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for the Study of Sea Pollution

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MATHEMATICAL MODEL

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by

Jacques C.J. NIHOUL *

Abstract

The system analysis approach is applied to the problem of sea pollution. To describe a given sea region, a tractable number of state variables are proposed and partial differential equations governing their evolution in space and time are established and discussed with a view on their application to knowledge, monitoring and management of the ocean.

* Prof. Dr. Ing. Jacques C.J. NIHOUL,
Institut de Mathématique,
Avenue des Tilleuls, 15,
B-4000 LIEGE (Belgium)

1.- Introduction

There is a growing public concern at the increasing deterioration of the environment by urban and industrial pollution. One realizes that the uncontrolled use and abuse of the sea for the disposal of waste has created serious ecological problems which threaten the health and welfare of man himself. An urgent need is felt for a more thorough understanding and a more rational and severe control of the marine environment. After centuries of contemptuous exploitation, one covets the management of the ocean.

This objective cannot be achieved however without a complete conversion of the traditional methods of physical, chemical and, above all, biological oceanography. The old fashioned naturalist's approach must give way to the rigour of system analysis. The oceanic region one wishes to manage must be regarded as a system described, from a physical, chemical and biological point of view, by a tractable number of state variables, governed by a closed set of evolution equations and subject to well defined and continuously surveyed boundary conditions.

Then, and only then, will it be possible to apply the theory of optimization to find a compromise between the requirements of the increasing industrialization and the affluent society and the necessity to preserve the natural resources so essential to mankind's survival.

2.- The state variables

The parameters which have to be determined as functions of space and time to provide a detailed description of a given sea region are, beside the physical parameters (velocity \mathbf{v} , pressure p , temperature θ , ...), the concentrations of the various constituents of the sea. The word "constituent" is introduced here to denote any chemical substance or living organism which participates to the ocean mixture with an individual behaviour. Thus completely dissolved NaCl is not a constituent but Na^+ and Cl^- are; a substance imprisoned in a complex aggregate is not a constituent; living organisms, animals are constituents, not the substances of which their tissues are made up. Water is a constituent and, actually, by far the most abundant one.

Dissolved substances are mixed with water at the molecular scale, non-dissolved substances are found in the form of a suspension (or emulsion) of small particles which, according to their weight and size, may tend to float or sediment. Colloidal solutions can also occur when the mixing is effected at the scale of macro-molecules or aggregates of molecules (10^{-3} - 10^{-1} microns); constituting an intermediate case between the solutions and the suspensions.

There is no objection to include living species in this description. They will be regarded as "substances" mixed with water; the nature of the mixture depending upon their size - migration of certain varieties may be incorporated in the model in roughly the same way as sedimentation and be accounted for by a "migration flux" with respect to the moving water masses.

Let $\rho_0, \rho_1, \dots, \rho_N$ denote the specific masses of the various constituents (ρ_0 referring to water) i.e.

$$(1) \quad \rho_i = \frac{\text{mass of constituent } S_i}{\text{total volume}} .$$

It is possible to establish a system of partial differential equations governing the evolution with space and time of the concentration functions $\rho_i(\mathbf{x}, t)$ and the coupled thermomechanical parameters, velocities, pressure, temperature.

Unfortunately, not only will these equations contain multiple interaction terms which are little known by the chemists and the biologists but also the size of the system - if one were to include every chemical substance and living species - would make its analytical or numerical solution utterly impossible.

One has thus to accept a simplified description in terms of a restricted number of state variables and evolution equations, defined as to make their study both a tractable problem and a significative undertaking with regard to the understanding and monitoring of pollution.

An attempt is made here to derive a consistent model on the following basis.

(i) A detailed description of every substance (or living organism) would be irksome and would not, in any case, be amenable to experimental

verification or interpretation.

(ii) More directly utilizable would be the knowledge of selected element's concentrations in a limited number of "phases", a phase denoting - by lack of a better word - a class of constituents having similar properties with respect to their mixing with sea water and, for instance, being distinguished by the scale or the degree of refinement of their dispersion in the sea.

Thus, phases could be constituted by (i) all dissolved chemical substances, (ii) suspended particles, (iii) minute living organisms carried along by the sea (like plankton and phytoplankton), (iv) different groups of animals at different stages of the food chain, (v) bottom sediments, etc.

A more refined classification could also be suggested and progressively incorporated in the model, provided it is amenable to analysis. For instance, a distinction could be made between mineral and (dead) organic suspensions, etc.

In this approach, a pollutant like mercury, for instance, would not be studied by following the evolution of every of the numerous mercury compounds which can be present in the sea but in a simpler way, by determining, as a function of space and time, the total concentration of mercury in each phase, say the total concentration of mercury in solution independently of the various solutes in which it may be involved.

Hence if φ is the number of phases and e the number of elements selected for their importance with respect to pollution, one may define a limited number of $n = e\varphi$ generalized state variables as follows.

Let b_j^k denote the weight fraction of element j (say mercury) contained in constituent k , one may define the total concentration of element j in phase m as

$$(2) \quad \rho_{jm} = \sum_{(\text{over phase } m)} b_j^k \rho_k$$

the sum being carried over all constituents present in phase m .

One may now relabel the new variables $\rho_{jm} : \rho_\alpha$ with $\alpha = 1, 2, \dots, n$, a greek index referring to a state variable.

[For instance ρ_1 could be the total concentration of mercury in solution, ρ_2 the total concentration of mercury in suspension, etc.]

In addition to the "pollution variables" ρ_α , it will be useful to know the specific mass of each phase defined as the sum of the specific masses of all constituents belonging to that particular phase.

Let ρ^d , ρ^s , ρ^b ($b = 1, 2, \dots$) denote the specific masses of respectively the phase of dissolved substances, the phase of suspensions, the biological phase b . The largest contribution to ρ^d comes from the dissolved salts and ρ^d may be regarded as a measure of the salinity; ρ^s is related to turbidity and the ρ^b 's are specific biomasses^(*).

One may regard however these additional variables as included in the definition (2) by considering for each phase an extra element for which all the b_j^k 's are equal to 1. Hence ρ^d , ρ^s , ... need not be considered separately from the ρ_α 's if α now runs from 1 to $n + \varphi$.

The equations describing the evolution of the concentrations with space and time will be completed by hydrodynamical and thermodynamical equations written in terms of a pressure p , a temperature θ , a specific mass ρ and a velocity \mathbf{v} of the sea water which is really pure water + dissolved substances.

Hence, for instance,

$$(3) \quad \rho = \rho_0 + \rho^d .$$

3.- The dynamical equations

Let V denote an arbitrary fixed volume in the sea region under consideration and let S be the surface including V .

The total amount of constituent S_i present in V can only change in time either because S_i flows in or out of V or because it is produced or destroyed inside V . The production or destruction

(*) One notes that the variables ρ_α represent concentrations if the concentration is defined as the "mass of pollutant per unit volume". In the case of a biological phase, a concentration defined as the ratio of the mass of pollutant to the phase's biomass would be more significant. This is obtained by dividing the specific mass ρ_α by the specific biomass ρ^b of the corresponding phase.

of S_i inside V can result from external sources or from internal interactions (chemical, biochemical, ...) with other constituents.

Hence

$$(4) \quad \frac{\partial}{\partial t} \int_V \rho_i \, dV = - \int_S \rho_i \mathbf{v}_i \cdot \mathbf{n} \, dS + \int_V (Q_i + Y_i) \, dV$$

where \mathbf{v}_i denotes the velocity of S_i , \mathbf{n} the unit vector along the normal to the surface S , Q_i and Y_i the rates of production or destruction of S_i per unit volume by, respectively, external sources (release, etc.) and internal interactions.

Transforming the surface integral by Gauss's theorem, one can write

$$(5) \quad \int_V \left(\frac{\partial \rho_i}{\partial t} + \mathbf{v} \cdot \rho_i \mathbf{v}_i \right) \, dV = \int_V (Q_i + Y_i) \, dV$$

where \mathbf{v} is the differential vector operator

$$\mathbf{v} = \mathbf{e}_1 \frac{\partial}{\partial x_1} + \mathbf{e}_2 \frac{\partial}{\partial x_2} + \mathbf{e}_3 \frac{\partial}{\partial x_3} .$$

Since the volume V is arbitrary, one must have

$$(6) \quad \frac{\partial \rho_i}{\partial t} + \mathbf{v} \cdot \rho_i \mathbf{v}_i = Q_i + Y_i .$$

Now

$$(7) \quad \rho_i \mathbf{v}_i \equiv \rho_i (\mathbf{v}_i - \mathbf{v}) + \rho_i \mathbf{v} .$$

The second term in the right-hand side $\rho_i \mathbf{v}$ represents the flow of constituent S_i as it is carried along by the ocean water. The first term in the right-hand side represents the "slippage" flow of constituent S_i with respect to the bulk motion. One generally calls the former the flow of S_i and the latter the flux of S_i .

The flux of a given constituent S_i is due to molecular diffusion and in certain cases to the net migration (sedimentation for instance) of the substance through the water.

The molecular contribution can be expressed by assuming that it obeys the Fourier-Fick law according to which the flux is proportional to the gradient of the concentration.

It turns out however that, in the sea, this contribution is always negligible compared with that part of the flow which is associated with erratic motions producing a general stirring and mixing

of the sea constituents analogous to diffusion but many times more efficient.

Let \mathbf{m}_i denote the net migration flux. [This flux is often zero or negligible as, for instance, in the case of water itself, dissolved substances, neutrally buoyant particles, minute organisms carried along by the sea, etc.] Eq. (7) may now be written (neglecting molecular diffusion)

$$(8) \quad \rho_i \mathbf{v}_i = \rho_i \mathbf{v} + \mathbf{m}_i .$$

The rate of release Q_i is a given quantity in any specific problem. The interaction rate Y_i can be written

$$(9) \quad Y_i = \sum_{\beta=1}^R P_{i\beta}$$

where $P_{i\beta}$ is the rate of production or destruction of S_i per unit volume in the β^{th} reaction and the sum is over all reactions.

In the case of chemical reactions, one may write

$$(10) \quad P_{i\beta} = v_{i\beta} J_{\beta}$$

where J_{β} is the rate of reaction β and $v_{i\beta}$ is proportional to the stoichiometric coefficient of S_i in reaction β counted positive when S_i appears in the right-hand side (production) and negative when it appears in the left-hand side (destruction). [For instance, if J_{β} is expressed in moles per unit volume and unit time, $v_{i\beta}$ is the stoichiometric coefficient multiplied by the molecular mass of S_i .]

One notes that the summation in (9) always includes a chemical reaction and its reverse with opposite stoichiometric coefficients. The two reactions only contribute to Y_i inasmuch as the two reaction rates are different.

Combining (6), (8) and (9), one obtains

$$(11) \quad \frac{\partial \rho_i}{\partial t} + \mathbf{v} \cdot \rho_i \mathbf{v} = - \mathbf{v} \cdot \mathbf{m}_i + \sum_{\beta=1}^R P_{i\beta} + Q_i .$$

Multiplying every term of (11) by b_j^i and summing over all constituents of each phase, one gets

$$(12) \quad \frac{\partial \rho_{jm}}{\partial t} + \nabla \cdot \rho_{jm} \mathbf{v} = - \nabla \cdot \mathbf{m}_{jm} + Q_{jm} + \sum_{\beta=1}^s P_{j\beta}^m$$

where

(i)

$$(13) \quad \mathbf{m}_{jm} = \sum_{(\text{over phase } m)} b_j^i \mathbf{m}_i$$

represents the net migration of element j in phase m [say, the net sedimentation of the mercury in suspension no matter which mercury compounds are actually sedimenting] (for many phases, of course,

$\mathbf{m}_{jm} = \mathbf{0}$);

(ii)

$$(14) \quad Q_{jm} = \sum_{(\text{over phase } m)} b_j^i Q_i$$

represents the external production (or destruction) of constituent j in phase m [say, the total source of mercury in solution no matter which mercury compounds are actually dissolved];

(iii)

$$(15) \quad P_{j\beta}^m = \sum_{(\text{over phase } m)} b_j^i P_{i\beta}$$

represents the rate of production (or destruction) of constituent j in phase m by reaction β ; this term is obviously zero for all the reactions which do not imply a change of phase, hence the summation in (12) is limited to a smaller number of reactions (s , say).

Relabelling the variables ρ_α ($\alpha = 1, \dots, n+\phi$), one may write (12) in the form

$$(16) \quad \frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot \rho_\alpha \mathbf{v} = Q_\alpha - \nabla \cdot \mathbf{m}_\alpha + \sum_{\beta=1}^s P_{\alpha\beta}$$

An equation for the specific mass ρ is readily obtained from (16) but the contribution to water or salts concentrations of eventual sources or reactions can be neglected (in view of the enormous reservoir of water and salts). Hence

$$(17) \quad \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0$$

Neglecting molecular diffusion of momentum and heat as compared with turbulent diffusion, one may write, for the velocity and temperature fields

$$(18) \quad \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = - \frac{1}{\rho} \nabla p + \mathbf{g} - 2 \boldsymbol{\Omega} \wedge \mathbf{v}$$

where $\boldsymbol{\Omega}$ is the rotation vector of the earth, \mathbf{g} the acceleration of gravity and where the term representing the centrifugal force is incorporated in the pressure,

$$(19) \quad \frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = Q_{\theta}$$

where Q_{θ} represents the production of heat (by radiation, chemical or biological reactions, etc.).

Eq. (16), (17), (18) and (19) must be complemented by an equation of state.

In the case of well mixed water, it is permissible to assume that ρ is a constant. Eq. (17) reduces then to

$$(20) \quad \nabla \cdot \mathbf{v} = 0$$

and form with (18) a closed system for the determination of \mathbf{v} and p .

In the test region selected for the Belgian National Program (see Appendix I), this approximation is good everywhere except in the vicinity of an estuary where fresh water may be treated as a "pollutant" originating from a boundary source [the absence of volume sources in (17) does not of course exclude boundary sources].

If the mixing is not complete, the sea may display various forms of stratification and a better approximation for the state equation is obtained by Boussinesq approximation (e.g. Nihoul 1969).

In the following, one will restrict attention to perfectly mixed sea regions in order to present the philosophy of the subsequent approximations in the simplest context possible. There would be no difficulty in refining the model taking into account, for instance, stratification and Boussinesq approximation.

4.- Application of the K.B.M. Method

In the sea, the velocity field is always extremely complex. Different types of motions occur, characterized by different time scales and different length scales, from the quasi-steady currents to the

rapid small turbulent eddies, interacting with each other and forming an intricate pattern amenable only, in most cases, to a statistical analysis.

An attempt to follow a pollutant as it is convected by the fastest motions would be preposterous. Not only would such a study be beyond reach of any mathematical or experimental analysis but it would also have no significance as those rapidly changing erratic motions tend to cancel each other over any reasonable length of time, contributing only to the dispersion of the pollutant in much the same way (but many times more efficiently) as molecular diffusion.

Let T be a characteristic time for the study of pollution in the sense that one does not require the knowledge of the state of pollution, say, every second but only every T (T may be an hour, a day or two, a month, ... according to the problem in consideration).

Processes which have a characteristic time larger than T change only a little over T . They will be called "slowly varying".

Among the fast processes which have a characteristic time smaller than T , one must distinguish between erratic oscillating processes which tend to cancel each other and may be regarded as having a zero mean over T and evolving processes the effects of which are cumulated over T .

To the first category belong all types of motions from waves (of frequency larger than T^{-1}) to turbulence of which no mean current results although their mean square amplitude is not zero accounting for their extremely efficient mixing effect.

To the second category belong fast chemical or biological reactions which can be regarded as completed in a time short as compared to T .

Normally the sources will not release the reactants at such a high rate and the fast reactions will have to adapt their pace to that of the sources. In other words, if a source releases a substance A which is involved in a fast reaction to produce a substance B , it will look, over a time T , as if A being almost instantaneously transformed into B - the source had released B directly. Hence, if one is mainly interested in averages over T , one may disregard the fast reactions in the interaction term and take them into account by

correcting the sources, writing them down as releasing the products of these reactions directly.

One may then consider only two kinds of processes : those whose characteristic time is larger than T and those whose characteristic time is smaller and have a zero mean over T .

Let q denote any of the state variables v_i , ρ , θ , ρ_α , ... one may write

$$(21) \quad q = \bar{q} + \hat{q}$$

where

$$(22) \quad \bar{q} = \frac{1}{T} \int_t^{t+T} q \, dt,$$

$$(23) \quad \int_t^{t+T} \hat{q} \, dt \sim 0,$$

$$(24) \quad \int_t^{t+T} \frac{\partial \hat{q}}{\partial t} \, dt \sim 0$$

(because $\frac{\partial \hat{q}}{\partial t}$ refers also to rapidly changing intricate processes which roughly cancel each other over a time T).

Hence

$$(25) \quad \frac{1}{T} \int_t^{t+T} \frac{\partial q}{\partial t} \, dt \sim \frac{1}{T} \int_t^{t+T} \frac{\partial \bar{q}}{\partial t} \, dt = \frac{\bar{q}(t+T) - \bar{q}(t)}{T} \sim \frac{\partial \bar{q}}{\partial t}$$

(because the time T is small compared with the characteristic time of evolution of \bar{q} and the finite difference may be approximated by the differential).

Also (q and q' being any two state variables)

$$(26) \quad \frac{1}{T} \int_t^{t+T} qq' \, dt \sim \bar{q} \bar{q}' + \overline{\hat{q} \hat{q}'}$$

[because as \bar{q} and \bar{q}' vary little over a period of time T , they may in first approximation be taken out of the integration sign; then cross products $\bar{q} \hat{q}'$, ... vanish in the mean as a result of (23)].

Averaging eq. (16) and (18) to (20) over T , one obtains thus, taking ρ constant (well mixed water) :

$$(27) \quad \frac{\partial \bar{v}}{\partial t} + \mathbf{v} \cdot \bar{\mathbf{v}} \bar{\mathbf{v}} = - \frac{1}{\rho} \nabla \bar{p} + \mathbf{g} - 2 \boldsymbol{\Omega} \wedge \bar{\mathbf{v}} - \mathbf{v} \cdot \overline{\hat{\mathbf{v}} \hat{\mathbf{v}}}$$

$$(28) \quad \frac{\partial \bar{\theta}}{\partial t} + \mathbf{v} \cdot \bar{\theta} \bar{\mathbf{v}} = - \mathbf{v} \cdot \overline{\hat{\theta} \hat{\mathbf{v}}}$$

$$(29) \quad \mathbf{V} \cdot \bar{\mathbf{v}} = 0$$

$$(30) \quad \frac{\partial \bar{\rho}_\alpha}{\partial t} + \mathbf{V} \cdot \bar{\rho}_\alpha \bar{\mathbf{v}} = \bar{Q}_\alpha - \mathbf{V} \cdot \bar{\mathbf{m}}_\alpha + \sum_{\beta=1}^s \bar{P}_{\alpha\beta} - \mathbf{V} \cdot \hat{\rho}_\alpha \hat{\mathbf{v}}$$

The last terms in the right-hand sides of (27), (28) and (30) represent the net contribution of all the faster motions to the dispersion of momentum, heat and pollutants.

The averaging technique employed here with assumptions (25) and (26) is known as the Krylov-Bogoliubov-Mitropolsky method.

5.- The quasi-static approximation

The vertical component of eq. (27) reads (the vertical axis pointing upwards) :

$$(31) \quad \frac{\partial \bar{v}_3}{\partial t} + \mathbf{V} \cdot \bar{\mathbf{v}} \bar{v}_3 = - \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_3} - g - 2(\Omega_1 \bar{v}_2 - \Omega_2 \bar{v}_1) - \mathbf{V} \cdot \hat{\mathbf{v}} \hat{v}_3$$

where Ω_1 and Ω_2 are the horizontal components of $\mathbf{\Omega}$. The terms on the left-hand side represent the acceleration of the vertical mean motion. This is presumably negligible as compared to the acceleration of gravity which is of the order of 10 m/s^2 . The angular velocity of the earth is of the order of 10^{-4} s^{-1} . If the horizontal velocity is of the order of 1 m/s , the Coriolis term is 10^5 smaller than the gravity term. Observations in sea areas comparable to the Southern North Sea test region investigated by the Belgian - Nato program seem to indicate that the last term on the right-hand side of (31) is also much smaller than the gravity term (Bowden, 1956, 1966).

If these terms are neglected, (31) reduces to

$$(32) \quad \frac{\partial \bar{p}}{\partial x_3} = - \rho g$$

and, integrating over x_3 ,

$$(33) \quad \bar{p} = - \rho g x_3 + f(x_1, x_2) .$$

Let $z = \zeta$ represent the equation of the mean free surface.

At the free surface, the pressure must be equal to the atmospheric pressure p_a . Hence

$$(34) \quad p_a = - \rho g \zeta + f(x_1, x_2) .$$

This determines \bar{p} . Eq. (33) may thus be written

$$(35) \quad \bar{p} = p_a + \rho g \zeta - \rho g x_3 .$$

The horizontal components of the Coriolis force read :

$$(36) \quad f \bar{v}_2 - 2 \Omega_2 \bar{v}_3$$

$$(37) \quad - f \bar{v}_1 + 2 \Omega_1 \bar{v}_3$$

where the vertical component of the rotation vector $\mathbf{\Omega}$ has been written $\frac{1}{2} f$ to conform to usual notations.

It is reasonable to assume that the vertical mean velocity is much smaller than the horizontal mean velocity. Hence the last term may be neglected in (36) and (37).

Combining eq. (27), (35), (36) and (37), one has, then, for the horizontal components of the mean velocity vector

$$(38) \quad \frac{\partial \bar{v}_1}{\partial t} + \mathbf{\nabla} \cdot \bar{\mathbf{v}} \bar{v}_1 = - \frac{\partial}{\partial x_1} \left(\frac{p_a}{\rho} + g \zeta \right) + f \bar{v}_2 - \mathbf{\nabla} \cdot \hat{\mathbf{v}} \hat{v}_1 ,$$

$$(39) \quad \frac{\partial \bar{v}_2}{\partial t} + \mathbf{\nabla} \cdot \bar{\mathbf{v}} \bar{v}_2 = - \frac{\partial}{\partial x_2} \left(\frac{p_a}{\rho} + g \zeta \right) - f \bar{v}_1 - \mathbf{\nabla} \cdot \hat{\mathbf{v}} \hat{v}_2 .$$

The approximation made in writing (35), (38) and (39) is equivalent to assuming static equilibrium in the vertical direction and neglecting all components of the earth rotation vector but the vertical one. This may be termed the "quasi-static approximation".

6.- The vertically integrated equations of motion

If one is mainly interested in the horizontal distribution of pollutants, it is convenient to integrate eq. (29), (30), (38) and (39) over depth.

Let $z = 0$ denote the free surface at equilibrium, $z = \zeta$ the perturbed free surface and $z = -h$ the surface of the bottom and let :

$$(40)(41) \quad U = \int_{-h}^{\zeta} \bar{v}_1 dz , \quad V = \int_{-h}^{\zeta} \bar{v}_2 dz ,$$

$$(42)(43) \quad S_\alpha = \int_{-h}^{\zeta} \bar{Q}_\alpha dz , \quad I_\alpha = \int_{-h}^{\zeta} \sum_{\beta=1}^s \bar{P}_{\alpha\beta} dz$$

$$(44) \quad M_\alpha = \int_{-h}^{\zeta} \left(\frac{\partial \bar{m}_{\alpha,1}}{\partial x_1} + \frac{\partial \bar{m}_{\alpha,2}}{\partial x_2} \right) dz ,$$

$$(45) \quad R_\alpha = \int_{-h}^{\zeta} \rho_\alpha \, dz$$

One notes that, except for animals migrating in the horizontal direction, M_α is zero; the migration vector \mathbf{m}_α being vertical for sedimentation, floatation as well as for diurnal migration of certain species with light (in most of the latter cases, anyway $\overline{\mathbf{m}_\alpha}$ is zero whenever the characteristic time T is larger than one day).

The kinematic boundary condition at the free surface is

$$(46) \quad \frac{d\zeta}{dt} \equiv \frac{\partial \zeta}{\partial t} + \overline{v_1} \frac{\partial \zeta}{\partial x_1} + \overline{v_2} \frac{\partial \zeta}{\partial x_2} = [\overline{v_3}]_{z=\zeta}.$$

Let

$$(47) \quad H = \zeta + h.$$

Integrating (38), (39), (29) and (30) over depth, one gets :

$$(48) \quad \frac{\partial U}{\partial t} - f V = -H \frac{\partial}{\partial x_1} \left(\frac{p_a}{\rho} + g\zeta \right) - \overline{\frac{\partial}{\partial x_1} v_1 v_1} - \overline{\frac{\partial}{\partial x_2} v_2 v_1} \\ - \overline{\frac{\partial}{\partial x_1} \hat{v}_1 \hat{v}_1} - \overline{\frac{\partial}{\partial x_2} \hat{v}_2 \hat{v}_1} - \left[\overline{v_3 v_1} + \overline{\hat{v}_3 \hat{v}_1} \right]_{z=-h}^{z=\zeta}$$

$$(49) \quad \frac{\partial V}{\partial t} + f U = -H \frac{\partial}{\partial x_2} \left(\frac{p_a}{\rho} + g\zeta \right) - \overline{\frac{\partial}{\partial x_1} v_1 v_2} - \overline{\frac{\partial}{\partial x_2} v_2 v_2} \\ - \overline{\frac{\partial}{\partial x_1} \hat{v}_1 \hat{v}_2} - \overline{\frac{\partial}{\partial x_2} \hat{v}_2 \hat{v}_2} - \left[\overline{v_3 v_2} + \overline{\hat{v}_3 \hat{v}_2} \right]_{z=-h}^{z=\zeta}$$

$$(50) \quad \frac{d\zeta}{dt} + \overline{\frac{\partial v_1}{\partial x_1}} + \overline{\frac{\partial v_2}{\partial x_2}} = 0$$

$$(51) \quad \frac{\partial R_\alpha}{\partial t} = S_\alpha - M_\alpha + I_\alpha - \overline{\frac{\partial}{\partial x_1} \rho_\alpha v_1} - \overline{\frac{\partial}{\partial x_2} \rho_\alpha v_2} - \overline{\frac{\partial}{\partial x_1} \hat{\rho}_\alpha \hat{v}_1} \\ - \overline{\frac{\partial}{\partial x_2} \hat{\rho}_\alpha \hat{v}_2} - \left[\overline{\rho_\alpha v_3} + \overline{\hat{\rho}_\alpha \hat{v}_3} + \overline{m_{\alpha,3}} \right]_{z=-h}^{z=\zeta}$$

where \sim denotes an integral over depth.

Eq. (50) may be simplified as follows. One may write :

$$(52) \quad \int_{-h}^{\zeta} \left(\frac{\partial \overline{v_1}}{\partial x_1} + \frac{\partial \overline{v_2}}{\partial x_2} \right) dz = \frac{\partial}{\partial x_1} \int_{-h}^{\zeta} \overline{v_1} dz + \frac{\partial}{\partial x_2} \int_{-h}^{\zeta} \overline{v_2} dz \\ - \frac{\partial \zeta}{\partial x_1} (\overline{v_1})_{\zeta} - \frac{\partial \zeta}{\partial x_2} (\overline{v_2})_{\zeta}$$

Combining with (46) and (50), one obtains

$$(53) \quad \frac{\partial \zeta}{\partial t} + \frac{\partial U}{\partial x_1} + \frac{\partial V}{\partial x_2} = 0 .$$

Apart from the pressure terms in (48) and (49) and the source, migration and interaction terms in (51), the terms in the right-hand side of these equation represent respectively :

(i) Mean Horizontal Advection

$$\frac{\partial}{\partial x_1} \overline{v_1 v_1} + \frac{\partial}{\partial x_2} \overline{v_2 v_1} \quad \text{in (48)}$$

$$\frac{\partial}{\partial x_1} \overline{v_2 v_1} + \frac{\partial}{\partial x_2} \overline{v_2 v_2} \quad \text{in (49)}$$

$$\frac{\partial}{\partial x_1} \overline{\rho_{\alpha} v_1} + \frac{\partial}{\partial x_2} \overline{\rho_{\alpha} v_2} \quad \text{in (51)}$$

These terms are generally neglected or approximated by (e.g. Wolff, Hansen and Joseph, 1970)

$$\frac{\partial}{\partial x_1} R_{\alpha} U + \frac{\partial}{\partial x_2} R_{\alpha} V$$

and similar expressions for the advection of momentum.

There is no real ground for this simplification except when these terms are sufficiently small that it doesn't matter whether they are neglected or incorporated in one form or another.

(ii) Mean Horizontal Mixing

$$\frac{\partial}{\partial x_1} \widehat{v_1 v_1} + \frac{\partial}{\partial x_2} \widehat{v_2 v_1} \quad \text{in (48)}$$

$$\frac{\partial}{\partial x_1} \widehat{v_2 v_1} + \frac{\partial}{\partial x_2} \widehat{v_2 v_2} \quad \text{in (49)}$$

$$\frac{\partial}{\partial x_1} \widehat{\rho_{\alpha} v_1} + \frac{\partial}{\partial x_2} \widehat{\rho_{\alpha} v_2} \quad \text{in (51)}$$

These terms may be expressed in a simpler form by introducing eddy viscosities v_1 , v_2 and eddy diffusivities λ_1 , λ_2 (e.g. Bowden 1966) such that :

$$(54) \quad \frac{\partial}{\partial x_1} \overline{\hat{v}_1 \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{v}_2 \hat{v}_1} = \frac{\partial}{\partial x_1} (v_1 \frac{\partial U}{\partial x_1}) + \frac{\partial}{\partial x_2} (v_2 \frac{\partial U}{\partial x_2})$$

$$(55) \quad \frac{\partial}{\partial x_1} \overline{\hat{v}_2 \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{v}_2 \hat{v}_2} = \frac{\partial}{\partial x_1} (v_1 \frac{\partial V}{\partial x_1}) + \frac{\partial}{\partial x_2} (v_2 \frac{\partial V}{\partial x_2})$$

$$(56) \quad \frac{\partial}{\partial x_1} \overline{\hat{\rho}_\alpha \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{\rho}_\alpha \hat{v}_2} = \frac{\partial}{\partial x_1} (\lambda_1 \frac{\partial R_\alpha}{\partial x_1}) + \frac{\partial}{\partial x_2} (\lambda_2 \frac{\partial R_\alpha}{\partial x_2})$$

(iii) the boundary interaction terms

$$\left[\overline{v_3 v_1} + \overline{\hat{v}_3 \hat{v}_1} \right]_{-h}^{\zeta} \quad \text{in (48)}$$

$$\left[\overline{v_3 v_2} + \overline{\hat{v}_3 \hat{v}_2} \right]_{-h}^{\zeta} \quad \text{in (49)}$$

$$\left[\overline{\rho_\alpha v_3} + \overline{\hat{\rho}_\alpha \hat{v}_3} + \overline{m_{\alpha,3}} \right]_{-h}^{\zeta} \quad \text{in (51)}$$

The first two are generally approximated by introducing the concept of surface stresses (due to wind) and bottom stresses (e.g. Groen and Groves, 1966). The third one - which actually accounts for bottom and air-sea interactions - is generally not taken into account except, in a very crude way, by summarizing the combined effect of this term and I_α on the model of radioactive decay by a term $k R_\alpha$ (k positive or negative).

The surface and bottom stresses are generally denoted τ_s and τ_b . If a similar notation is used for the boundary interaction term in (51) (still to be determined), one may write :

$$(57) \quad - \left[\overline{v_3 v_1} + \overline{\hat{v}_3 \hat{v}_1} \right]_{-h}^{\zeta} = \tau_{s1} - \tau_{b1}$$

$$(58) \quad - \left[\overline{v_3 v_2} + \overline{\hat{v}_3 \hat{v}_2} \right]_{-h}^{\zeta} = \tau_{s2} - \tau_{b2}$$

$$(59) \quad - \left[\overline{\rho_\alpha v_3} + \overline{\hat{\rho}_\alpha \hat{v}_3} + \overline{m_{\alpha,3}} \right]_{-h}^{\zeta} = \tau_{s\alpha} - \tau_{b\alpha}$$

7.- Discussion

Eq. (48), (49), (51) and (53) form a closed system for the variables U , V , ζ and R_α . This system cannot be solved however without the specification, in terms of these variables, of (i) the advection terms, (ii) the horizontal mixing terms, (iii) the boundary interaction terms, (iv) the internal interaction terms I_α , (v) the migration terms M_α .

The criticisms one can make of the previous models (e.g. Wolff, Hansen and Joseph, 1970) are the following ones

(i) the advection terms are either neglected or replaced by an approximation which has no real justification;

(ii) the horizontal mixing terms are approximated with the help of eddy viscosities and diffusivities but very little effort is made to understand better and predict more accurately these parameters. Introduced in the scope of the theory of turbulence, they are now being extensively used to account for larger scale erratic motions which are not "properly" turbulent. Experimental and theoretical progresses on this subject are not sufficiently incorporated in the models;

(iii) the boundary interaction terms are usually approximated with more concern for the simplification of the equations than for the adequate representation of the phenomenon;

(iv) the bottom and air-sea interaction terms and the internal interaction terms are either ignored or so crudely approximated that it is difficult to regard the existing models as anything more than simple hydrodynamical models with little bearing on pollution;

(v) the migration terms are nowhere mentioned.

The present model has the merit of leaving as little as possible in the shadow but the critical discussion above also points out to several aspects of it which require further study.

Progress here is difficult because it relies on successful incursions into Chemistry, Biology, Sedimentation Analysis, Fishery Predictions and Air-Sea Interactions.

The explicit form of m_α and $P_{\alpha\beta}$ could in principle be determined from physical chemistry, sedimentation theory, biochemistry, etc.

[analysed along the line of irreversible thermodynamics (e.g. De Groot and Mazur, 1962; Fujita, 1962)] fisheries observations on animal's migrations and rivalry of species, etc., but again there are so many chemical compounds and biological species in the sea and there are still so many unknowns, especially in the field of biochemical interactions, that the calculation would be both irksome and very little reliable.

However it should not be difficult to determine experimentally the form of the resulting migration and interaction terms m_α and $P_{\alpha\beta}$. By the introduction of the concepts of phase and element concentration per phase, the number of variables is greatly reduced and the parameters to be measured are amenable to experiments^(*).

It should be noted however that the enormous simplification brought by the model does not exclude the possibility of using its predictions for control and monitoring of the sea.

[Let us suppose for instance that one is concerned with the effect of mercury on shellfish. One of the generalized state variables, say ρ_α , is taken as "constituent mercury in phase shellfish". The other state variables are defined in order to form a closed system with ρ_α . They include at least mercury in phases which may interact with phase shellfish (say mercury in solution, ...). Knowing the amount and location of mercury release and its repartition among the different phases (i.e. how much mercury is incorporated into the sea in chemical substances which dissolve or remain in suspension, etc., and where and when the releases take place) and knowing (after eventually an experimental survey) the boundary conditions (i.e. the concentrations, ρ_α on the boundary of the sea region under examination), one can predict by the model the concentration of mercury in shellfish as a function of time and space and predict when and where the critical concentration - whose definition is answerable to other, medical or legal, studies - will be reached.]

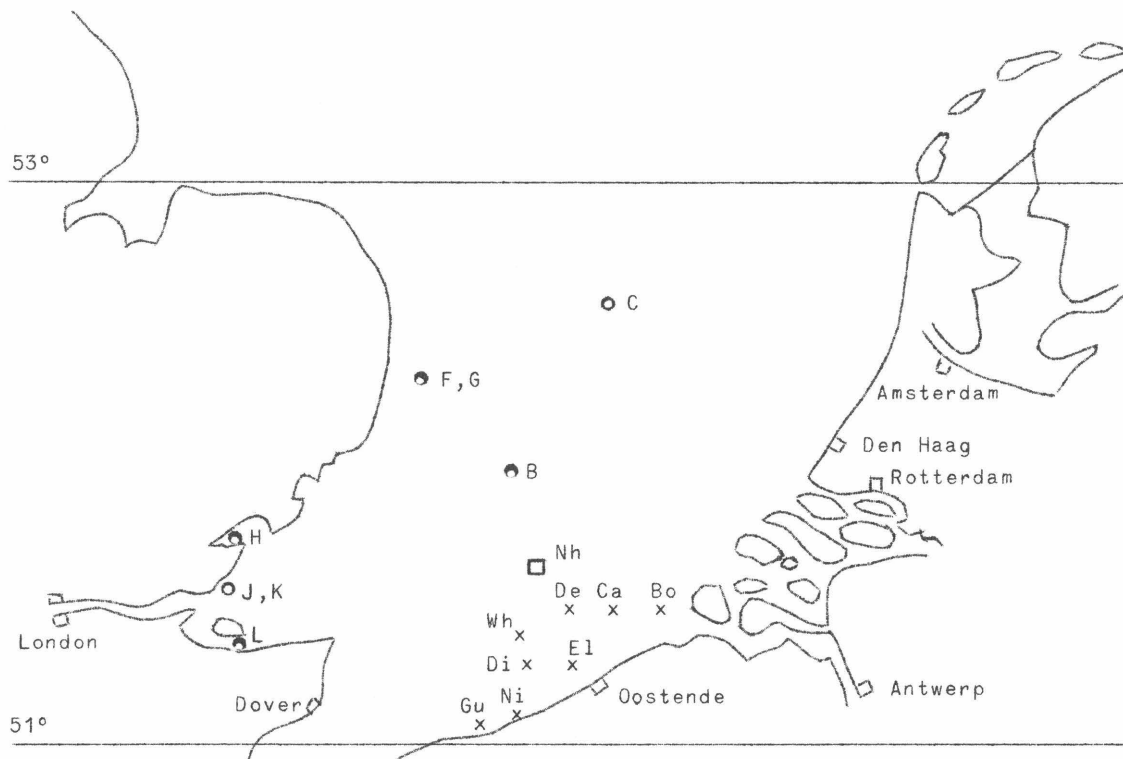
(*) Note that the system of dynamical equations can always be closed at any order by excluding a phase for which the terms in the equations are too little known (say migration of fish) and taking into account its interaction with other phases by some term of global decay or increase whose form is easier to determine experimentally.

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Appendix I

Test region under investigation by the Belgian National Program



● Location of ICES experiments on dispersion

x Location of measurements made in the scope of the Belgian National Program during a first experimental cruise

Appendix II

University departments participating in the program

Professeur A. BOEYE,
Laboratorium voor Microbiologie,
Farmaceutisch Instituut,
Vrije Universiteit te Brussel,
P. Hegerlaan,
1050 BRUSSEL.

Professeur J. BOUILLON,
Laboratoire d'Anatomie comparée,
Faculté des Sciences,
Vrije Universiteit te Brussel,
Avenue F. Roosevelt, 50,
1050 BRUXELLES.

Professeur CAPART,
Institut royal des Sciences naturelles,
Rue Vautier, 31,
1050 BRUXELLES.

Professeur L. DE CONNINCK,
Instituut voor Dierkunde,
Laboratorium voor Morfologie en Systematiek,
Rijke Universiteit te Gent,
Ledeganckstraat, 35,
9000 GENT.

Professeur A. DISTECHE,
Institut de Biologie générale,
Université de Liège,
Quai Van Beneden, 22,
4000 LIEGE.

Professeur ELSKENS,
Analytische sheikunde met. en Toeg-Wetenschappen,
Vrije Universiteit te Brussel,
Avenue F. Roosevelt, 50,
1050 BRUXELLES.

Professeur GODEAU,
Laboratoire de Morphologie et d'Ecologie animales,
Quai Van Beneden, 22,
4000 LIEGE.

Professeur GULLENTOPS,
Geologie en Sedimentologie Laboratorium,
Katholieke Universiteit te Leuven,
Naamsestraat, 59,
3000 LEUVEN.

Professeur LOUIS,
Botanische Instituut,
Katholieke Universiteit te Leuven,
Naamsestraat, 59,
3000 LEUVEN.

Professeur Jacques C.J. NIHOUL,
Mécanique des Fluides géophysiques,
Institut de Mathématique,
Université de Liège,
Avenue des Tilleuls, 15,
4000 LIEGE.

Dr. Guido PERSOONE,
Laboratorium voor Oecologie,
Ledeganckstraat, 35,
9000 GENT.

Professeur POLK,
Laboratorium voor Systematiek en Oecologie,
Vrije Universiteit te Brussel,
P. Hegerlaan,
1050 BRUSSEL.

Professeur WOLLAST,
Laboratoire de Géologie et de Sédimentologie,
Université libre de Bruxelles,
Avenue F. Roosevelt, 50,
1050 BRUXELLES.