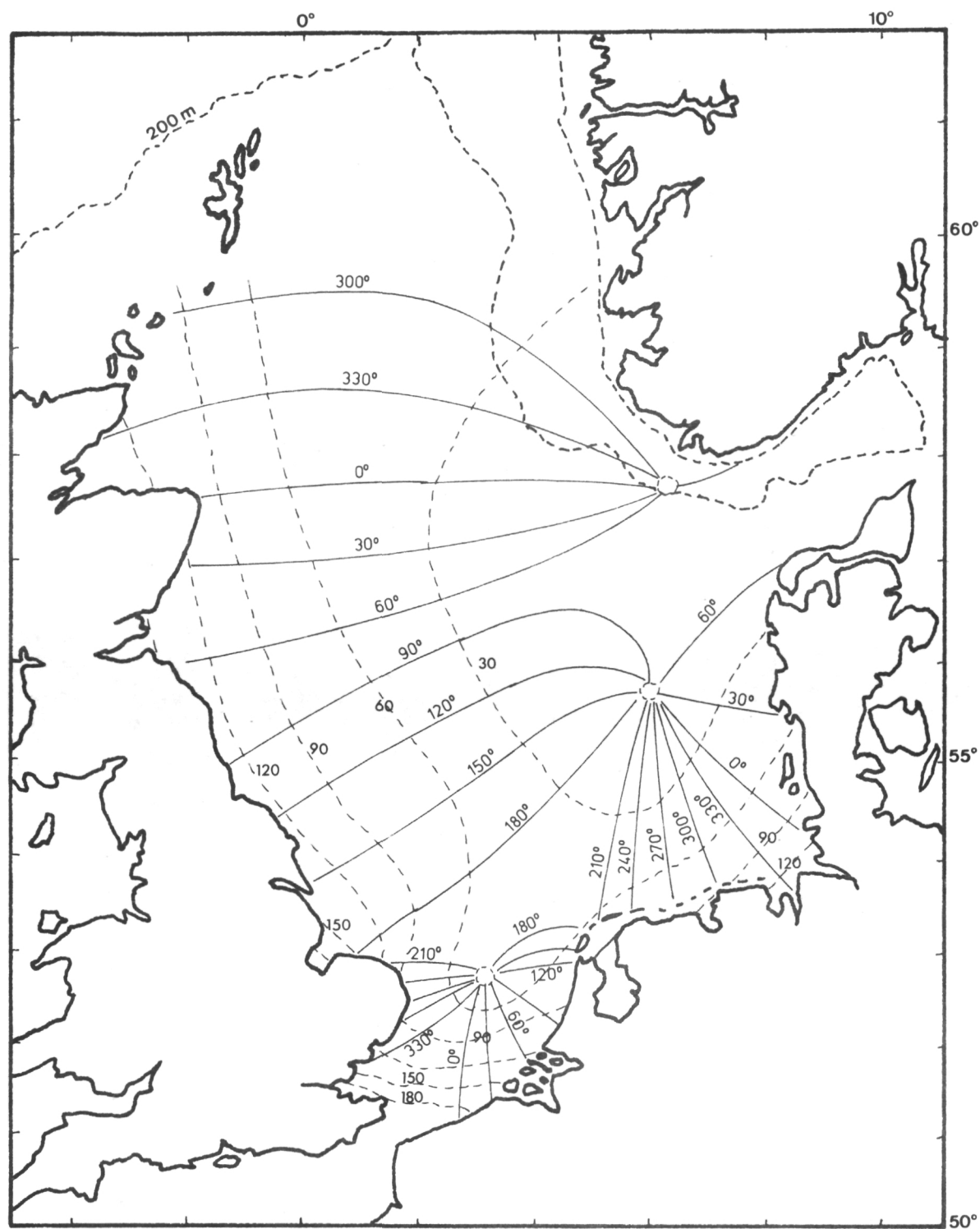


fig. 1.4.- Lines of equal tidal phases and amplitudes in the North Sea according to the mathematical model (after Røndal, 1973).

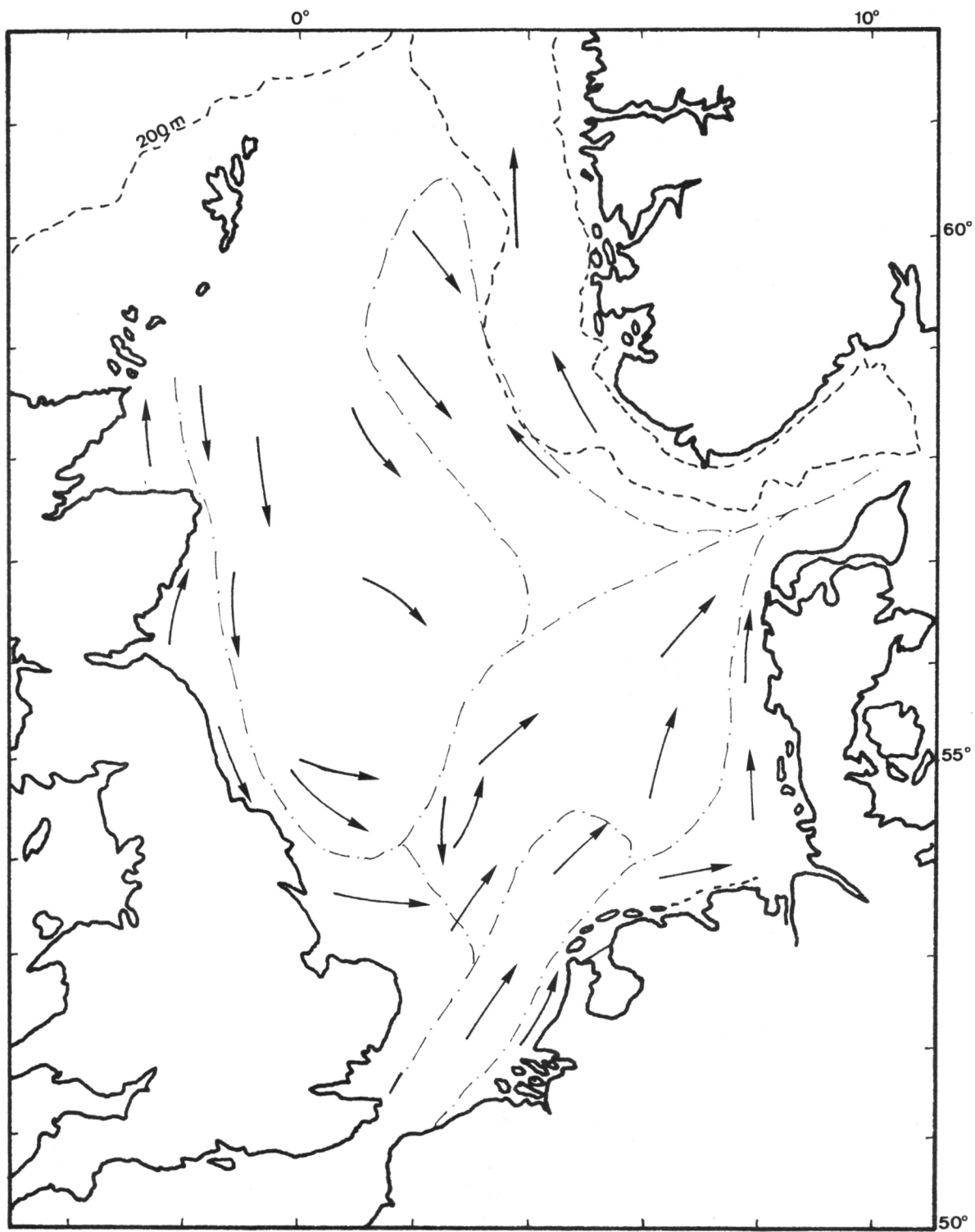


fig. 1.5.- Water masses in the North Sea according to Laevastu (1963).

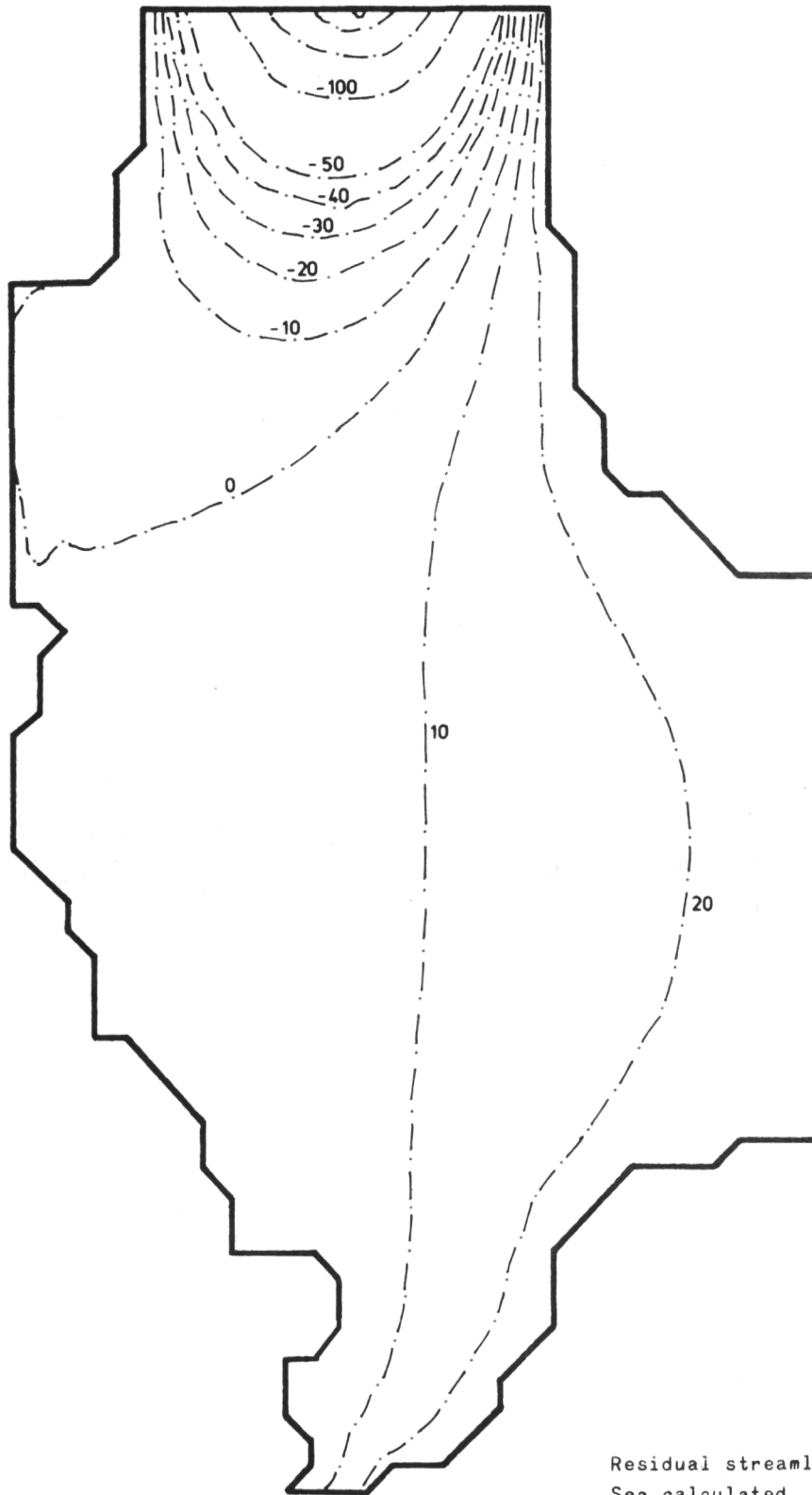


fig. 1.6.

Residual streamlines $\psi = \text{const}$ in the North Sea calculated, assuming constant depth (after Røndal, 1972). The actual values of ψ are 10^4 times the indicated figures.

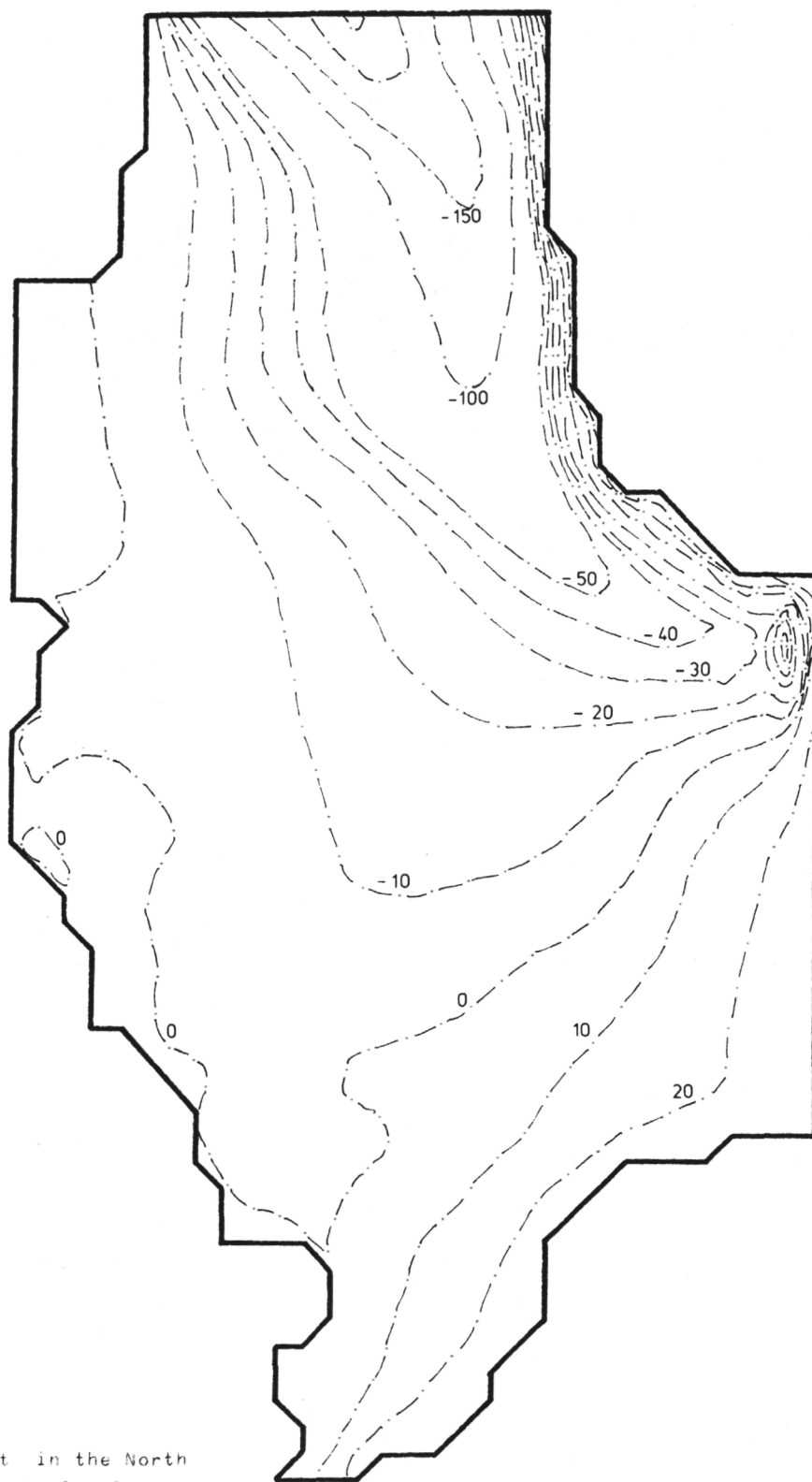


fig. 1.7.

Residual streamlines $\psi = \text{const}$ in the North Sea (after Røndal, 1972). The actual values of ψ are 10^4 times the indicated figures.

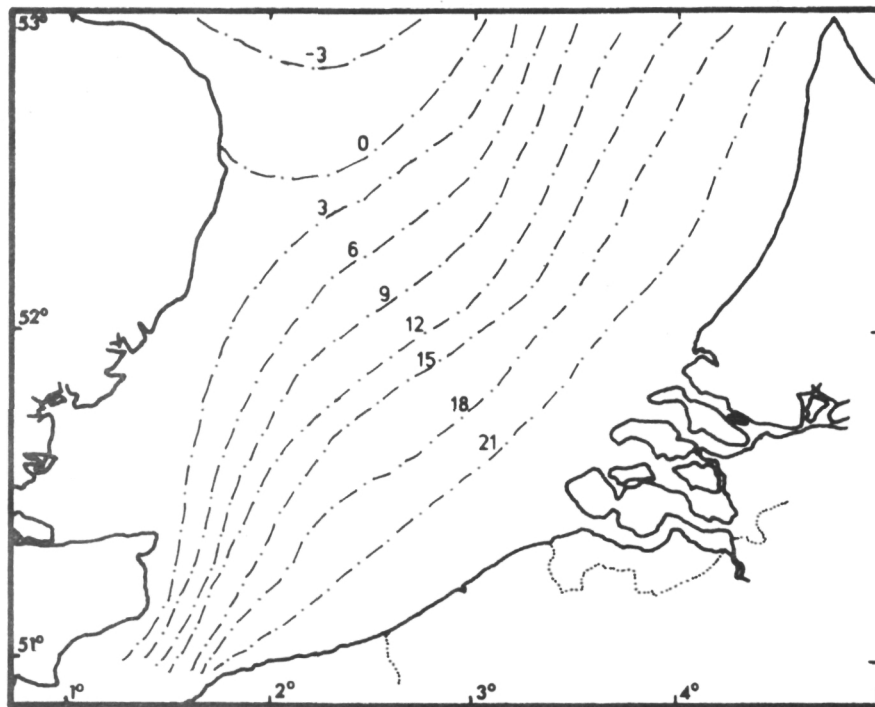


fig. 1.8.- Residual circulation in the Southern Bight without tidal stress.
Streamlines $\psi = \text{const}$ (in $10^4 \text{ m}^3/\text{s}$). (After Nihoul and Runday, 1974).

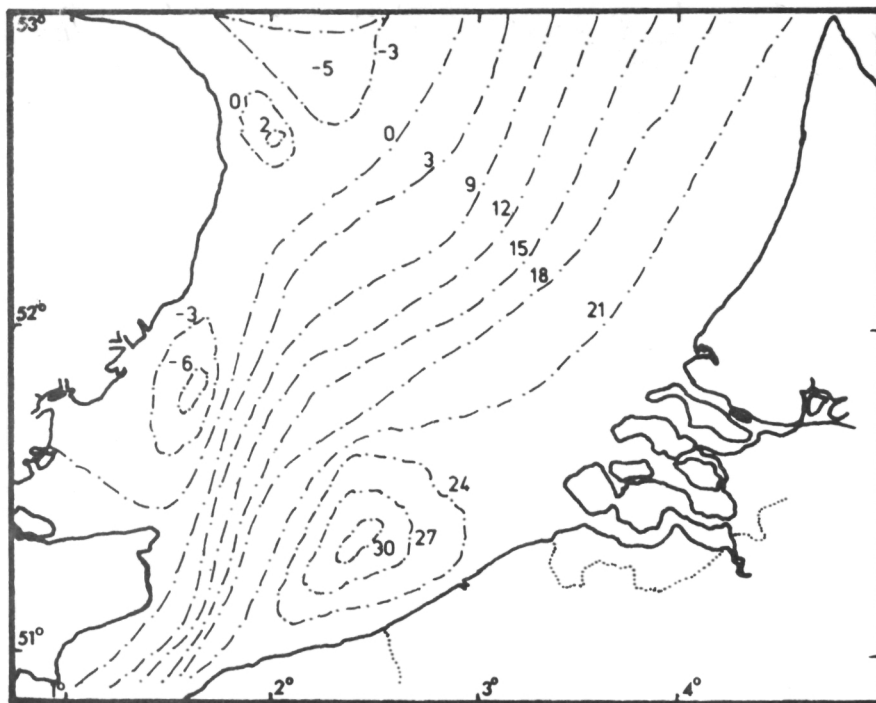


fig. 1.9.- Residual circulation in the Southern Bight with the tidal stress.
Streamlines $\psi = \text{const}$ (in $10^4 \text{ m}^3/\text{s}$). (After Nihoul and Runday, 1974).

Figure 1.9 shows the calculated streamlines in the Southern Bight taking the tidal stress (calculated from the tidal model) into account and demonstrating its cogent influence on the residual circulation.

8.3.- Passive dispersion model

The model has been applied with success by Nihoul (1972) and by Adam and Runfolla (1972) to the determination of the dispersion pattern subsequent to a dye release or a dumping.



fig. 1.10.

Simulation of a dye-release experiment in the North Sea
[after Adam and Runfolla (1972)].

Position : 51°20' N , 1°34' E .

Curves : 1/50 of initial central concentration 48 h -
72 h - 96 h - 108 h after release.

Figure 1.10 illustrates the influence of the shear effect on the anisotropy of the patch of dye.

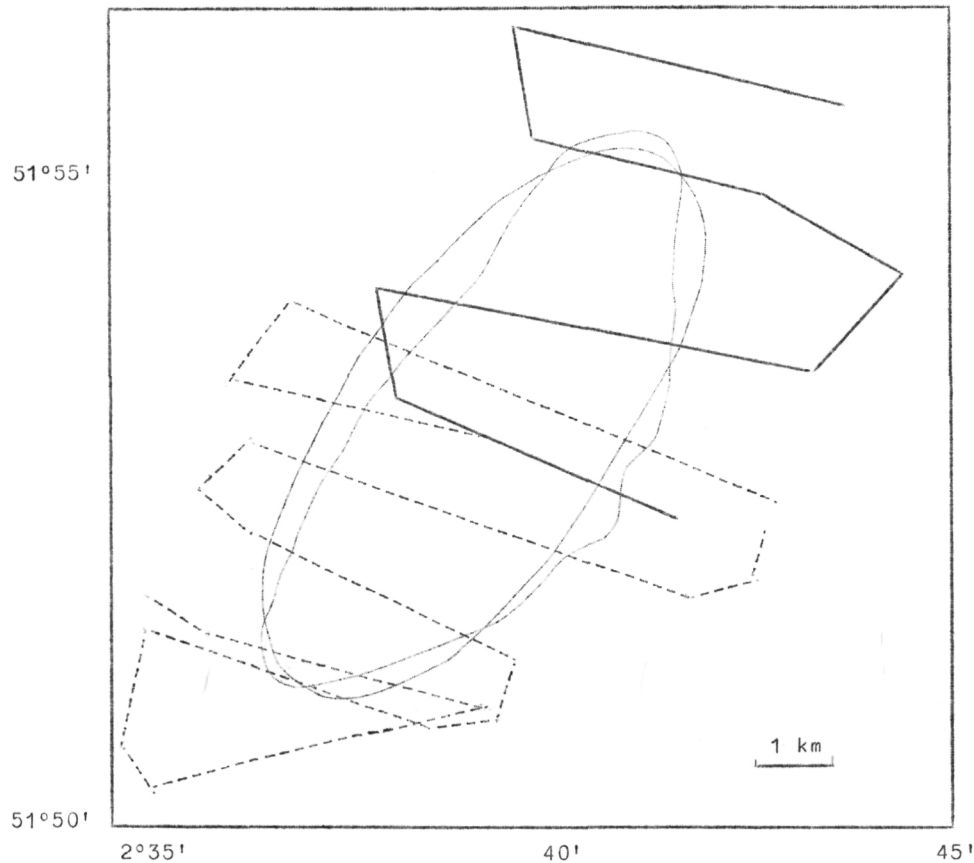


fig. 1.11.

Comparison between observed and predicted shape of a patch of rhodamine B 68 hours after release.

The experimental curve is the irregular curve drawn by Talbot (1970) [The broken piecewise straight lines are the ship's trajectories]. The theoretical curve is the regular ellipse predicted by the simplified model [Nihoul (1972)].

Figure 1.11 shows a comparison between the observed and predicted shape of a patch of rhodamine B, sixty-eight hours after release. The theoretical curve is calculated using a simplified version of the model which fits the best ellipse to the tidal velocity vector diagram.

8.4.- Niche interactions model

The model has been applied with success by Pichot and Adam to the study of chemical, biochemical and ecological interactions in the Ostend *Bassin de Chasse*

Figures 1.12, 1.13 and 1.14 show the evolution of six different forms of phosphorus :

- x_1 dissolved phosphate in sea water;
- x_2 P in non-living matter in suspension;
- x_3 dissolved phosphate in interstitial water;
- x_4 P in bottom sediments;
- x_5 P in plankton;
- x_6 P in benthos.

They illustrate the cogent influence of the non-linear terms in the interaction laws on the existence of a steady state and the time necessary to reach it.

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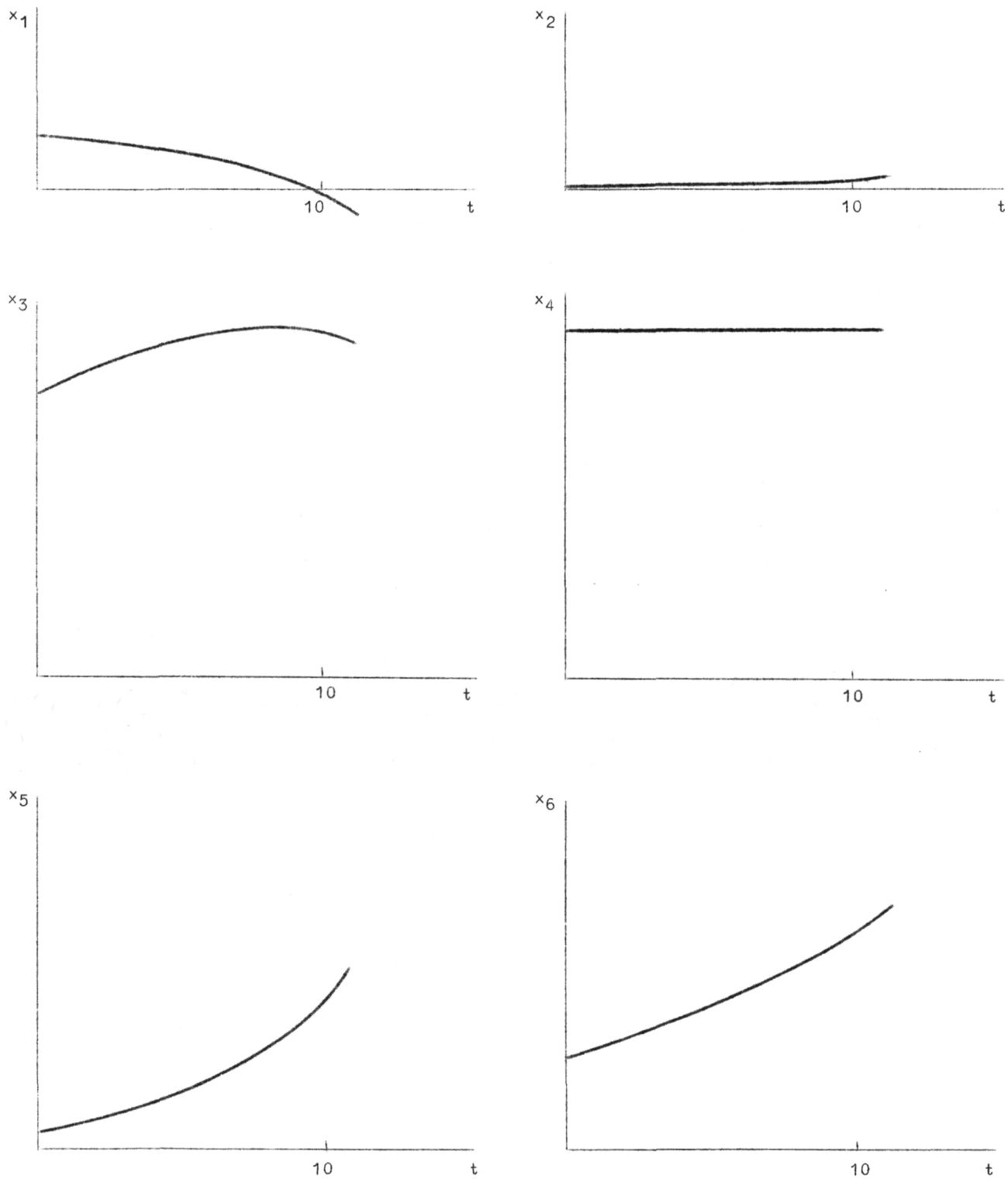


fig. 1.12.

Evolution of six different forms of P in a closed sea basin assuming completely linear interactions [after Adam (1973)].

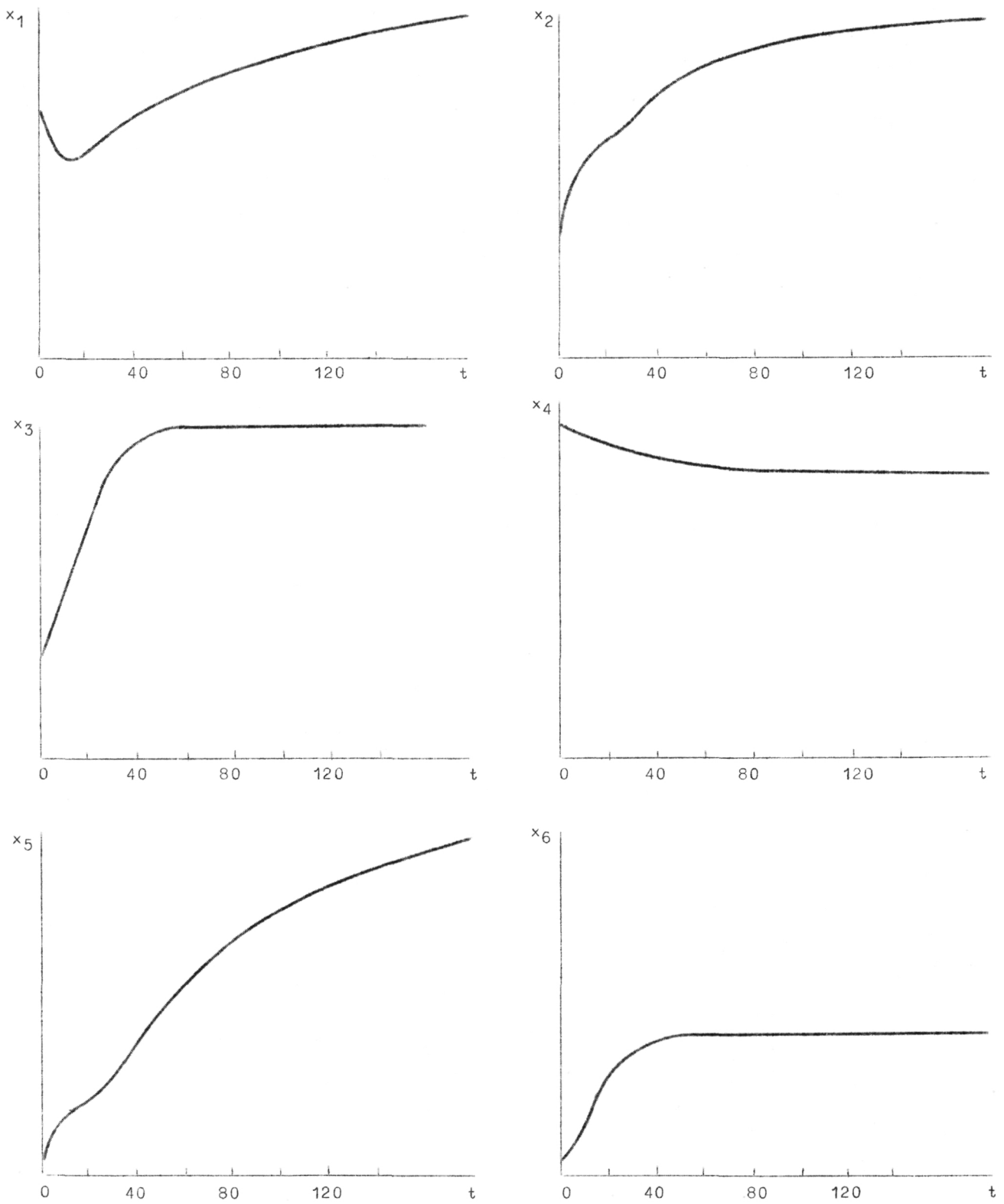


fig. 1.13.

Evolution of six different forms of P in a closed sea basin assuming quadratic-bilinear interactions [after Adam (1973)].

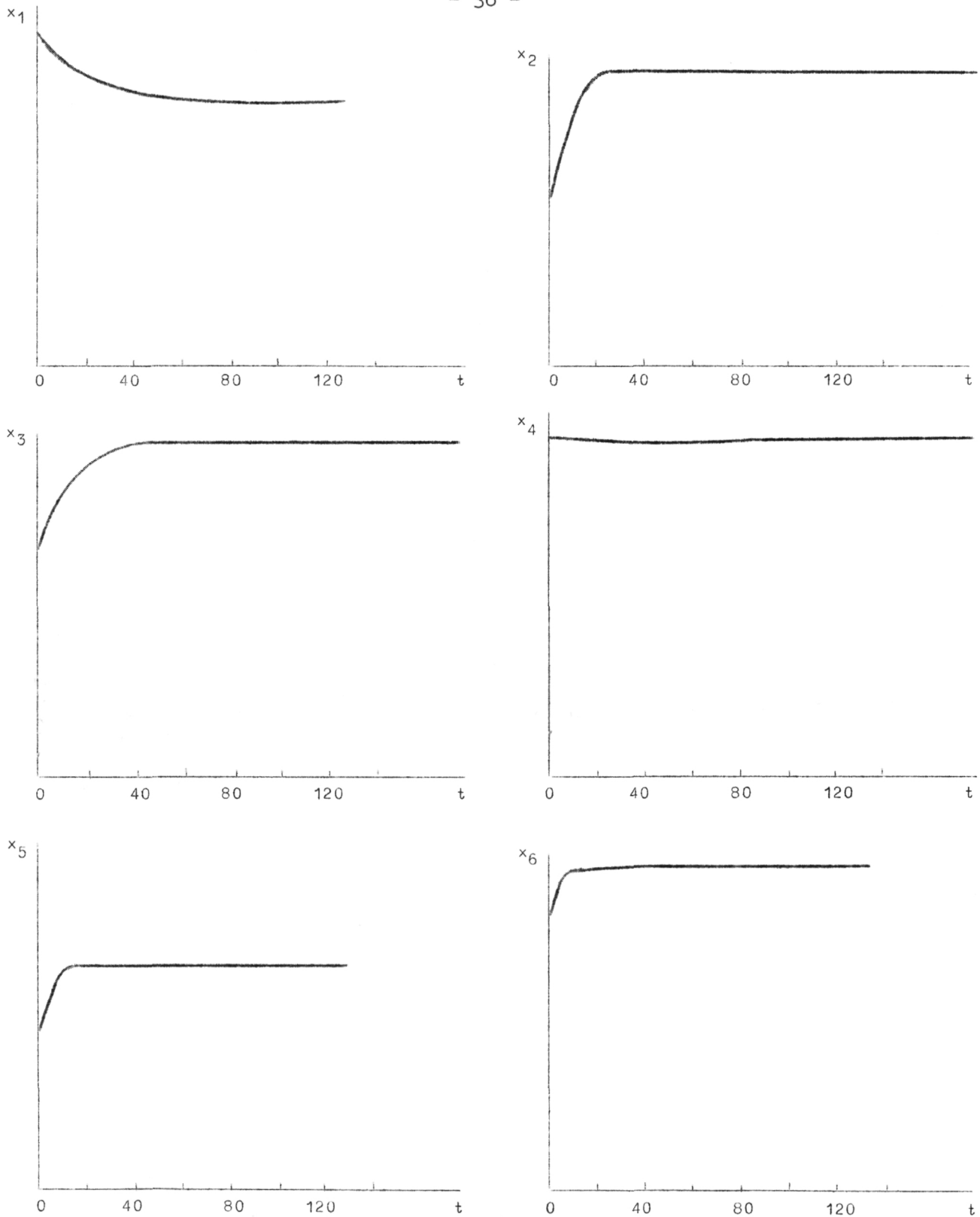


fig. 1.14.

Evolution of six different forms of P in a closed sea basin assuming strongly non-linear interactions [after Adam (1973)].

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- N 1 NIHOUL, Mathematical Model for the Study of Sea Pollution.
- N 2 NIHOUL, Application of Averaging Techniques to the Mathematical Modelling of Sea Pollution.
- N 3 NIHOUL, Mathematical Model, Proc. ICES, Meeting on Pollution in the North Sea, Lowestoft, March 25-26, 1971.
- N 4 RONDAY, Etude de la dispersion d'un polluant en mer du Nord.
- N 5 NIHOUL, Shear Effect and Eddy Diffusion in the Southern North Sea.
- N 6 NIHOUL, Ecosystemology applied to Sea Pollution.
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