

I.- Mathematical Model

The presence of many strongly interdependent variables makes ecosystems difficult to describe. The simple collection of data and their descriptive ordering are such formidable tasks that one has often ignored the need for doing more than this.

The present alarming state of ecological problems, however, calls for a more thorough understanding and a more rational and strict control of the environment.

Monitoring, control and management are achievable only if, for a selected number of representative variables, one can *predict evolution* and, within appropriate constraints and tolerances, one can find, by *optimization*, the necessary compromises between the requirements of increasing industrialization and affluent society and the necessity to preserve the valuable natural resources.

To predict the evolution of the selected variables, one must have some modelled idea of their behaviour.

A model can be of many sorts. It can be a fairly literal model like a mechanical model demonstrating the possible motions of an animal's limb; it can be a more elaborate physical model operating in quite another energy sphere as an electrical network simulating dynamical interactions in the food chain. It can also be a *mathematical model*.

The mathematical model is the ultimate goal. Indeed, if several distinct physical processes can be used to simulate the same phenomenon, it is because fundamentally, they are described by the same equations and that the *same* equations (submitted to the *same* boundary and initial conditions) yield the *same* solution independently of the particular significance of the variable, whether it represents an electric potential, a stream function, a temperature ...

Hence one mathematical model incorporates all the equivalent physical models. It is appropriate not only for analogue computation and simulation but also for analytical and numerical analysis.

1.- Construction of a mathematical model

1.1.- State variables and control parameters

The first step in constructing a mathematical model is the definition of a *limited number of representative state variables*. There must be sufficiently few of them for their evolution equations to be amenable to analysis but also sufficiently many of them to describe adequately the system's behavior. State variables should not be confused with *control parameters*. These are additional parameters which influence the evolution of the system (hence appear in the evolution equations) but for which no specific evolution equations are written; either because they are determined by a separate model or sufficiently known already or because the additional equations would jeopardize the model by their difficulty, their dubiousness or simply by increasing the system beyond computers' ability. Atmospheric conditions, intensity of light at the sea surface are control parameters, for instance, and several more are also involved in the coefficients of (chemical and biochemical) interactions.

It is inherent in the nature of models that experimental data should be needed to ascertain the values of parameters. The restriction of the number of state variables to be studied (i.e. the closure of the system of evolution equations) necessarily relegates to the parameters' group several which would be state variables in a perfect but unpractical model and which one prefers to evaluate separately by sideways theoretical or experimental reflection. On the other hand, the expression of interaction terms in analytical form always involves some kind of approximation and introduces empirical coefficients.

Examples of such control parameters in models of plankton production are for instance transparency of water [Riley, Stommel and Bumpus (1949)], coefficient of mixing accross the thermocline (Steele, 1958), etc.

In addition to the hydrodynamical and thermodynamical variables, the state variables are typically densities (mass of a chemical substance per unit volume, specific biomass, concentration of a pollutant at one stage of the food chain, ...).

1.2.- Evolution equations

The state variables are governed by a system of evolution equations which may be algebraic or differential. They express the complete local budget of mass, momentum, energy, species concentrations, etc.

The diagram shown in figure 1 recapitulates that the state variables may change in time or in space as a result of releases (from external sources) or withdrawing (to external sinks), internal interactions and displacement of material induced by sea motion or migration (for instance sedimenting particles have a vertical migration through the water).

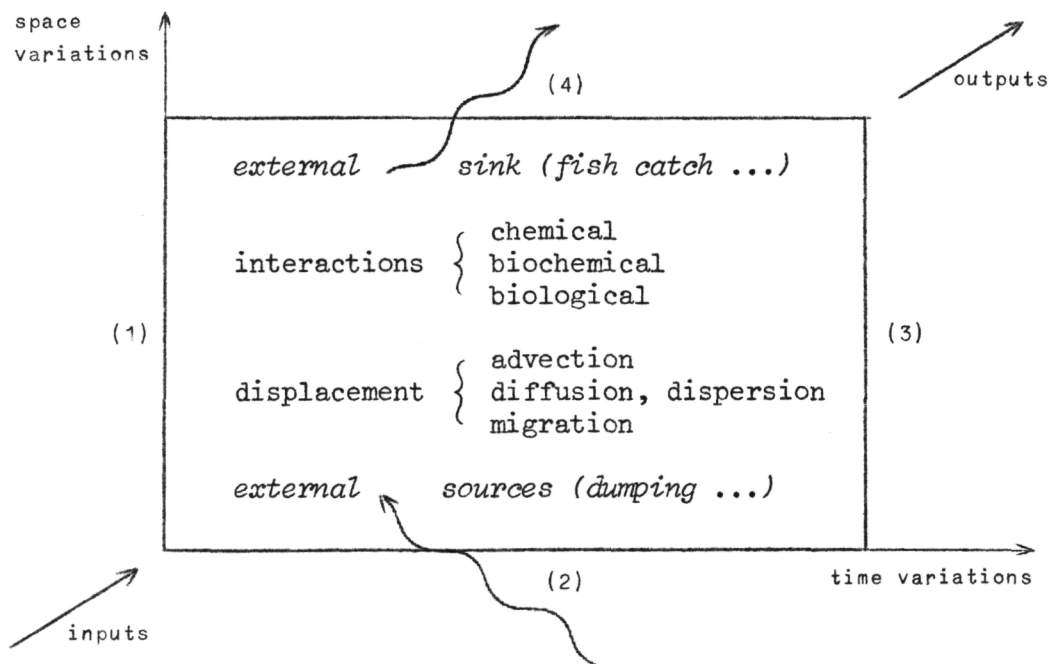


fig. 1.- Diagram of the marine system.

1.3.- Initial and boundary conditions

The evolution equations must be solved subject to given initial and boundary conditions.

The solution is usually obtained by numerical techniques which imply at one stage or another a discretization in space and time replacing the region under study by a numerical grid of points⁽¹⁾.

(1) For a clear introduction and a critical review of numerical methods adapted to mathematical models of the type discussed here, the reader is referred to the excellent paper by Emmons (1970).

This grid is adapted in each problem to the phenomenon under investigation and the mathematical method used and the mesh size is chosen from the consideration of the length and time scale of the former and the stability of the latter. There is thus an infinite variety of numerical grids for any mathematical model. These adaptable grids should not be confused with experimental grids of points where samples are taken to determine some initial state of the region or check some results of the model, in most cases, with respect to a particular phenomenon.

One example of numerical grid is shown in figure 2. The grid covers the Southern Bight and, for the simplicity of currents' calculation, extends to the English coast. Experimental surveys by the Belgian ships are however limited to the eastern part of the Southern Bight and completed by British data in the western part. Cross signs \times indicate points where samples were taken and analysed during the 1971 cruises. Whenever possible the samples were taken simultaneously by three ships anchored at the vertices of a small triangle centered at the sampling point; thus providing information on the spatial variations of the observations. For the same reason, one additional cruise took samples at intermediate points (situated half way on the mesh sides).

The meshes in front of the Belgian coast are covered by a finer grid (not shown in the figure) both for numerical calculation of currents and experimental surveys of the state of pollution.

Boundary conditions are provided by larger scale models, charts or measurements with the collaboration of neighbouring countries and in particular England, Germany, Holland, France and Danemark.

The experimental surveys have two main objectives :

- (i) determine the actual state of pollution and thus feed the model with initial conditions,
- (ii) estimate the control parameters and thus determine the form of the interaction terms appearing in the model.

Once these are determined with sufficient accuracy the model is able to predict the subsequent evolution of the system taking into account eventual changes in the boundary conditions and accidental or intentional releases of pollutants.

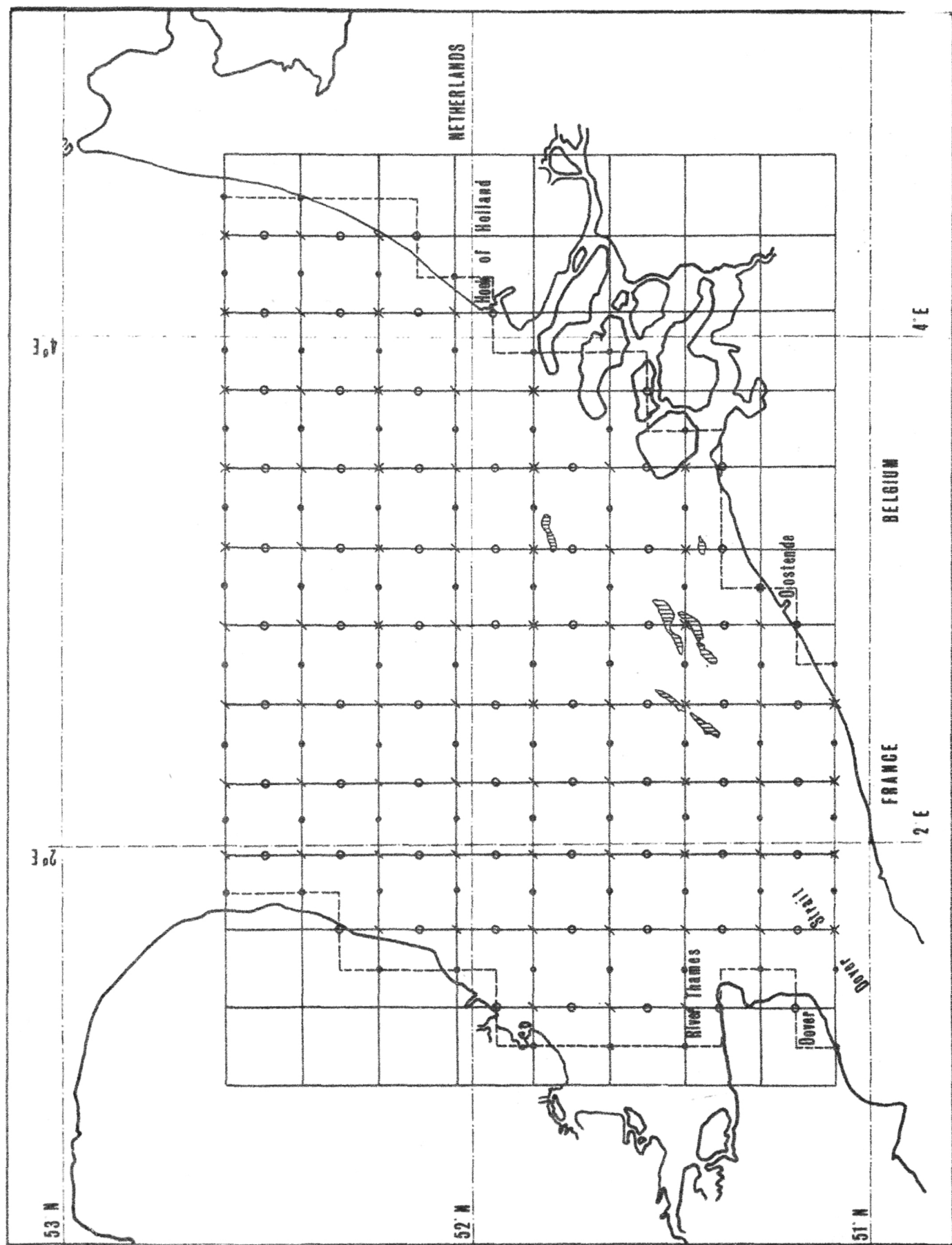


FIG. 2

The results presented in the present report must therefore be regarded as much more than an inventory as the mathematical model gives the computer the means to extrapolate and interpolate between sampling points and simulate the dynamics of the marine system.

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 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 macromolecules 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 $\rho_i(x,t)$ 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 utilisable 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⁽¹⁾.

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 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

(1) 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 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

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

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

(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 ($\alpha = 1, \dots, n+\varphi$), one may write (12) in the form

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

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

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

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

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

where $\mathbf{\Omega}$ 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 figure 2), 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 (fig. 3)].

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.

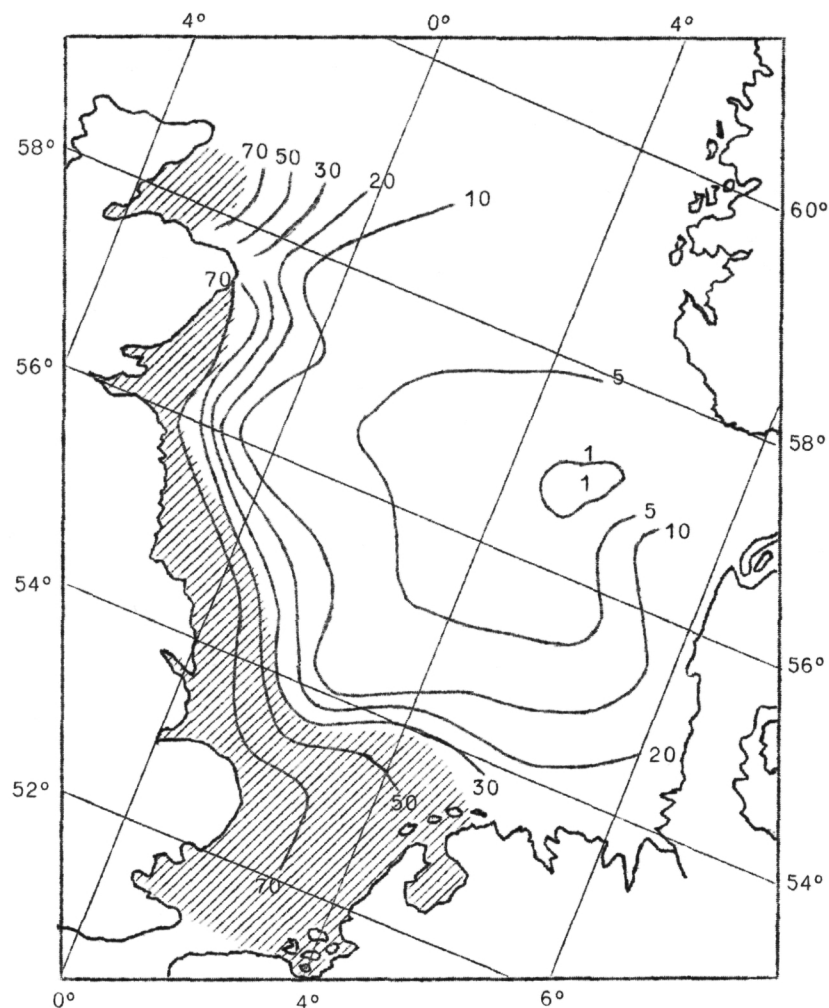


fig. 3.- Distribution of thickness of the boundary layer in the North Sea, m.;
The area where the mixing layer depth extends to the bottom of the
sea is shown by shading (reproduced from Kraav, 1969).

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 signification 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 time 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) :

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

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

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

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

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 $\boldsymbol{\Omega}$. 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 National 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 f . 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 Ω 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

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

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

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 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 $\overline{m_{\alpha}}$ 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 :

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

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

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

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

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

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

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

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

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

$$\frac{\partial}{\partial x_1} \overline{\hat{v}_1 \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{v}_2 \hat{v}_1} \quad \text{in (48)}$$

$$\frac{\partial}{\partial x_1} \overline{\hat{v}_2 \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{v}_2 \hat{v}_2} \quad \text{in (49)}$$

$$\frac{\partial}{\partial x_1} \overline{\hat{\rho}_{\alpha} \hat{v}_1} + \frac{\partial}{\partial x_2} \overline{\hat{\rho}_{\alpha} \hat{v}_2} \quad \text{in (51)}$$

These terms may be expressed in a simpler form by introducing eddy viscosities ν_1 , ν_2 and eddy diffusivities λ_1 , λ_2 (e.g. Bowden 1966) such that :

$$(54) \quad \overline{\frac{\partial}{\partial x_1} \hat{v}_1 \hat{v}_1} + \overline{\frac{\partial}{\partial x_2} \hat{v}_2 \hat{v}_1} = \frac{\partial}{\partial x_1} (\nu_1 \frac{\partial U}{\partial x_1}) + \frac{\partial}{\partial x_2} (\nu_2 \frac{\partial U}{\partial x_2})$$

$$(55) \quad \overline{\frac{\partial}{\partial x_1} \hat{v}_2 \hat{v}_1} + \overline{\frac{\partial}{\partial x_2} \hat{v}_2 \hat{v}_2} = \frac{\partial}{\partial x_1} (\nu_1 \frac{\partial V}{\partial x_1}) + \frac{\partial}{\partial x_2} (\nu_2 \frac{\partial V}{\partial x_2})$$

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

(iii) the boundary interaction terms

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

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

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

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 summerizing 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 :

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

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

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

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⁽¹⁾.

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.]

(1) 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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