

Marine Ecological Geography

Theory and Experience

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1. Auflage 2011. Buch. xxvi, 434 S. Hardcover

ISBN 978 3 642 17443 8

Format (B x L): 15,5 x 23,5 cm

Gewicht: 931 g

[Weitere Fachgebiete > Geologie, Geographie, Klima, Umwelt > Geologie > Marine Geologie, Ozeanographie](#)

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Chapter 2

Mathematical Modeling of Marine Ecosystems: Geographic and Ecological Aspects

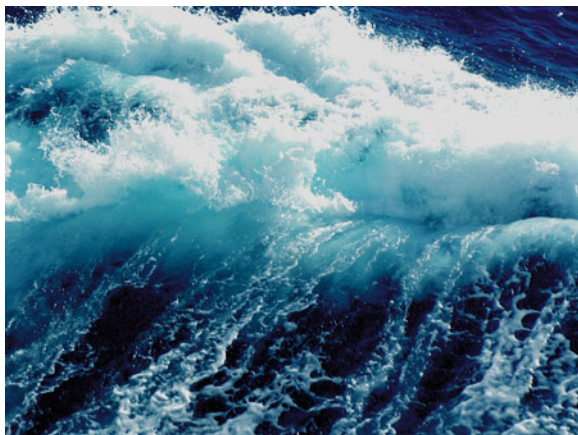
Owing to efforts of the classics of modern natural science, during the history of its development the qualitative model of the outside world was formed. So, V.I. Vernadsky laid the basis for the doctrine about living matter and marine geochemistry (Vernadsky 1923, 1934), A.P. Vinogradov started to study a chemical composition of microorganisms (Vinogradov 1935), N.M. Knipovich was the pioneer of fishery research of the seas and brackish waters (Knipovich 1938), S.V. Bruevich developed the analytical methods of marine hydrochemical investigations and formulated the fundamentals of hydrochemistry, biohydrochemistry, and chemical dynamics of the seas (Bruevich 1933, 1978), L.A. Zenkevich studied fauna and bioproductivity of sea waters (Zenkevich 1947), A.B. Skopintsev started the investigations of nutrients and organic matter in water reservoirs and streams (Skopintsev 1950), G.G. Vinberg considered the problems of biological productivity formation in the seas (Vinberg 1960).

These works have served as the methodological and theoretical basis of regular investigations on the ecological state of marine ecosystems, hydrochemical features of formation of fishery resources and bioproductivity of natural waters; regularities of development of chemical and biological processes of organic matter transformation and disintegration; mechanisms of nutrient substrate regeneration in connection with study of the cycle of matter conditions in biosphere (Leonov 1999) which started in the second half of the twentieth century worldwide, and also methods of systematization and analysis of the obtained information (Fashchuk 1997; Fashchuk et al. 1997).

2.1 Types of Mathematical Models of Marine Ecosystems

According to the known mathematician, academician I.M. Yaglom: “*The maturity level of any discipline is determined to a great extent by degree of the use of*

Photo 2.1 Today mathematical models of marine ecosystems, together with field observations at sea, have become a basis of scientific understanding of ocean nature. (Atlantic Ocean by J. Gangnus)



mathematical apparatus in it, content-richness of “mathematical models” inherent in the discipline and associated deductive conclusions...” (Photo 2.1).

By the second half of the twentieth century marine ecology “has matured” as a science so much that mathematical modeling of marine ecosystem state became an independent scientific direction in natural science. Within its framework the World Ocean is considered as a complex dynamic system of physical, chemical, biological, geological and other processes. The development of computer aids and apparatus of applied mathematics resulted in the intensive building of mathematical models of marine ecosystems which allowed to systematize the obtained knowledge in various fields of marine science for the purpose of forecasting and management of marine basin state.

There are several types of mathematical models of marine ecosystems. *Depending on the purposes of modeling*, they can be divided into *simulation models* confined to specific basins or regions and developed for specific purposes, and *qualitative*, theoretical models used for elucidation of the general regularities of process development and their analysis. In simulation models scientists aim to consider the maximum number of variables, while in qualitative models only the most important characteristics are counted. Therefore, the main problem for them is associated with a choice of priority variables (Smith 1976).

By method of realization, the models are divided into *deterministic* models which use functional dependences for description of the relationships among variables, and *stochastic* models based on statistical relationships. The former are used more often because they permit infinite set of components and do not consider random fluctuations of environmental parameters. They are convenient in terms of interpretation of the results (Aizatulín and Lebedev 1977). There are also *stochastic and deterministic* models in which at the first stage the solution is sought deterministically, and then, by means of Monte-Carlo technique the variability of various parameters is modeled and response of the solution to this variability is studied.

By method of representation of the phenomenon spatial structure models are separated into *point* (parameters are concentrated in one point), *reservoir*

(distribution of parameters is limited by borders—box walls), and *continuous* (real spatial distribution of parameters is taken) models.

In point model the characteristics are integrated by whole volume of the considered area. In reservoir model each element of spatial area described by the space-averaged parameters (river section, ocean layer), is called *reservoir* (box), and in state space (food link, suspension, dissolved matter) it is called *block*. Transfer of properties from one reservoir to another is conventionally called *flux*, and that from one block to another—*transition* (Niul 1978).

In reservoir models the considered volume is divided into separate reservoirs, for each of which only the reservoir—averaged concentration of substance is considered and the point model is constructed. It allows to account with some degree of certainty the spatial heterogeneity and to define any structural objects. The main advantage of reservoir models is simplicity of their realization, though in the real nature it is difficult to identify the representative system of reservoirs and to attribute the appropriate parameter values to them. Moreover, these models are sensitive to small fluctuations of parameters (Kagan and Ryabchenko 1978).

In continuous models there is no spatial averaging, and at every instant the solution is represented by the smooth curve (or field) of parameter distribution. These models are usually reduced to solution of the simplified thermodynamics differential system (two motion equations, static equation, equation of continuity of incompressible fluid, heat and salt-transfer equation, equation of state), and equations for the studied characteristics similar to equations of heat and salt balance.

When implementing the problems of modeling of chemical and biological characteristics, the solution of system of thermohydrodynamics equations (simulated fields of current velocity, temperature, salinity) is substituted in the parameter—transfer equations. Thus, the chance to study their transformation caused by chemical, biological, and biochemical processes, together with their mass transfer, appears (Aizatulin 1974).

The choice of a particular model type depends on the problem facing the researcher. Thereupon, sometimes the preference is given not to complex but primitive models, because of their ability to answer the specific questions.

2.2 Objectives of Mathematical Modeling in Marine Ecology

The development of methods of oceanological investigations including all fields of marine science (physics, chemistry, biology, geology) and interdisciplinary sciences—hydrobiology, biophysics, biochemistry, biogeo—and hydrochemistry, has determined the accumulation of the huge factual material reflecting various aspects of marine ecosystem functioning during the 1930s–1960s (Photo 2.2). As a result, the necessity to systematize and generalize the obtained data, formalize the existing ideas in the form of mathematical models to forecast the dynamics of natural water properties by main chemical and biological parameters, has appeared.

Photo 2.2 Changes in character of water consumption occurred in the 1940s–1960s, growth of waste water discharge volumes put ecologists before necessity to study the prospects of marine and lake ecosystems variability with use of mathematical models. (Atlantic Ocean by Yu.Maslyaev—top; Balaton Lake by [www.hungarystartshere.com]—bottom))



At the first stages of such systematization in the 1920s–1930s, the integral indicators of matter transformation in natural waters and water basin state were studied, with use of the models reproducing (*the dissolved oxygen regime, depending on content of labile organic matter (OM) in units of chemical or biochemical oxygen demand*) (COD and BOD, respectively). Moreover, the attention was given to *the trophic interpopulation relationships of organisms* (e.g., “predator–prey”).

Among the chemical and biological processes developing in marine environment, the special attention under modeling is given to the mechanisms determining transformation and biogeochemical cyclicity of elements entering into the composition of living matter (*C, N, P, S, Si*). Thus, at the first stages of modeling the attention was drawn to *rates of decrease in concentration of chemicals, utilization and consecutive transformations of substrata by organism community, and rates and mechanism of transformation of chemicals*. As a result, the following important practical problems have been solved:

- (1) The quantitative information on spatiotemporal changes in chemical and biological characteristics of marine ecosystem, depending on intensity of

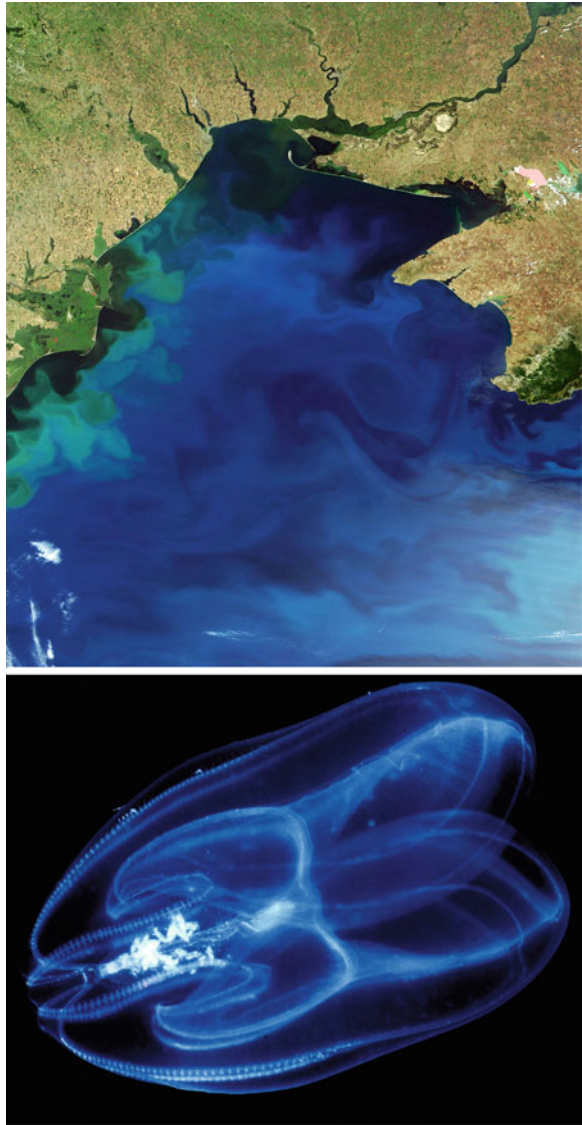
impact of environmental factors (temperature, light conditions, transparency, water regime, nutrient load) on it, was obtained.

- (2) Pollution assimilative capacity of marine ecosystem was assessed, and recommendations on creation of the most effective conditions for this process were developed.
- (3) The matter balance in natural waters with account of exchange fluxes at the water-atmosphere and water-bottom interfaces, supply of matter with waters of tributaries and atmospheric precipitation, and losses of matter at their export by water masses from the basin, was drawn up.
- (4) A role of natural and anthropogenic processes in nutrient cycle of marine ecosystems was established. On this basis the measures on water resources conservation were developed; natural water reserves and potential of their quality were estimated; methods of pollution control and mechanisms of water purification were defined.
- (5) The nutrient stock in natural waters and its spatial and temporal variability influenced by processes of their consumption by planktonic organisms and regeneration under the OM destruction was estimated. The bases of primary production in basins and their biological productivity at the higher trophic levels were studied.
- (6) The behaviour and distribution of populations, communities of organisms in marine environment were studied; the features of vertical heterogeneity and horizontal patchiness of hydrobionts distribution were reproduced (Vinberg and Anisimov 1966); the role of predators in regulation of photosynthetic activity of phytoplankton was defined (Vinberg and Anisimov 1969).
- (7) The vertical structure of microorganism communities—biomass of various phyto- and zooplankton groups, detritus, in tropical zone of the ocean (Vinogradov et al. 1972), in pelagial of the Sea of Japan (Menshutkin et al. 1974) an Peruvian upwelling (Fleishman and Krapivin 1974) was studied.
- (8) The reasons of intensification (outbursts) of biological communities development (Petrovsky et al. 1998), invasion of new species in ecosystems (Keondzhyan et al. 1990), and blooming of certain alga groups were investigated (Photo 2.3).

Now the relevant objectives of mathematical modeling of biogeochemical processes in marine ecosystems are: study of chemical and biological process rates, cycle of matter in natural waters, conditions of biological productivity formation in basins, estimation of balance of organogenic element compounds in aquatic environment, and the complex research on processes of chemical exchange at interfaces “water–atmosphere,” “water–bottom” and chemical and biological transformation of matter in aquatic environment and bottom sediments.

When studying a complex of hydrodynamic processes developing in marine environment, the great attention under mathematical modeling of marine ecosystems state is given to problems of horizontal and vertical transfer of pollutants, establishment of conditions of formation and disintegration of marine organism (phyto- and zooplankton, pelagic and bottom commercial objects) concentrations, redistribution of life by depth (Menshutkin and Finenko 1975).

Photo 2.3 Development of “red tides”, outbursts of phytoplankton blooming, in marine basins ((*top*)—Black Sea NW shelf, by [veimages.gsfc.nasa.gov]) and populations of new invading species ((*bottom*)—*Mnemiopsis Leidy*, by [www.people.bu.edu]) is one of the major spheres of “interests” of marine ecosystems modeling today



2.3 Models of Biochemical Processes in Marine Ecosystems

According to existent ideas of character of ecological data generalization, there is a predominance of mathematical analysis of information at its first stage, modeling at the second stage, and development of the mathematical theory at the third stage. By the 1980s the level of mathematization of marine ecological science has corresponded to the first stage, though the first tenuous steps within the second

stage have been made yet in the beginning of the twentieth century, when Streeter–Phelps model of oxygen regime of rivers and Lotka–Volterra model of predator–prey interactions were developed, and in the world there were about 150 mathematical models of water basins and watercourses of various complexity (Aizatulin and Shamardina 1980).

More than hundred from this number have been developed for lakes and reservoirs, with a third of them created by native authors. The ecosystems of Great Lakes, Bratsk, Ivankovo, Rybinsk, Mozhaisk, Zeya, Dnieper and other reservoirs were modeled.

Thus, together with problems of basin eutrophication, estimation of energy fluxes and productivity, the questions on influence of intermittent land flooding on ecosystem, mass blooming of reservoirs were solved. The majority of these models are the point correlation—regression and point or two-reservoir models of primary production and budget of phosphorus as limiting factor and factor of eutrophication of water systems. Simulation models comprised only 10% in the total number of mathematical developments and numerical experiments.

By 1980 a large number of the developed models were used for ecosystem study of continental sources, rivers, brooks, and also intermittent water bodies and ponds as the simplest modeling objects. There were only a few models which tried to describe state of the whole marine ecosystem or its specific areas.

By the beginning of the twenty first century many simulation models capable of analytically and numerically investigating changes in the major chemical and biological characteristics, occurring in aquatic ecosystems, have been already developed in the world. Their detailed review is presented in numerous literary sources (Vavilin 1986; Dombrovsky et al. 1990; Tskhai 1995; Leonov 1999), etc.

Nevertheless, the majority of models concerning the problems of transformation of matter in marine environment under biochemical processes are the point or reservoir models. In spatial models these problems receive less attention, and emphasis is made on the analysis of spatiotemporal variability of hydrochemical and biological components of aquatic ecosystems (Fashchuk et al. 2005).

2.3.1 Formalization of Biochemical Processes in Mathematical Models

Biogeochemistry studies chemical biogenic (organogenic) elements and their mineral compounds. Among them the main elements are those composing living organisms: carbon, oxygen, phosphorus, nitrogen, sulfur, silicon and some other (Ivanenkov 1979). Moreover, micronutrient elements, among which iron and manganese are the most important, include almost all elements found in the ocean. Vernadsky (1934) defined organogenic elements as cyclic elements undergoing the reversible processes. Their cycles are reversible only in body of atoms, and part of atoms comes out of the circulation (Vernadsky 1934).

The spatial and temporal variability of nutrients participating in reversible cycle, determines two groups of processes in the ocean. The first group includes chemical and biological redox and absorption—desorption processes changing concentrations of properties in specific volume of water. The hydrophysical processes of advection and turbulence belong to the second group, responsible for transfer of chemical elements conditionally considered as passive impurity. For suspended forms of nutrients the processes of their passive settlement (sedimentation) are also of great importance. All these processes determine the dynamics of chemical substances in marine ecosystem. Moreover, the exchange processes at the atmosphere—water and ground—water interfaces are also very important in mathematical ecological modeling (Bruevich 1978).

Unlike distribution models of hydrophysical parameters of marine ecosystem state, based on solution of standard differential equation system, in biochemical models there is no such system of equations. There are only accepted methods of parametrization of modeled processes. Thus, the ratios between space and time scales of hydrophysical processes within which they are capable of affecting the formation of spatial distribution of hydrochemical and biological parameters, are enormously important. According to Monin (1982), the spatial heterogeneities are characterized by typical time scales of processes generating them (Table 2.1): *small scale* (fractions of millimeter—tens of meters)—from 10^{-3} s to tens of hours;

- *mesoscale* (hundreds of meters—kilometers)—from hours to days;
- *synoptic* (tens and first hundreds of kilometers)—from days to months;
- *global* (thousands and tens of thousands kilometers)—from years to hundreds of years.

Table 2.1 Processes affecting distribution and variability of chemical substances in the ocean (Monin 1982)

Process	Scale (sec)	Lifetime	Source
Gaseous interchange between ocean and atmosphere	10^1	Tens of seconds	Emerson (1995)
Hydrolysis of gases and processes in carbonate system	10^1	Tens of seconds	Emerson (1995)
Physiological rhythms of marine organisms	10^{5-6}	Hours—months	Rudyakov (1986)
Advective and turbulent transfer (surface waters)	10^{6-7}	Days—year	Monin et al. (1974)
Chemical and biological	10^{6-7}	Days—year	Monin et al. (1974)
Anthropogenic CO ₂	10^9	30–40 years	Gruber et al. (1996)
Oxidation of persistent aquatic humus (suspended organic matter)	10^{11}	2,000 years	Skopintsev et al. (1979)
Advective and turbulent transfer (deep waters)	10^{11}	1,000 years	Monin et al. (1974)
Sedimentation	$>10^{12}$	$>10,000$ years	Monin et al. (1974)

It is obvious that at any time scale several processes actively affect the formation of hydrochemical fields that should be taken into account, when creating the mathematical model. In the upper ocean layer where chemical and biological processes are the most important, every process is corresponded by certain characteristic time and characteristic values of component concentrations. With depth this regularity is broken. In this case, the concentrations of living organisms and organic matter decrease exponentially, while concentrations of nutrients (e.g., phosphates) grow. With that, the characteristic scales of change in concentrations of dissolved inorganic forms of nutrients and their suspended organic forms, including those in living organisms, differ by more than 4 orders of magnitude. Thus, the method of parametrization of chemical and biological processes should be connected with scales of variability in concentrations of chemical forms in the selected modeling object and spatiotemporal scale of the solved problem.

The chemical and biological processes imply a complex of processes, including the synthesis of organic matter from inorganic compounds, its transfer in trophic chain, elimination of organic and inorganic substances from living and dead organisms, autolysis of suspended material, and organic matter degradation. The process of OM synthesis and degradation proceeds under the classical Redfield stoichiometry (Redfield 1934) with account of interchange of matter among various organisms within an ecosystem.

When modeling (*nutrient uptake under the synthesis of organic matter photosynthesis*), the following statements are taken into consideration (Sergeev 1979):

- Specific rate of photosynthesis is directly proportional to phytoplankton biomass and rate of nutrient uptake;
- Average sizes of phytoplankton cells and their chemical composition are identical and constant; autotrophic growth ceases at zero values of sunlight and nutrient concentrations.

With that, the complex ambiguous dependence of photosynthetic intensity on intensity and duration of sunlight, nutrient concentrations in the environment and cell, water temperature and salinity, size and species of alga is considered (Photo 2.4).

When describing photosynthesis, the majority of ecosystem models lean on the concept of limiting factor governing the rate of this process. According to Liebig's Law formulated in 1840, the rate of photosynthesis is limited by that chemical element, for which ratio of its concentrations in the environment and marine organisms, is minimal. In 1905 Blackman expanded this law with the concept of limiting factor, and in 1911 Shalford formulated the more general principle of 1 tolerance, lying in the fact that tolerance of organism (species) was determined by both maximum and minimum of ecological factor range (Aizatulina and Shamardina 1980; Reimers 1980). When modeling marine ecosystems, one of nutrients (nitrogen, phosphorus, or more rarely silicon) is usually used as limiting factor. However unlike Liebig's Law, the concentration of limiting factor only in water but not in organisms figures in these models.

Photo 2.4 Experimental study of mysteries of photosynthesis performed by fluorocarbons (*on photo*) of phytoplankton cells seems quite difficult without mathematical modeling



When modeling *the elimination of nutrient compounds from autotrophic organisms*, their entry into marine environment in the process of breathing (inorganic compounds), exudation (loss of organic matter as a result of vital activity of marine algae which can reach 40% of net daily production), and at die-away is taken into account (Parsons et al. 1982).

When modeling *the transformation of nutrient compounds by heterotrophic organisms*, their uptake by autotrophs (phytoplankton) and formation of dead organic matter (detritus) by zooplankton (Menshutkin and Finenko 1975; Aizatulin and Leonov 1975, 1977; Leonov 1980; Fasham et al. 1990), elimination of these compounds in the process of breathing, metabolism (Sergeev 1979) and die-away of zooplankton in the form of dissolved inorganic and suspended organic matter (Shushkina 1977; Sazhin 1982; Rudyakov et al. 1984), and also at grazing of some heterotrophic organisms by others is considered.

2.3.2 Point Models

In the 1960s K. Wyrski modeled the vertical distribution of hydrochemical characteristics in marine ecosystems. In his one-dimensional model the formation of layer of oxygen minimum and phosphate maximum in intermediate waters of the ocean was investigated. The model considered biological oxygen demand and vertical turbulent exchange that allowed obtaining the good agreement with picture observed in the ocean and running numerical experiments on change in the studied characteristics under the influence of model parameters (Wyrski 1962).

In that time Watt and Hayes, based on the analysis of samples taken in the area of Halifax (Canada), have proposed the model considering three forms of phosphorus: dissolved inorganic (DIP), dissolved organic (DOP), and particulate (PP). The fitted coefficients reflected adequately the dynamics of phosphate formation in the sea even during the expedition (Watt and Hayes 1963).

In the 1970s this model has been improved by division of particulate phosphorus into 3 constituents (bacteria, zooplankton and detritus). For description of phosphorus transformation with account of bacteria and zooplankton the first-order chemical equations, equations in the form of the Michaelis–Menten scheme, and a number of other schemes of consecutive transformation of chemical forms of phosphorus were used (Aizatulin and Leonov 1975; Leonov and Aizatulin 1977).

The point non-stationary Steel's model reflects the common features of seasonal dynamics of phosphates and phytoplankton concentrations in the photic layer of the North Sea. The model considers the phosphate amount and phytoplankton biomass. For description of their dynamics in open system the seasonal variability of sunlight, mixing, sedimentation, concentration of zooplankton consuming phytoplankton as food were taken into account (Steel 1959, 1962; Steel and Frost 1977). The similar problem for the Baltic Sea was solved in more detailed model considering the seasonal transformation of nitrogen compounds. In this model, along with nitrates, nitrites, ammonium and dissolved organic nitrogen, phyto- and zooplankton were introduced also (Savchuk 1977).

The point simulation Hornberger-Spear model is devoted to study of estuary eutrophication impact on growth of benthic algae. In the model the transformation of phosphorus forms in estuary waters, sediments, phytoplankton, and benthic algae is considered. It uses the Michaelis–Menten dependences and first-order equations and accounts the influence of sunlight, temperature and phosphorus intake from external sources (with river and rain waters). The seasonal variability of *P* forms, with the estimation of contribution of various processes, is calculated (Hornberger and Spear 1980).

In 1990 the Fasham-Ducklow-McKelvie model describing seasonal dynamics of nitrogen compounds in the upper mixed ocean layer has appeared. In this model the transformation of nitrates, ammonium, the labile dissolved organic nitrogen and detritus with the participation of phyto-, zooplankton and bacteria was considered. The model became the reference standard for modeling of both the large-scale features of global biogeochemical cycles and other, faster, processes in aquatic environment (Fasham et al. 1990).

The seasonal variability of vertical hydrochemical structure was investigated with use of the Fasham's model by the example of real observational data (Fasham et al. 1993; Kawamiya et al. 1995). Further, Savchuk and Wulff (1996) studied the vertical distribution of various forms of phosphorus (phosphates, detritus), nitrogen (nitrates, ammonium, detritus), oxygen and biological characteristics (phyto- and zooplankton), with estimation of a role of various factors in formation of vertical hydrochemical structure of deep Baltic Sea, using their own model (Savchuk and Wulff 1996).

2.3.3 Box Models

In the set of models of this type initiated by Swedish scientists, the components of mass transfer are estimated by nutrient deficit in box, based on investigations of the World Ocean circulation (Bolin et al. 1983).

The Postma's box model considers the phosphorus balance in the World Ocean divided into 9 homogeneous boxes with account of the processes of consumption, regeneration, sedimentation, and exchange. Using the same model, Sarmiento et al. (1990) investigated the influence of Atlantic subtropical gyre on transport of radioactive tracers, nitrates, and oxygen that allowed them estimating the characteristics of new production by nitrates and biological oxygen demand (Sarmiento et al. 1990).

The box model was successfully applied to studying the Lake Balaton ecosystem in Hungary (Leonov 1986), dynamics of phosphorus forms, functioning conditions of some aquatic ecosystems of Finland (Varis et al. 1986; Leonov and Niemi 1989; Leonov 1989a). One of the versions of this model involving forms of nitrogen and dissolved organic matter, was used for research of the Lake Ladoga ecosystem (Leonov et al. 1991). The later model version allows estimating the transformation of main compounds of organogenic elements (carbon, nitrogen, phosphorus, oxygen) (Leonov et al. 1994). The modern model version accounts the characteristics of pollution (oil products, pesticides, heavy metals, phenols), phytoplankton production, and concentration of substances in bottom sediments (Leonov 2000). Several complex developments were used for study of the Okhotsk (Leonov and Sapozhnikov 1997; Pishchalnik and Leonov 2003) and Caspian (Leonov and Sapozhnikov 2000) Sea ecosystems. When modeling the Sea of Okhotsk, the cycles of nitrogen, phosphorus, and silicon were studied in parallel. In total, 18 blocks were considered, six of which included living organisms. The sea was divided into 8 boxes ("aquatories"), with mass transfer among them. The similar calculations were made for ecosystem of Aniva Bay on the Sakhalin shelf (Leonov and Pishchalnik 2005) and northwestern shelf of the Black Sea (Leonov and Fashchuk 2006).

It should be noted that a great contribution to studying biohydrochemistry of natural waters, developing the methods of mathematical modeling of simultaneous biological and chemical transformation of matter in marine ecosystems was made by T.A. Aizatulin. For the first time in native practice he has directed attention to formalization of cycles and mechanisms of transformation of nutrient compounds under the analysis of dynamics of hydrobiont biomass and nutrient concentrations in the sea. He proposed the chemical and kinetic apparatus describing the regeneration of mineral components of nutrients (Aizatulin 1967) and processes of transformation of organic and inorganic metabolites as an important link of the whole chemical - ecological system (Aizatulin 1974).

The models based on such chemical and kinetic approach were intended first for study of dynamics of dissolved oxygen concentration and oxidation of organic matter (Aizatulin and Leonov 1975) and joint cycles of sulfur and oxygen (Aizatulin and Leonov 1990), nitrogen and oxygen, phosphorus and oxygen,

carbon, phosphorus and oxygen (Leonov and Aizatulin 1977), nitrogen, phosphorus and oxygen (Leonov 1989b) in closed systems. In later developments the joint cycles of nutrients in their various combinations in marine environment were modeled, using from several to several tens of equations describing the dynamics of biological community, concentrations of various nutrient forms, and biomass of organisms transforming matter (Vinogradov et al. 1989; Leonov and Aizatulin 1995; Leonov and Sapozhnikov 1997; Yakushev 1998).

2.3.4 Continuous Models

In the middle of the twentieth century the large-scale meridional distribution of phosphates in the Atlantic ocean was investigated with use of the continuous model. With that, the currents were calculated by dynamic method on a $5 \times 5^\circ$ grid, in each point the difference between consumption and elimination of phosphates was compensated by their transfer due to physical processes (Riley 1951). It was the first attempt to investigate the distribution of hydrochemical characteristics in the ocean by means of mathematical modeling.

The oxygen distribution at meridional section of Atlantic ocean was studied by means of continuous two-dimensional model, in which the surface oxygen distribution and its biological consumption in water column were prescribed. The accepted scheme of circulation reflected two gyres in the Southern Hemisphere and one gyre—in the Northern Hemisphere (Bubnov and Krivilevich 1973).

To analyze oxygen regime in waters of the World ocean the integral two-dimensional scheme of the World Ocean circulation calculated on a $5 \times 5^\circ$ grid, was used. With that, the oxygen flux through the ocean surface, spatial variability of production, and oxygen consumption were considered. In this case, for construction of hydrochemical model the “prepared” scheme of water circulation was used (Ryabchenko 1977).

In last decade such approach has become dominating. In coupled models the hydrophysical representation of specific object is combined with model of biogeochemical transformation nutrients. For the Black Sea the scheme of biogeochemical sources “phytoplankton–zooplankton–dissolved organic matter–nitrates–ammonium” is used (Gregoir et al. 1997), and elements of global transport of organic matter are studied with use of the three-dimensional circulation model and simplified model of biogeochemical transformation of phosphorus (Najjar et al. 1992).

The complex simulation model of the Sea of Azov considered the problems of economic activity impact on water resources of the basin (Gorstko 1976; Bronfman 1976; Gorstko et al. 1982) (Photo 2.5). Along with biological components of various trophic levels, the model takes into consideration the concentration of nutrients as an indicator of eutrophication level of marine ecosystem. The cycle of phosphorus, nitrogen and silicon compounds with account of the processes of

Photo 2.5 In the 1970s Rostov scientists developed the first continuous complex model of the Azov Sea ecosystem (Cape Kazantip—Azov Sea in summer and winter – photo by V. Kaminsky)



their transfer, disintegration, consumption, abrasion of coast and other factors is described. The modern development of the Rostov modeling school is reflected in monograph (Matishov [2001](#)).

2.3.5 Hydroecological Model of Organogenic Element Transformation

After the analysis of existing experience in study of marine basin nature by mathematical methods (Fashchuk et al. [2005](#)), the simulation box hydroecological model of organogenic element transformation in marine environment, developed in the late twentieth century by A.V.Leonov, was chosen for solving the problems of marine ecological geography. To study the regime of oil product transformation in marine ecosystem, the chosen model, instead of *abundance and biomass* of oil oxidizing bacteria, considers *their biochemical activity*, i.e. ability to perform the cycle of processes including consumption of food substrates, elimination of microbial products, formation of detritus. The model describes the interrelated biogeochemical cycles of such elements as N and P, and also includes the

description of transformation rates of Si, dissolved organic C (DOC) and oxygen O_2 in a two-layer aquatic ecosystem. Thus, the dynamics of concentrations of DOC, O_2 , N^- , P^- , and Si-containing substances is estimated under their biotransformation and development of exchange processes at the water–air and water–bottom interfaces. The model accounts the following P, N and Si compounds: detritus P, dissolved inorganic P, organic P, organic N, ammonium N (NH_4), nitrite N (NO_2), nitrate N (NO_3), urea N and free nitrogen (N_2), inorganic Si, organic Si, detritus Si.

The biotransformation of organogenic element compounds reproduced by the model is performed by community of microorganisms: *heterotrophic bacteria (B) consume organic compounds and in the process of metabolism form a pool of inorganic substances; phytoplankton (F1, F2, and F3) utilizes inorganic substances and forms a reserve of organic substances in aquatic environment; zooplanktonic organisms (Z1 and Z2) regulate the dynamics of community organisms and through their own activity affect the development of production—destruction processes.*

Actually, the model reproduces transient processes and describes response of aquatic ecosystem to changes in environmental conditions or to change in at least one of factors considered in the model (water regime, temperature, sunlight, nutrient load). It contains 226 equations describing:

- change in concentrations of components under study;
- specific rates of organogenic substance utilization by heterotrophic bacteria, phyto- and zooplankton;
- functions and correction coefficients on temperature and sunlight intensity for constants of substrate utilization rates by hydrobionts;
- specific rates of metabolic eliminations and elimination activity of organisms;
- specific rates of organism die-away;
- total rates of change in microorganism biomass due to interaction of chemical and biological components of community under consideration;
- total rates of change in nutrient concentrations in aquatic environment and sediments;
- rates of substance supply from external sources (atmospheric precipitation, distributed sources).

When estimating the rates of change in concentrations of organogenic substances due to horizontal and vertical transport, the following is considered:

- entry of these substances into marine aquatories with tributary waters;
- replenishment of substance reserve due to vertical exchange with underlying layer;
- transport of substances from adjacent aquatories within the marine ecosystem and their loss under an export outside the ecosystem by water flow.

The block of biochemical transformation of oil products by oil-oxidizing bacteria includes 10 equations describing:

- change in concentrations of oil products and biomass of oil oxidizing bacteria;
- total and separate utilization of substrates (oil products and DOC) by oil oxidizing bacteria;
- activity function of oil oxidizing bacteria, depending on temperature;
- specific rates of elimination of metabolic products and die-away of oxidizing bacterium biomass.

Thus, the model describes the intraannual dynamics of chemical and biological indicators of aquatic environment state, instantaneous rates of the processes responsible for change in concentration of substances, internal and external substance flows in various parts of the investigated ecosystem, and turnover time of all chemical and biological components considered in model (Leonov 2008).

2.4 Hydrodynamic Models of Marine Environment

Time scales of biochemical transformation of oil products in marine environment amount months, years, and in some cases decades. At the same time, having appeared in water, oil spill undergoes the shorter-term transformations (hours, days) caused by synoptic variability of hydrometeorological and hydrodynamic conditions in the basin and over its aquatory.

In the late twentieth century, owing to use of advanced measuring equipment and adequate space–time measuring strategy, the qualitatively new data on structure, synoptic and mesoscale variability of hydrophysical patterns in the World Ocean have been obtained. The real dynamic state of marine aquatories is determined by such processes as synoptic eddies, fronts, meanders of currents, shelf wind currents. Herewith, the progress in weather forecast reached by modern atmospheric models, allows using the modeling parameters of surface layer in dynamic models of the ocean in real time mode (unlike prescription of climatic atmospheric fields practiced in the 1960s–1980s). Thus, now there are prerequisites for creation of joint dynamic models of ocean and atmosphere and their coupling, capable of reproducing the state of marine environment hydrodynamics and, consequently, investigating dynamics of its oil and chemical pollution at synoptic time scales.

Over the last thirty years various aspects of the problem of accidental oil spills in the sea are discussed at annual international conferences “Oil Spill Conference” held in the USA. During the first decade after sensational wreck of tanker *Torrey Canyon* a great attention was given to study of physical and chemical oil transformation. Today it is uncontroversial that, when investigating oil behavior in the sea, first of all it is necessary to consider the following processes:

- surface oil transport under the combined effects of wind, waves and currents;
- surface oil spreading;
- turbulent diffusion of oil at sea surface and in water column;
- oil evaporation under natural conditions;

Photo 2.6 Along with processes of transport, spreading, dissolution, and evaporation of oil, hydrodynamic models describe its emulsification—formation of “chocolate mousse” [www.inapcache.boston.com]



- oil penetration in water column from the air-sea interface as droplets;
- formation of water-in-oil emulsion, “chocolate mousse” (Photo 2.6).

Thus, the adequacy of physical and mathematical models of oil spreading after accidental spill depends on the level of our knowledge of hydrophysical, hydrochemical and hydrobiological parameter distribution in specific place and time. At present, degree of exploration of the mentioned processes is different. For some of them the mathematical models corresponding to the present level of physical ideas have been already formulated, for others only empirical parameterizations or qualitative representations exist.

Nevertheless, the Oil Spill Models are created and used for various calculations and forecasts worldwide. Currently the most known models include: American OILMAP-WOSM (Worldwide Oil Spill Model) (Anderson et al. 1995), ADIOS (Automated Data Inquiry for Oil Spills), and GNOME (General NOAA Oil Modelling Environment); American–Norwegian COZOIL (Coastal Zone Oil Spill Model) (Hewlett and Jayko 1998); British OSIS (Oil Spill Information System) (Leech et al. 1993), and Russian SPILLMOD (Oil Spill Modelling) (Ovsienko et al. 2005).

Model OILMAP-WOSM (Worldwide Oil Spill Model) was created by request of American oil companies and today is used by them in those areas, where the companies have business. At calculations in parameterized form the processes of oil spreading, evaporation and dispergation are considered. Model COZOIL has “grown” from the same “incubator” as OILMAP and developed by joint efforts of the American and Norwegian specialists. Today this model is the most complicated by its architecture, as it includes block for calculations of coastal wave dynamics and uses the knowledge of morphological features of coastal zone and offshore strip.

Model OSIS differs principally from the above two models by method of mathematical description of oil spreading because oil spill in this model is represented as an ensemble of oil droplets of different size which in the process of

modeling sink into the water column and then rise to the surface under buoyancy force, participating simultaneously in diffusional dispersion and transfer in the upper mixed layer of the sea.

2.4.1 Russian Hydrodynamic Model of Oil Spills “SPILLMOD”

To date the Russian model SPILLMOD has rather wide geography of application both in Russia and international projects. The main model feature is associated with computing technology allowing estimating the change in configuration of oil spill and its properties in the area with arbitrary geometry of contacting boundaries. Unlike other known models, in SPILLMOD the processes of oil spreading and transport are calculated “hydrodynamically” but not “parametrically” that allow reproducing the oil spill dynamics most adequately. The computing algorithms allow to consider almost all known processes of oil spill transformation and to include the operations on mechanical oil recovery (oil skimmers), use of chemical dispersants, localizations of oil with booms, oil combustion in the model. It is notable that since 1998 the model is a basis of computer simulators of Marine Academy of US Coast Guard, developed by British company TRANSAS MARINE.

For the Caspian Sea, for example, the program complex SPILLMOD includes models: circulation dynamics, sea ice dynamics, joint model of circulation and ice dynamics, models of wind wave and dynamics of oil spill with processes of its physical and chemical transformation.

The possible directions of oil spill model application are—forecast of accident occurred previously—retrospective forecast (calculation) for analysis of accident consequences—estimation of hypothetical accidents for assessment of possible consequences—training of specialists with use of computer simulators of accident—development and selection of effective strategies of application of technical means for localization and elimination of oil spill accidents.

2.4.1.1 Accident Simulation

In most cases accidents at sea occur under the severe hydrometeorological conditions, and time for decision making on specific response measures is limited. For this reason the preliminary estimated scenarios of possible accident development can provide actual benefit. Modeling of oil spreading gives a possibility to assess the probable scales of damage for marine environment before accident initiation. By results of computer simulation the experts engaged in development of oil spill response (OSR) plans, can draw conclusion on how resources and facilities for prevention or minimization of resultant emergencies should be organized, and models of spill technology application allow assessing various strategies of oil localization and minimization of accident consequences.

Having used, for example, the data of geographic and ecological model of the Kerch Strait as source information, in 2006 we implemented 16 prognostic numerical calculations (scenarios) of oil spill transformation under the influence of physical and dynamical processes with the SPILLMOD model (Fashchuk et al. 2007) (see Fig. 1.16, Chap. 1). Similar calculations were made for the northeastern Sakhalin shelf (Ovsienko et al. 2005).

Figure 2.1 demonstrates another example of model accident simulation—estimation of oil stain configuration forming under different wind situations in 2 h after the 1500 ton oil spill during transfer operations in the terminal area of port of Tuapse (Black Sea).

2.4.1.2 Identification of Risk Zones and Probability of Object impact by Oil Spill in the Aquatory or in Coastal Zone of the Sea

The risk zone of object impact in the aquatory or in coastal zone over the certain periods of time is an important statistical characteristic of possible oil spreading area. Figure 2.2 shows embedded areas, boundaries of which can be reached by oil spill if the response measures have not been taken.

The technique of risk zone construction consists in the following. The aquatory around a source is divided into subareas or cells of rectangular grid with sides such as all oil slick motion trajectories would enter the selected zone. Then, for each grid element the minimum time, necessary for oil spill to enter the specified cell is estimated. By the obtained grid dataset the contours of areas or risk zones, where oil spill can appear within the chosen timeframes or, in other words, transport of oil spill outside the corresponding zones in specified time is unlikely, are constructed.

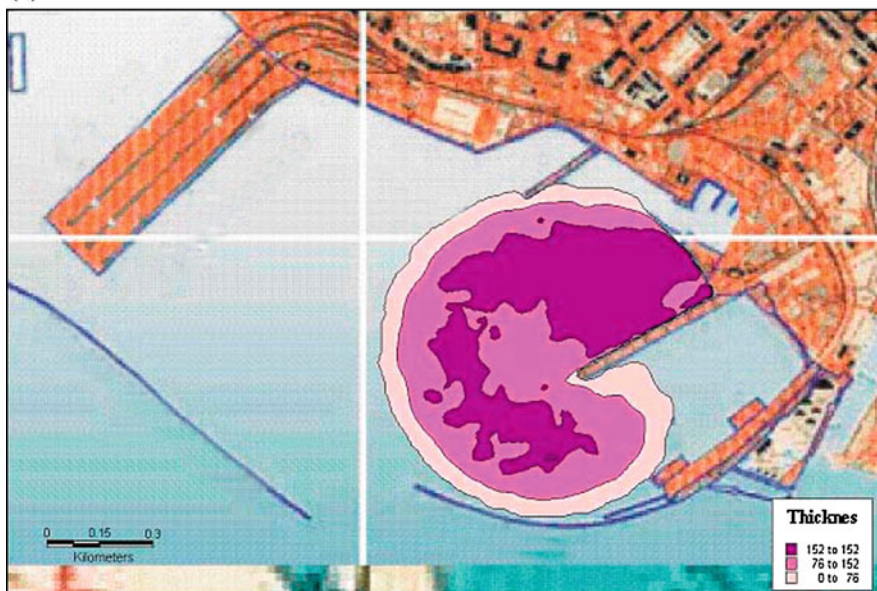
The probability of object impact within a certain zone can vary in wide range and depends on time since accidental oil spill, relative positions of accident source and impacted object, linear and area characteristics of protecting object, volume and regime of oil dumping. As a rule, the conditional probability of object impact, i.e. *provided* that spill has occurred, is calculated. The probability of occurrence of oil spill of various volumes is calculated at estimation of industrial risk.

Figure 2.3 shows distribution of impact probability of the 10 km “squares” on the aquatory at volley of oil in the Varandey terminal area of the Pechora Sea and conventional point 8 in the Baltic Sea.

2.4.1.3 Forecast of Development of Accident Situation After Oil Spill

The operational forecast of situation development is an important element of the negative consequence prevention management system of actual (already happened) accidental oil spills in the sea. The *forecast* of oil slick motion trajectory and changes in characteristics of oil or oil products allows setting the

(a)



(b)

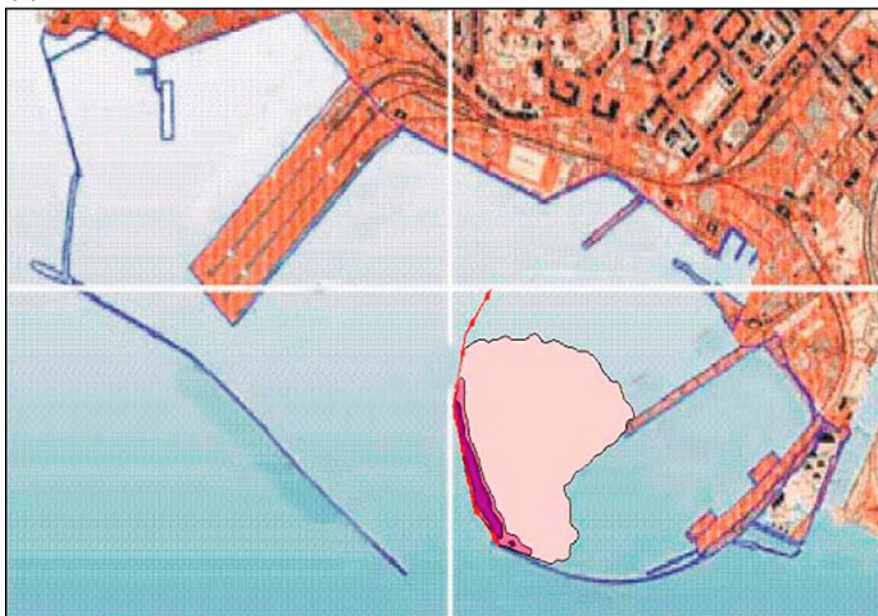


Fig. 2.1 Scenario of oil stain transformation (thickness of oil film, micron) in 2 h after the 1,500 ton oil spill in port of Tuapse (Ovsienko et al. 2005) (Wind: **a** still; **b** northeast, 6 m/s)

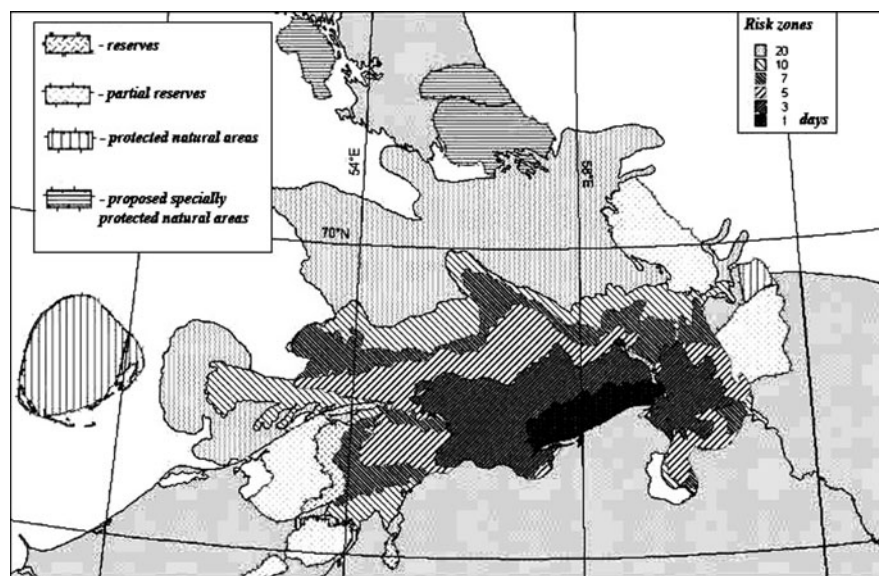


Fig. 2.2 Risk zones of oil spreading at accident in the area of Varandey terminal (Pechora Sea) (Ovsienko et al. 2005)

effective response measures. For these purposes the program complex SPILLMOD, based on the system of mathematical models describing main hydrometeorological processes which determine oil behavior in marine environment, can be used also.

The first version of model SPILLMOD developed in 1990, has been used in real-time regime for the forecast of development of catastrophic crude oil spill in the Persian Gulf during military operations in January–February, 1991 when within four days about 6 million barrels of oil were dumped from several points of the Kuwait coast into the northwestern Persian Gulf. Three months after the estimations their results were compared with satellite observations in the military zone. Despite the limited set of input data, the results of comparison have appeared rather encouraging (Fig. 2.4).

2.5 Conclusions

Using the methods of mathematical modeling, based on the system interrelated description of chemical, biological and physical processes (geographic and ecological information models), the problems of the long-term chemical composition of natural waters and its long-term changes in space and in time are studied. Moreover, on the basis of current information, numerical methods and computing

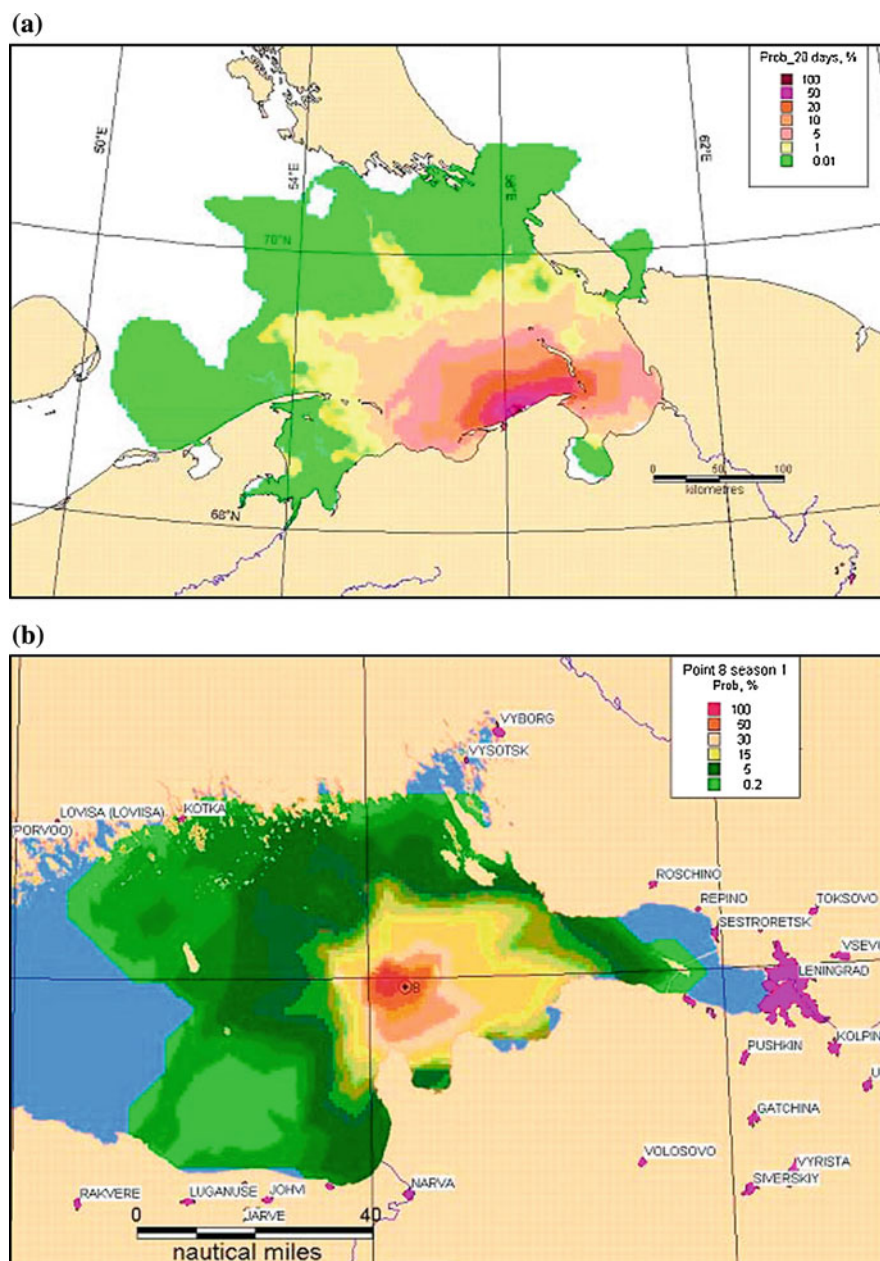


Fig. 2.3 Probability of marine aquatory impact as a result of oil volley in the Varandey terminal area of the Pechora Sea (a) and in the zone of hypothetical oil spreading in the Baltic Sea (b) (Ovsienko et al. 2005)

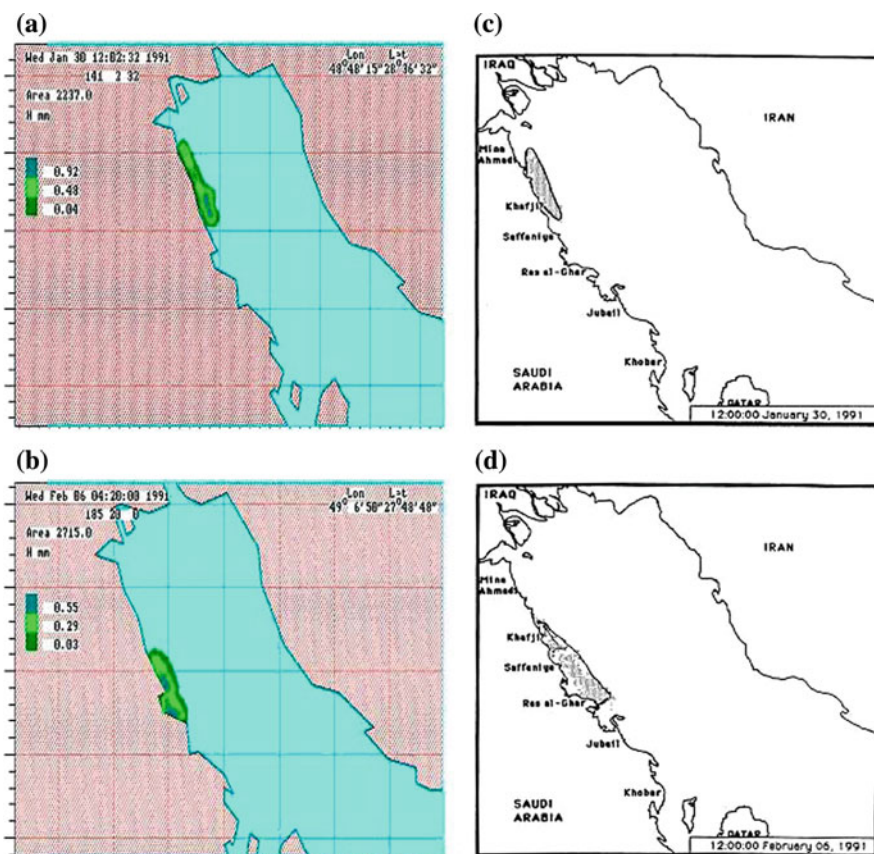


Fig. 2.4 Model calculations of oil spill dynamics in the Persian Gulf (a, c) and its actual position by satellite observations (b, d) (Ovsienko et al. 2005)

facilities, the mathematical models, capable of describing the main dynamic processes in the ocean at synoptic spatiotemporal scale are created.

In prospect, this apparatus can be applied to control of the water body state, tracing of anthropogenic factor role in formation of water resource quality, properties of natural waters in specific water bodies and streams, and also in different basins and aquatories of marine ecosystems. In particular, the investigations seem rather actual at solving of the environmental problems, planning of nature protection actions, rationalization of use of biological and mineral resources of the Caspian, Barents, Black, White, Okhotsk, and other Russian seas with account of the forthcoming development of their shelf oil and gas fields, building of terminals and ports for treatment and transportation of oil hydrocarbons.

Today, for the known economic reasons the complex observations on the state of ecosystems of these basins practically are not conducted or have episodic character. In these circumstances, the methods of mathematical modeling get a

special applicability. On the basis of available scarce and irregular information, they allow:

- assessing the volumes of nutrients entering into the water basin with river discharge, atmospheric precipitation, and as a result of interchange at the water-bottom interface;
- assessing the ecosystem response on variations in intensity of these sources by change in nutrient flows due to development of biotransformation processes (nutrient uptake, elimination of metabolic products, die-away of hydrobionts, intensity of trophodynamic interactions) and under the transfer of water mass components across the boundaries of adjacent aquatories;
- assessing the eutrophication effects by increase in hydrobiont biomass, intensity and duration of phytoplankton blooming, changes in conditions of nutrient limitation of bioproduction processes (P or N);
- assessing the intensity of vertical transfer and nutrient and organic matter exchange between the upper and deeper sea layers, conditions of oxygen deficit formation in the near-bottom water;
- identifying and assessing quantitatively the role of main biological components participating in production cycle and favoring the redistribution of nutrient forms in water column by their intraannual supply and subsequent biotransformation in marine ecosystem;
- defining the priority processes determining the production capacity of marine basins and, on this basis, providing recommendations on their rational natural resource use and environment protection;
- studying the dynamics of oil spills under the influence of hydrometeorological factors;
- making the model reconstructions of hypothetical oil spill dynamics under the different scenarios of synoptic situations, ice conditions, real coastal orography and seafloor topography.

Mathematical modeling of marine ecosystems on the basis of adequate data of geographic and ecological information models—"portraits" is one of the prospective lines of marine ecological geography.

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