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OPERATIONAL OCEANOGRAPHY

Textbook

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This textbook represents a summary of problems of organization of operational work on provision of end-users with marine hydrometeorological information, including the discussion of modern oceanographic systems, development of continuous ocean monitoring systems, description of forecasting hydrodynamic models, procedure and basic approaches to data assimilation by forecasting models, methods of storage and processing of observational data, and information products.

The textbook is suitable for students and PhD students studying "Applied Hydrometeorology" and specializing in the area of Applied Marine Sciences, and is recommended by Academic Association of Universities for Hydrometeorology of the Russian Federation.

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ISBN

PREFACE

Global climate warming and resulting possible rise of sea level, elevated risk of occurrence of hazardous hydrometeorological phenomena and accidents, promoted a better understanding of the need of development of ocean observation operational systems and further development of forecasting methods and technologies. The process of integration of mathematical model technology together with processing and presentation of observational data in a user-friendly form and their real time transfer is widely applied and introduced into the routine of hydrographic services and agencies. Such technologies got the name "operational oceanography" and have been rapidly developing in the last two decades. Creation and development of operational oceanographic systems allows to ensure the safety at sea, to use such systems in management of marine resources and coastal activities, for prevention of oil spills, for operational control of sea oil pollution and spreading of other types of pollution, for studying of ice conditions and control of climate change. In order to prevent or reduce the damage from adverse weather conditions around the world the early warning systems of natural hazards, such as tsunami, tropical hurricanes, storm surges, etc. are being developed. The key role in such systems is assigned to operational provision with oceanographic data and forecasting information [Abuzyarov, 2009]. Operational transfer of oceanographic information, production of forecasts and making them available to a consumer using modern technologies allows to optimize the economic activity at sea and coastal zone. Development of operational oceanographic systems is also aimed at provision of decision-makers with operational information, decrease of life and human health risks as a result of natural and technogenic catastrophes, conservation of marine ecosystems and mitigation of climate change consequences.

Informational basis of preparation of different types of operational oceanographic production makes the monitoring of parameters of marine and air environment that serves the basis for diagnostic fields that are further used for making forecasts of the characteristics of the World Ocean marine environment. In order to ensure the needs of operational oceanography it is necessary to create the systems of routine monitoring, of both World Ocean and its enclosed and shelf seas [Shiller et al., 2011].

Development of forecasting products is based on the extensive arrays of data of observations in the World Ocean accumulated for many decades. In order to provide the management, access and distribution of data, operational oceanographic information, scientific products and knowledge based on the data obtained from oceanographic vessels, new automatic observation systems in the seas and satellite observations the national and international centers of data storage and processing are being created. The use of network standards for in-situ marine data and satellite information transfer in real time, as well as the latest achievements of information technologies allow to provide the archiving and saving of data for their use in a scientific research, expands the possibilities of availability of existing data for both scientific community and other consumers in general. At the same time the use of a common procedure of databases quality check allows to give metadata, data and high quality products to consumers.

There are powerful computers installed in the data reception centers that make possible the assimilation of observational data by forecasting models. Results of model calculations are used for production of forecasts, such as warnings of coastal floods, storm and ice conditions, blue-green algal blooms and pollution. Also, electronic maps, reference books, catalogues of oceanographic products are made, and ocean currents, wind conditions, sea level, etc. are predicted. Such forecasting information is rather rapidly transferred to consumers.

Due to the difficult economic situation in 1990s there was a lag in Russia in the field of development of operational oceanographic systems. However, the economic growth in the 21 century and the related development of marine activity in the Russian Federation required the development of the latest methods and technologies of forecasting for the seas of Russia. The accumulated earlier extensive experience of making measurements at sea, the saved scientific potential in the field of modeling, as well as the opportunities for use of the accumulated European experience and existing technologies due to participation of the Russian scientists in the European programmes and projects created the prerequisites to the development of modern national technologies in the field of operational oceanographic systems.

In recent years the system of operational oceanographic service in Russia has improved within the frames of the subprogramme “Uniform System of Information on the State of the World Ocean (in Russian: ESIMO) of the Federal Target Program “World Ocean”. One of the main modules in this subprogramme is the operational module based on technologies of creation and distribution of various diagnostic and forecasting products of global and regional character using modern computers, GIS-technologies and means of telecommunication [Abuzyarov, 2009].

Separate components of the operational subsystem ESIMO have been already introduced in the operational routine of scientific and operational institutions of Roshydromet and marine hydrometeorological services. The ESIMO Web portal (http://www.oceaninfo.ru) has been put into operation providing the remote search and access to information resources of national and foreign sources of operational information, data arrays and databases in the ESIMO subject field, including forecasting products and data.

Thus, operational oceanography includes a wide range of tasks: creation of routine systems of monitoring, hydrodynamic modeling of water dynamics, operational data transfer and assimilation by forecasting models, observational data storage and processing, user-friendly transformation of model data (visualization), creation of information products each of which is a separate field of knowledge.

The purpose of the present text-book is to give an idea of modern oceanographic systems. There is a summary of problems of organization of the operational routine of providing the consumers with forecasting products. There is also a description of the main programmes and projects existing within the international cooperation in operational oceanography. The special attention in the text-book is given to numerical models of sea state forecast, pollution distribution, and ways of field data assimilation. There is also the information on the "Uniform System of Information on the State of the World Ocean (in Russian: ESIMO) and modern European regional forecasting systems.

The book is aimed at students (Bachelor and Master level) studying in the field of Applied Hydrometeorology (Applied Marine Sciences), profile "Applied Oceanology" and specializing on fisheries oceanology, applied marine sciences and ICZM.

The text-book has been prepared within the international project "eMaris" of the TEMPUS programme.

Chapter 1. OPERATIONAL OCEANOGRAPHY: AIMS, OBJECTIVES, CURRENT STATE, PROBLEMS AND PROSPECTS

1.1. Operational Oceanography – basic provisions

Operational Oceanography (OO) is one of the applied sections of General Oceanography. Its development is closely related to the introduction of new methods of marine measurements, improvement of numerical models, development of modern technologies of data transfer and assimilation, and development of telecommunication facilities. The distinctive feature of OO is that the development of this area of marine sciences has been stimulated by the international organizations, such as World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission (IOC), etc. which activity is aimed at the development of oceanographic service.

There are various approaches to the definition "Operational Oceanography". At present, the definitions "operational" and "scientific" oceanography are not conventional. It is due mainly to the differentiation of research and operational activity in different countries depending on the existing structures of management and financing in each country. International experts have specified as a general principle of "operational" oceanography that it usually characterizes the activities resulting in a more effective prediction of the ocean state. Thus, Operational Oceanography provides the main infrastructure for work of services responsible for provision of consumers with operational information.

One of the definitions of OO is given at [EuroGOOS website: http://eurogoos.eu/]. According to this definition OO can be defined as the activity of systematic and long-term routine measurements of the seas and oceans and atmosphere, and their rapid interpretation and dissemination.

Important products derived from OO are:

– nowcasts providing the most usefully accurate description of the present state of the sea including living resources;

– forecasts providing continuous forecasts of the future condition of the sea for as far ahead as possible;

– hindcasts assembling long term data sets which will provide data for description of past states, and time series showing trends and changes.

Operational Oceanography usually proceeds by the rapid transmission of observational data to data assimilation centers. There, powerful computers using numerical forecasting models process the data. The outputs from the models are used to generate data products, often through intermediary value-adding organizations. Examples of final products include warnings (of coastal floods, ice and storm damage, harmful algal blooms and contaminants, etc.), electronic charts, optimum routes for ships, prediction of seasonal or annual primary productivity, ocean currents, ocean climate variability etc. The final products and forecasts must be distributed rapidly to industrial users, government agencies, and regulatory authorities.

The scheme of functioning of the operational system is presented on figure1.1 including various ways and technical tools for making measurements at sea, satellite data and modeling for the purpose of obtaining the forecast.

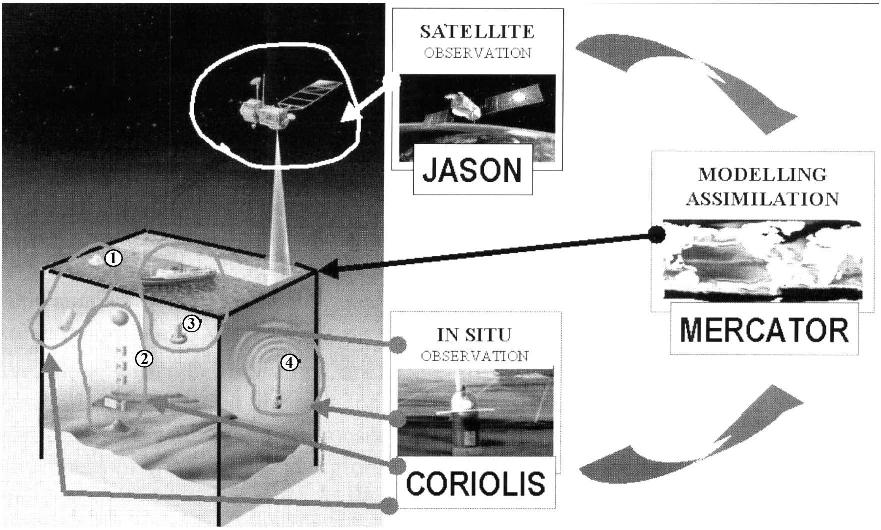

Figure 1.1 – Scheme of the operational system routine work [Proceedings of the Fourth international Conference on EuroGOOS]

Advanced methods in operational oceanography are dealing with top end technologies available to (i) enhance the capacity of numerical models to simulate and forecast the dynamics and functioning of the marine environment closest to reality, and (ii) extract information and generate useful applicative knowledge from the integration of data across different geographical and temporal scales, and across sectors.

Specialized numerical modeling aimes at different dynamical and functioning aspects of the marine environment. Data and information services are applied in a number of contexts including environmental monitoring and surveillance, assessment and mitigation of risks, marine science-based policy development and strategic planning, climate change, sustainable resource exploitation, ocean governance, marine industries and emerging challenges in the marine domain. In the process of Environment Impact Assessment (EIA), there are applications to local case studies, dealing with the merging of scientific, environmental, legal and socio-economic aspects, and focusing on the use and integration of multiple data sets to achieve the best assessments.

OO implies the monitoring and forecasting of the physical characteristics of the marine environment. However, in the last decade the biological indicators have also become a part of operational products being interesting from the scientific and economic points of view. Biological processes such as the phytoplankton development, influence on carbon cycle and penetration of light and heat into the deep layers of the subsurface layer of the ocean, biological productivity, water quality, population health – are the most important indicators of the state of the coastal zone experiencing the anthropogenic impact.

1.2. Global and regional operational oceanographic systems

Rapid development of OO is related to the foundation in 1990 of Global Ocean Observing System (GOOS). This is the system for coordination of the international programmes, each of which working in various directions supplementing each other for the purpose of maintenance of continuous and stable functioning of global ocean observing networks. The main objectives of GOOS are aiming at meeting the growing needs of various consumers in quality, quantity and operational efficiency of oceanographic information and include:

– Monitoring, study and prediction of weather and climate;

– Description and forecast of the ocean state, including living resources;

– Improvement of marine and coastal ecosystems and resources management;

– Reduction of damage from natural hazards and pollution;

– Protection of life and property on coasts and at sea;

– Stimulation of scientific research.

The main users interested in GOOS are: administrations of coastal areas, national oceanographic and meteorological services, hydrographic services, marine and coastal enterprises, marine transport, politicians and interested people.

The GOOS system includes two modules: global and coastal. The main objective of the global module is the identification of the large-scale changes in the ocean and assessment of their influence on climate. The objective of the coastal module is the assessment of large-scale changes effect on coastal regions, including ecosystems. In order to fulfill the objectives of the coastal module the GOOS regional systems are created that are united in a global network of coastal observations and data management.

In 1994 the European module was created – EuroGOOS - for development of operational oceanography in the European seas and adjacent parts of the oceans. The regional structure of EuroGOOS included 5 regions: 1) Atlantic Ocean; 2) Arctic seas; 3) Baltic Sea; 4) shelf of Northwest Europe; 5) Mediterranean Sea. These regions of the World Ocean have significant differences in the oceanological characteristics, degree of study and economic situation. Each regional system aims at promotion of solution of the GOOS objectives and tasks in the region. Distribution of regional systems is shown on figure 1.2.

EuroGOOS conducts regular information transfer to GOOS Committee. Presently, the EuroGOOS structure includes 36 organizations from 16 European countries. Members of EuroGOOS interact among themselves in order to have a uniform approach to solution of the following tasks: allocation of priorities of the European operational oceanography, stimulation of development of scientific, technical and computing bases for numerical oceanography and its introduction in routine of services and agencies, assessment of economic efficiency of forecast products use.

EuroGOOS activity aims at the assistance in planning of GOOS activity and promotion at national, European and global levels. At the same time, the most important task of EuroGOOS is to promote the European operational oceanography in GOOS, to stimulate the development of the European and regional services of operational oceanography taking into account GOOS modules: 1) coastal zone; 2) healthy ocean; 3) living marine resources; 4) climate; 5) marine services; to create a uniform routine of data processing including quality control and data management, to stimulate the research and to develop the technologies which will allow to solve problems of OO.

Activity of EuroGOOS aims at obtaining of the maximum economic efficiency during operation of existing systems, and by their introduction into larger systems of GOOS.

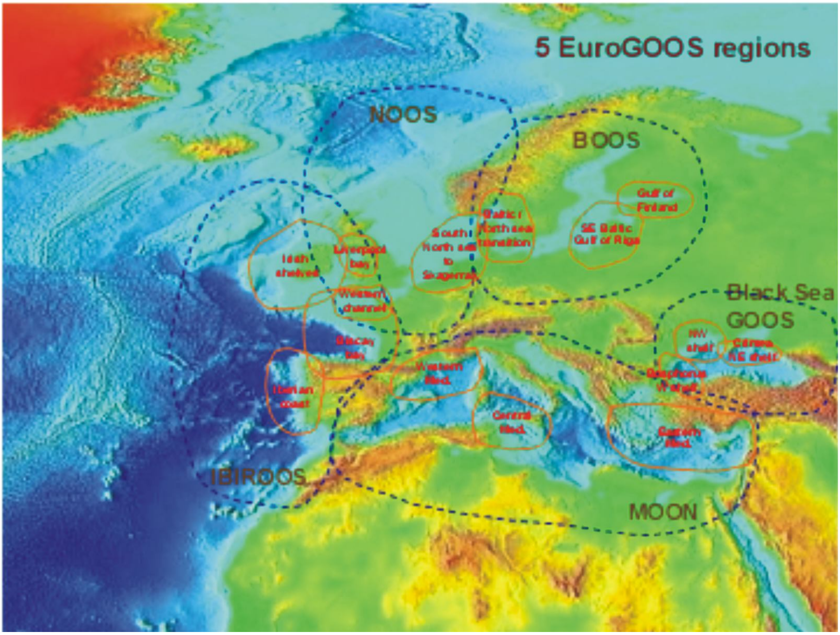

Figure 1.2 – European regional (blue dashed lines) and coastal (red lines) systems. BOOS – Baltic Operational Oceanographic System, NOOS - Northwest Shelf Operational Oceanographic System; MOON -Mediterranean Operational Oceanographic Network; IBIROOS - Irish, Biscay and Iberian Regional Operational Oceanographic System; Black Sea GOOS

GOOS implies the development, support and involvement in the programme of regional research groups for the purpose of organizing and conducting of marine observations. Besides the European module, GOOS also includes the regions of Northeast Asia, Africa, the Caribbean Sea, Australia, Arctic, etc.

GOOS is a component of Global Earth Observing System which unites the observations of all natural systems on the planet, including the sea.

GOOS is supported and funded by such organizations as:

- International Oceanographic Committee (IOC)
- World Meteorological Organization (WMO)
- United Nations Environmental Programme (UNEP)
- International Council of Scientific Unions (ICSU).

The participation of Russian organizations in GOOS is coordinated by the National Oceanographic Committee (NOC) of the Russian Federation. At the present stage Russian organizations contribute to the development of existing systems of observation and data exchange: using the ships of opportunity, Global Observation System of Sea level (GLOSS), International Exchange of Oceanographic Data and Information (IEODI), satellite sexisting systems of observation and data exchange: using the ships of opportunity, Global Observation System of Sea level (GLOSS), International Exchange of Oceanographic Data and Information (IEODI), satellite systems, as well as the development of GOOS regional projects in the Black, Baltic and Far East seas.

1.3. The main international programmes and projects in operational oceanography

Operational oceanographic systems for different parts of the World Ocean started to develop in the 1980s with the support of WMO. In the activity related to the development of operational oceanographic service WMO actively cooperates with the Intergovernmental Oceanographic Commission, International Maritime Organization (IMO), etc. So, in 1999 within the cooperation of WMO and IOC the WMO/IOC Joint technical Commission on Oceanography and Marine Meteorology (JCOMM) was created. JCOMM is an intergovernmental organization of experts which provides coordination, regulation and management of the systems of oceanographic and marine meteorological observations, data exchange and consumer service. One of the main objectives of this organization is to develop the operational oceanography on the basis of Global Ocean and Climate Observing Systems. JCOMM works within the four programme areas: 1) service; 2) observations; 3) data control; 4) education, training and capacity-building. One of the main objectives of the programme area Service is to support the systems of marine safety, prevention of hazardous phenomena, and mitigation of consequences of accidents. To provide the consumers with operational meteorological and oceanographic information the JCOMM Products Electronic Bulletin was created. Consumers by means of modern Web technologies can access and present various information in a convenient way [Abuzyarov, 2009].

A great role in the development of ocean and regional observing systems belongs to the two pilot projects, executed under the auspices of GOOS: Global Ocean Data Assimilation Experiment (GODAE) and ARGO project.

The GODAE project aimed at collection and assimilation of in-situ observational data and satellite data in global ocean models in real time. The main result of the project must have been the reproduction of ocean circulation in the synoptic scale with high spatial resolution – several tens of kilometers.

The ARGO project provided the release in the World Ocean of 3000 drifting diving buoys for measurement of temperature and salinity profiles down to 2000 m. More than 30 countries took part in the implementation of the project, including Russia. The first buoy was launched in 2000, and by 2007 the total number of buoys in the World Ocean reached 3000 allows now to receive annually more than 100000 profiles of temperature and salinity. It is about 20 times more than the annual number of similar shipboard measurements. ARGO information made a valuable contribution to the diagnosis and forecast of sea level changes, study of tropical cyclones and typhoons, and development of long-term weather forecasts.

The development of operational oceanographic systems is supported through the funding of scientific projects. The largest projects for the last decade can be considered such European projects as ECOOP – European Coastal Operational Observing and forecasting system, My-Ocean and MyOcean 2 (www.gmes.info/pages-principales/projects/marine-projects/myocean) which main objective is the integration of existing European and regional operational observing and forecasting systems into a single integrated Pan European System. Both projects are financed by the European Commission (7th Framework Programme). The European national meteorological and hydrographic services take part in the projects, as well as European Environment Agency, European Maritime Safety Agency, research institutes, European data centers such as Mercator Ocean, commercial organizations working in the field of software development, universities, etc. The main objectives solved within the ECOOP and MyOcean projects that united over 70 participants in ECOOP and 59 participants from 28 countries in MyOcean, is to provide the high-quality information on the entire ocean (global scale) and European shelf seas (regional scale) based on a combination of satellite and in-situ measurements together with 3-D hydrodynamic models that reconstruct the characteristics at the deep layers, give the short-term forecasts and forecasts of changes of the marine environment state, and restore the previous sea state in the last 20 years. One of the project tasks is to provide the information transfer in real time and its availability to the consumer see figure. 1.3.

It should be noted that the "delivery" of forecasting products to the consumer (end-user) is the most important link of the operational system

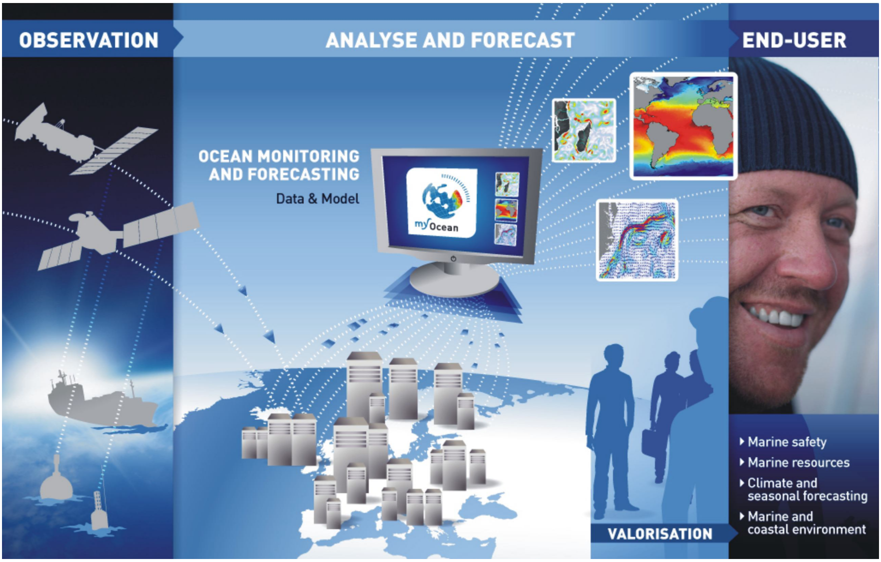

Figure 1.3 – Basic elements of the new Pan European service within the MyOcean project: observation, analysis and forecast (data and model), end user, economic efficiency (http://www.myocean.eu)

because the untimely or incomplete notification of the customer can lead to considerable financial losses, and even to human losses. Internet is the possible channel for data transmission. However, there are risks during its use, both to quality and safety of data transmission, and in certain cases Internet can not be installed or supported. Therefore for fast and reliable transfer of forecasting information and data it is necessary to use other opportunities of telecommunication facilities - satellite and telenavigation systems.

One of the most important results of the MyOcean2 project is the development of a catalogue of products for various consumers which includes over 100 different types of oceanographic information on water state of the World Ocean and its various regions. The information is published on the project website at http://www.myocean.eu and contains data on sea level, SST, ice cover, wind regime. The product catalogue contains the results of analysis of the World Ocean biogeochemical characteristics in the form of 3-D fields on a standard S deg. grid and with 50 vertical levels; weekly updated results of analysis and forecast of 3-D fields of the World Ocean physical characteristics of water; results of reanalysis of physical fields on a global scale for 1993-2011 and many other features (figure 1.4).

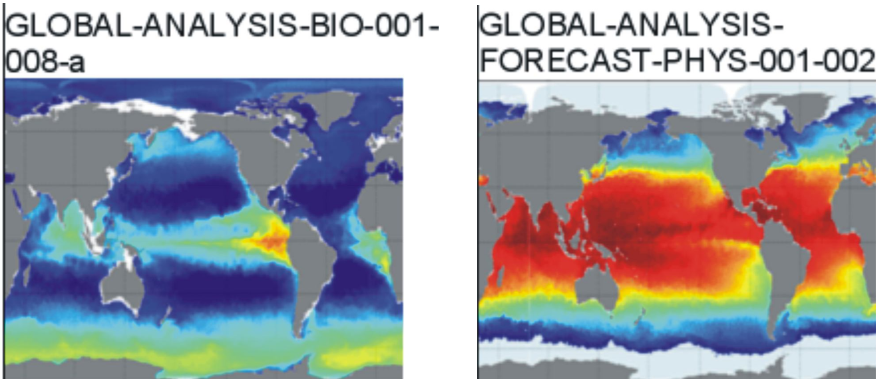

Figure 1.4 – Example of results of the World Ocean biogeochemical analysis of water (a) and global analysis and forecast of ocean physical characteristics (b)

Similar products are made for the seas and certain regions of the World Ocean.

MyOcean project is closely related to GOOS, EuroGOOS and projects aimed at the development of large data centers such as EMODnet and SeaDataNet.

The ultimate goal of MyOcean2 project is to make a Pan European structure (service) for monitoring and forecasting of ocean and sea state that will allow the countries to ensure the marine safety, to use the oceanographic system in management of marine resources and coastal activity, for prevention of oil spills and control of climate change, for study of ice conditions, water quality and distribution of pollution.

1.4. Observation systems in the World Ocean

Ocean observations come from a variety of sources, including satellite-based instruments, in-situ platforms such as surface and sub-surface buoys and floats, and volunteer observing ships (figure 1.5).

At present time, there are two main trends in the development of observation systems:

– automation of traditional contact methods of measurement of parameters of the marine environment;

– introduction of new tools of remote measurements of parameters of the marine environment (satellites, radars).

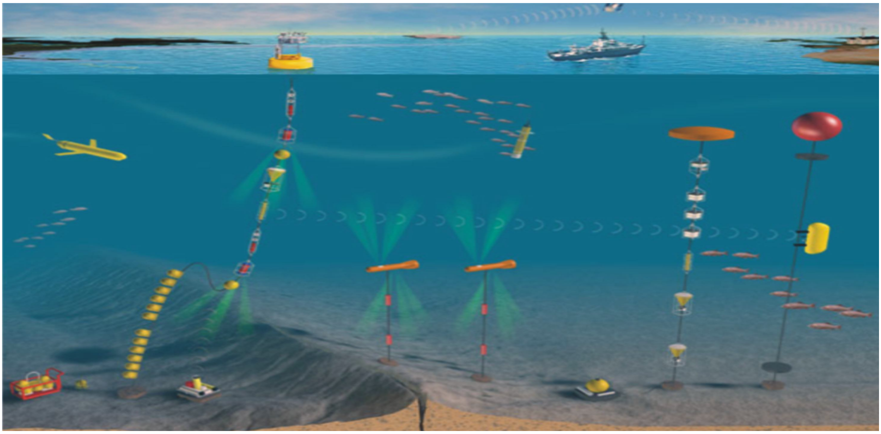

Figure 1.5 – Modern measurement systems in coastal zone (Ocean Observatories, Oceanus, 2006. http://ioi.research.um.edu.mt/cms/msc/index.php/2-uncategorised/)

The incoming data are used in three main aspects:

– for operational preparation of diagnostic and forecasting materials needed for hydrometeorological management of marine activity;

– for scientific research in the field of development and verification of models, methods and technologies of calculation and prediction of key parameters of the marine environment;

– for obtaining the necessary model parameters used at designing of vessels, various hydraulic engineering constructions, ports, platforms, etc.

Data of observations must meet some general requirements, they must be: global, 3D, complex, accurate, synchronized, regular and operational. All listed requirements must be fulfilled altogether because violation of one of them reduces the value of others.

The main ocean observing systems can be conditionally divided into three categories:

• global - cover the entire ocean (ARGO buoys, altimetry); measured parameters: sea surface temperature (SST), temperature and salinity profiles, sea level, currents;

• regional – for monitoring of individual phenomena (for example, the buoys TAO/TRITON/PIRATA are used for detection of El Nico, Arctic buoys for ice monitoring, etc.); temporary scales – from hours to days;

• coastal - monitoring of water quality, observations of wind, wave regime and tides near ports, radar information for monitoring of currents and waves at distances from 10 to 100 miles.

There are global data centers organized for data management. Now, there are two global ARGO Data Centers: in Monterrey (USA) and Toulouse (France). National data centers are in all member countries of the project (the USA, France, Great Britain, Canada, Australia, Germany, Japan, South Korea). All ARGO data are declared freely available to the world community (through the global GST network). Full observations that passed a control (with a time delay) are available through national ARGO data centers with a delay up to 5 months.

Observations Programme Area (OPA) was created in JCOMM, that is primarily responsible for the development, coordination and maintenance of moored buoy, drifting buoy, ship-based and space-based observational networks and related telecommunications facilities. It also monitors the efficiency of the overall observing system and, as necessary, recommends and coordinates changes designed to improve it. It has inherited lead responsibility for a number of important and well-established observational programmes, which are managed by bodies that now report through JCOMM (http://www.jcomm.info). The support center of in situ observing platforms created in JCOMM regularly updates the maps of the observing network in real time (figure 1.6).

Data of drifting diving buoys ARGO are updated daily, buoy data and data from vessels - monthly and are stored in a database of the support center.

Besides that, Observing System Monitoring Center (OSMC) is also created which is a web based tool to assist observing system managers and scientists with monitoring the performance of the global in situ ocean observing system, identifying problems in near-real-time, and evaluating the adequacy of the system (figure 1.7).

Since 1970, satellites started to be actively used for ocean observations. Presently, to obtain various satellite information the following satellite systems are used: NOAA, METEOSat, EUMETSAT, JANSON-1, JANSON-2, ENVISAT, etc.

The most important types of satellite information are:

– altimetry – necessary for definition of offshore surface currents and their mesoscale variability;

– thermal radiometry – allows to define with high resolution an SST field, including ocean fronts and eddies;

– visible spectrometry – measurements of ocean color are the basis for

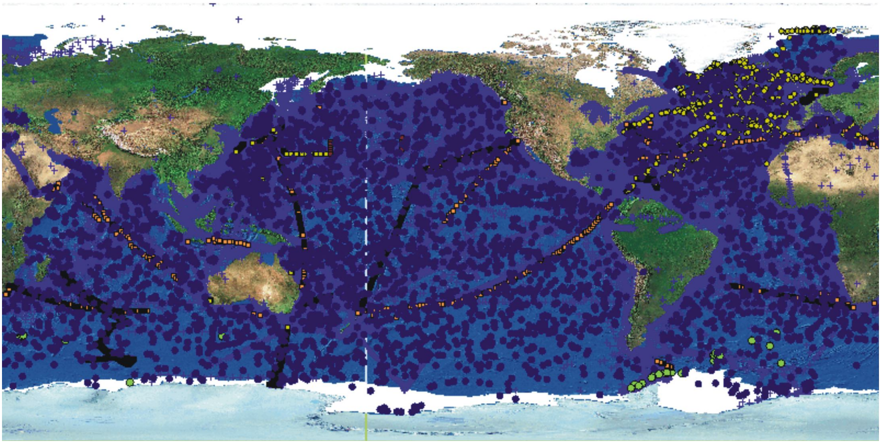

Figure 1.6 – Network status map from JCOMM/GOOS Network Status Map from JCOMMOPS generated using a Web Map Service (WMS) request

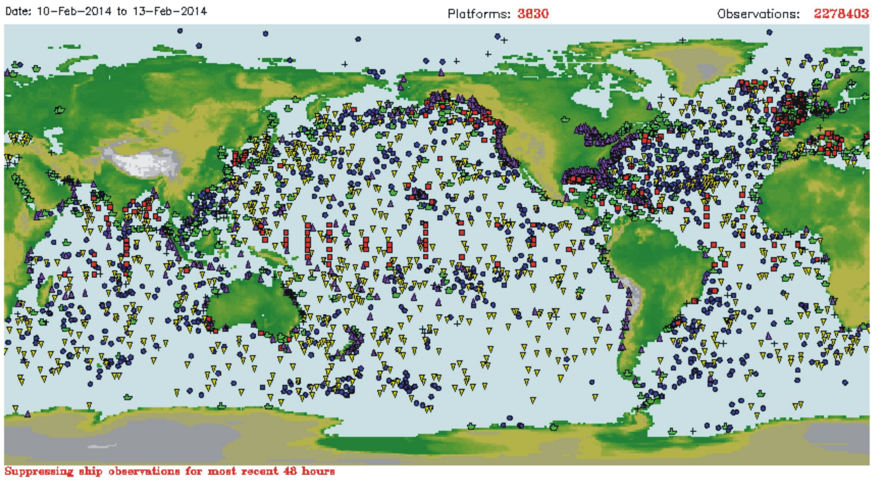

Figure 1.7 – Observing Platforms reporting in the last three days from OSMC

obtaining the data on chlorophyll and are also used in marine biogeochemical models.

Satellite radar data help greatly in the emergency situations during vessel pilotage in severe ice conditions and release of vessels from ice in the Arctic and Antarctica. Leaders of sea operations on the basis of radar ice charts (figure 1.8) analysis make the decisions on management of vessels and ice breakers in the Arctic and Antarctica.

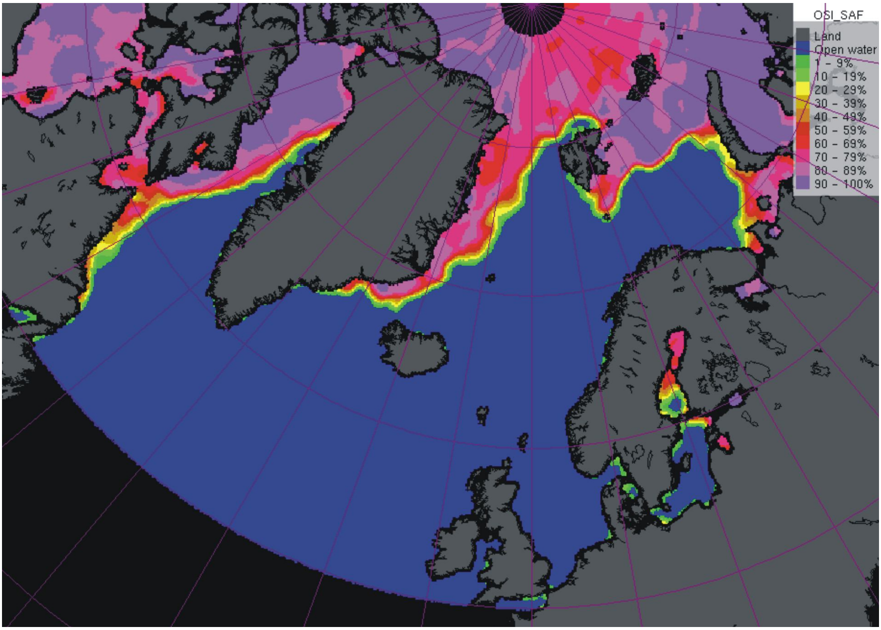

Figure 1.8 – Satellite ice monitoring chart

Chapter 2. OPERATIONAL FORECASTING OF STATE OF THE MARINE ENVIRONMENT

2.1. Hydrodynamic forecasting of the ocean state

Modern operational forecasting systems integrate the technology of a mathematical model together with the procedure of assimilation of observational data, processing and representation of forecast information in a user-friendly form during data transfer in real time. Hydrodynamic models make a basis of the forecast of the marine environment hydrophysical characteristics and pollution distribution. Now the general approach in development of forecasting systems is the integration of hydrodynamic models of atmosphere, ocean circulation, wind waves, etc. In recent years model complexes more and more often include models of transfer and transformation of oil pollution and ecosystem models.

In order to improve the quality of the forecast a procedure of assimilation by a mathematical model of observational data is used in operational forecasting systems. The main objective of the data assimilation method is to adapt the conditions of physical imitation models to the observed data. Thereby, this provides good initial conditions for a nonlinear model and interactive assessment of model parameters. The assimilation procedure is an essential component of operational forecasting; it is used for improvement of predictive qualities of a numerical model by constantly renewed forecasts based on a difference between the previous forecasts and recently obtained data.

2.1.1. Hydrodynamic models of ocean circulation and ice

The motion of ocean currents is usually studied with the use of a General Circulation Model (GCM). GCMs are used both for atmospheric and ocean modelling. These models make the core of both weather forecast models and climate models. Large scale wave motions, such as tidal waves, are usually well reproduced within the GCM framework, whereas other wave phenomena such as wind generated surface waves usually require the dedicated wave models in order to obtain a realistic representation of the physical processes. Although, further we will mainly focus on ocean models, it is important to have in mind that ocean processes and particularly motions near the ocean surface cannot be regarded in isolation from what is happening in the atmosphere [T.Soomere, 2013].

Despite the capabilities of Computational Fluid Dynamics (CFD) it is important to emphasize that our ability to simulate fluid motion does not diminish the importance of more traditional methods involving theoretical and experimental work and *in situ* and remote data recording.

Theoretical and experimental results are required to provide benchmark test cases, results that a CFD simulation must be able to reproduce to demonstrate that physical properties of the model are handled correctly. Such exercises are a part of model validation, and are essential in order to identify errors in the model and calibrate model parameters.

Once a model is deemed to produce results with acceptable accuracy and reliability, simulations can be used to provide information that is impractical or impossible to get through the other methods, e.g., filling out the gaps in field measurement data records due to sparse deployment of measurement instruments, analyzing flow scenarios that are too complicated for theoretical study, or providing forecasts of likely future events. Many scientists and engineers will not need to acquire the skills to develop CFD models, but as the use of CFD methods expands into new fields of science and engineering, more people will likely find that they need to work with data from simulations or even run CFD simulations themselves. It is therefore important also for non-specialists to have some idea about what goes on inside a CFD code, and what are the capabilities and limitations for these models.

The most important feature allowing to classify 3D ocean hydrothermodynamic models is a representation of local vertical direction, determined by the gravity. At present, there are three main representations of a vertical coordinate, however, none of them is universal.

The simplest choice of vertical coordinate is z-coordinate, that is a distance to calm sea surface $z=0$ with upward direction, so the seafloor is represented as $z = - H(x,y)$. This is an easy grid to work with from a design point of view, and has the advantage that the hydrostatic condition is represented exactly. Sloping bottom topography is a challenge when working with this grid. In practical applications with significant bathymetry variations the use of the z-coordinate system may result in a large number of inactive cells because the grid must extend globally to the maximum depth of the basin. The z -coordinate system is also problematic for locations where isopycnals are not horizontal surfaces, in which case pressure gradient errors may occur. The rigid structure of the grid also makes it difficult to combine with a free surface representation at the interface between ocean and atmosphere. Examples of models using z-coordinates for vertical discretization include

MOM (Modular Ocean Model, http://www.gfdl.noaa.gov/ocean-model) and MIT gcm (M.I.T. general circulation model, http://mitgcm.org/).

Another vertical coordinate can be potential density ρ related to specific pressure (close analogue of entropy or potential temperature in atmosphere). The isopycnal coordinate system defines vertical coordinates as isosurfaces of equal density. This solves the problem of artificial pressure gradients. This coordinate system makes it easy to obtain high grid resolution where density gradients are strong. A challenge with this method is that the vertical layers may become very thin or even vanish in parts of the model domain.

For instance, brackish coastal water usually has lower density than any water mass found in the middle of the ocean. Thin layers are also a source of numerical instabilities. Another potential problem is that the isopycnal coordinate system consolidates isopycnals as material surfaces, thereby restricting the cross-isopycnal mixing. Examples of models using isopycnal coordinates include MICOM (Miami Isopycnic Coordinate Ocean Model) and NLOM (Navy Layered Ocean Model,http://www7320.nrlssc.navy.mil/global_nlom/).

Finally, the third option is s-coordinate, defined by the formula

$$\sigma = (z - \eta)/(H + \eta), \tag{2.1}$$

where η - deviations of reservoir level from its undisturbed state at z = 0. As a result σ = 0 on the free sea surface at z = η and σ = -1 on the seafloor at z = - H (figure2.1).

A distinctive feature of models with s-coordinate is the smooth representation of bottom topography. This provides the best (in comparison with level and isopycnal models) description of current dynamics in the bottom boundary layer. s-models have also rather good description of thermodynamic effects caused by nonlinearity of the equation of state. Therefore, these models are very suitable for modeling of currents in the ocean shelf zone, shallow shelf seas, enclosed seas and river estuaries.

An example of models using s-coordinate as vertical is the three-dimensional model of ocean general circulation of Princeton University POM (Blumberg and Mellor, 1987) that is based on the full equations of hydrothermodynamics of the ocean. POMs additional advantage is that it describes vertical and horizontal turbulent transfer on the basis of tested and reliable parameterizations according to Mellor and Yamada (Mellor and

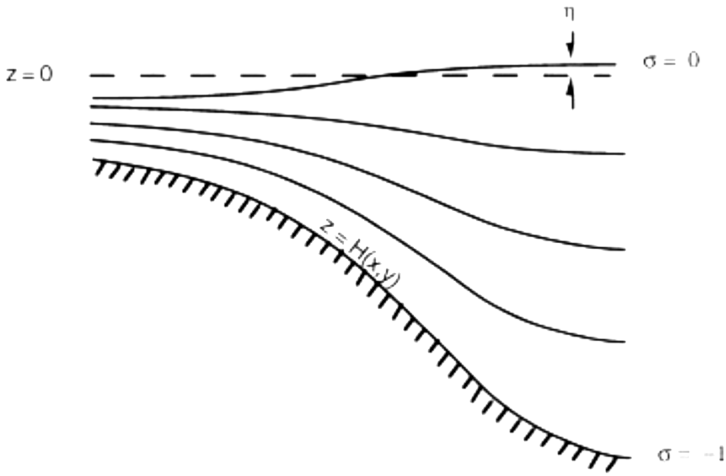

Figure 2.1 – Vertical structure of a model with σ - coordinate

Yamada, 1982) and Smagorinsky (1965). In particular, the terms F_x, F_y, F_T, F_S, F_c in the right parts of the equations of motion, heat, salt and admixture transfer, characterizing changes of horizontal components of respectively velocity, temperature, salinity and hydrodynamically passive admixture due to horizontal turbulent transfer, will be parameterized similarly to molecular processes as:

$$F_x = \frac{\partial}{\partial x}\left(H\tau_{xx}\right) + \frac{\partial}{\partial y}\left(H\tau_{xy}\right), \qquad F_y = \frac{\partial}{\partial x}\left(H\tau_{xy}\right) + \frac{\partial}{\partial y}\left(H\tau_{yy}\right),$$

$$F_\phi = \frac{\partial}{\partial x}\left(Hq_x\right) + \frac{\partial}{\partial y}\left(Hq_y\right), \qquad (2.2),$$

where

$$\tau_{xx} = 2A_M\frac{\partial U}{\partial x}, \tau_{xy} = \tau_{yx} = A_M\left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}\right), \tau_{yy} = 2A_M\frac{\partial V}{\partial y},$$

$$q_x = A_H\frac{\partial \phi}{\partial x}, q_y = A_H\frac{\partial \phi}{\partial y},$$

U, V - components of horizontal component of current velocity, $\phi = (T, S, C)$, T and S – temperature and salinity of water, C – concentration of passive admixture, A_M and A_H - coefficients of horizontal turbulent viscosity and diffusion. It is implied that $A_M = A_H$, and coefficient of horizontal turbulent viscosity A_M is defined by the Smagorinsky formula:

$$A_M = c_t \Delta x \Delta y \left[\left(\frac{\partial U}{\partial x} \right)^2 + \left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} \right)^2 + \left(\frac{\partial V}{\partial y} \right)^2 \right]^{1/2}, \tag{2.3}$$

where Δx and Δy - grid spatial sizes respectively along x and y axis; constant of proportionality c_t ($\approx$ 0.10 - 0.20) is an adjustment parameter and must be selected according to the results of calculations in order to provide the best compliance with data of observations.

Formula (2.3) considers the anisotropy of the field of current horizontal velocity, and coefficients of horizontal turbulent viscosity and diffusion vary in space and time depending on variations of velocity field.

Thus, the main advantages of POM model are: the detailed description of bottom boundary layer and modern parameterizations of vertical and horizontal turbulent diffusion considering the spatial heterogeneity and to a certain extent the anisotropy of the coefficient of horizontal diffusion.

Distribution of hydrodynamically passive dissolved admixture, not participating in any chemical and biological interactions, that spreads in the marine environment under the influence of currents and turbulence of point source admixture in case of use of s-coordinate is described by the equation:

$$\frac{\partial CD}{\partial t} + \frac{\partial CUD}{\partial x} + \frac{\partial CVD}{\partial y} + \frac{\partial CW}{\partial \sigma} = \frac{\partial}{\partial \sigma}\left[\frac{K_H}{D} \frac{\partial C}{\partial \sigma} \right] + \frac{\partial}{\partial x}\left[H A_H \frac{\partial C}{\partial x} \right] + \frac{\partial}{\partial y}\left[H A_H \frac{\partial C}{\partial y} \right] +$$

$$+ \quad \sum_i Q_i(t) \delta(x - x_i) \delta(y - y_i) \delta(\sigma - \sigma_i), \tag{2.4}$$

where, $D = H + \xi$, ζ - level deviations from undisturbed position;
W – vertical component of current velocity (projection of current velocity vector on σ-coordinate); C – admixture concentration; K_H – coefficient of vertical turbulent diffusion;
A_H – coefficient of horizontal turbulent diffusion; Q_i – speed of admixture input to the basin in i-source located at the point (x_i, y_i, σ_i);
δ – Dirac delta function.

Boundary conditions. In order to have a working numerical model, we need to specify boundary conditions, initial conditions and forcing mechanisms. These conditions will obviously depend to some extent on the particular application, so only a very general description of these features is presented here.

An ocean model typically has boundary conditions at the sea floor and at the sea surface. In addition, a numerical model covers a limited computational domain, and boundary conditions must also be specified for the lateral model boundaries.

During realization of a full system of three-dimensional equations of fluid hydrothermodynamics the boundary conditions on the sea surface are usually the flows of momentum, heat and salt, and for the sea floor it is most common to specify a no-flux condition.

The lateral boundary conditions are determined by the specific application. If the sidewall of the domain can be considered as a solid wall, as is the case when the sidewall is located on dry land, we can use the no-flux condition $u \cdot n = 0$, where n is the outward normal vector for the sidewall.

In many applications at least some of the lateral boundaries will intersect sea areas. In the case of global models, where the lateral boundary may be located along a line of longitude, periodic boundary conditions can be used at the east and west boundaries. The location of Antarctica at the South Pole allows the use of a no-flux wall condition, but the Arctic Ocean is difficult to represent in such a model. One solution to this problem is to model the Arctic Ocean and North Atlantic with a separate model using a rotated grid with poles at the equator, as is done in the OCCAM (Ocean Circulation and Climate Advanced Modelling Project) global ocean model. An alternative method is to apply a non-spherical coordinate system where polar singularities are hidden over land [T.Soomere, 2013].

The sea intersecting lateral boundary condition becomes more complicated for regional models which should allow flow exchange with sea areas not covered by the numerical model. Such open boundary conditions should be able to eliminate any reflection from waves and currents leaving the computational domain, and allow inflow of water masses according to parameters describing conditions in the exterior sea areas. The parameters for exterior sea areas may reflect transport due to major ocean currents and seasonal variability in average temperature and salinity, or may be extracted from a global ocean model in a similar way as the atmospheric climatology datasets. There is no universally accepted correct way to prescribe such open boundary conditions, and a single model may use a combination of several methods (zero gradient, radiation conditions, flow relaxation) to achieve the desired result.

Climatological datasets, including hydrographic data for potential temperature and salinity, are important for the initialization of ocean models. If a global ocean model is initiated with a homogeneous state, it will take thousands of simulated years for diffusive processes to generate realistic deep ocean water masses. Even if the model is initialized with hydrographic data close to the long term equilibrium state, the model will usually require some spin-up time before a realistic circulation pattern emerges. At the start of a simulation the initial density field is adjusted towards an equilibrium state. For a global circulation model it takes from a few weeks to a few months to set up the barotropic wind generated currents, whereas the baroclinic response is set up after a few years, and the thermohaline circulation is established after about a decade of simulated time. For regional scale models the spin-up time is much shorter, particularly if the model domain is influenced by large water exchange across open lateral boundaries.

To account for the atmosphere influence (forcing) in ocean circulation models the results of atmospheric forecasting models are used, such as air temperature, wind speed and direction, precipitation, etc. Usually atmospheric models give a short-term forecast for 48 hours that determines the terms of the forecast of ocean circulation models.

For freezing seas the ice model is usually added to the hydrodynamic module. The objective of ice cover mathematical modeling is the reproduction of main physical processes occurring at stages of formation, growth, redistribution, thawing and disappearance of ice in the sea. At the same time, a complex structure of sea ice cover, variety of forms, thickness, ridging, heterogeneity of wind and currents create a quite complex picture of ice drift.

At present, there are no universal models of ice which could be used for any of the freezing seas. In this regard, for each specific sea a parameterization is required for many characteristics of the environment influencing the ice processes.

In order to operationally use the sea ice model it must describe the dynamics and thermodynamics of snow and ice cover and allow to simulate changes of ice drift velocity, its thickness and area.

For example, for the description of ice cover evolution in the Baltic Sea the model with several categories of ice state is successfully used, that was developed by the Finnish researchers. In the model ice is divided in 2 main categories: undeformed and deformed ice. In turn, undeformed ice is divided into some categories, and deformed ice - in ridged and layered ice. Layered ice exists when ice thickness is below 17 cm (so-called transfer thickness); at high thicknesses ice belongs to ridged ice category. Evolution of each ice category is described by the equations for concentration (area) and mass of ice, and these equations are solved in the Lagrangian space of ice thicknesses. In each category ice thickness changes as a result of advection, deformation and thermodynamic processes. It is implied that fast ice exists in areas where reservoir depth is less than the set critical value. Also, the snow cover condition is considered in the model.

2.1.2. Models of wind waves

Wave forecasting is a process of assessment of how wave parameters will change under the influence of wind on water surface [Abuzyarov, 2009]. The dependence of wave fields on wind fields determines the close link between wave and meteorological models. Therefore, the development of atmospheric models is also followed by the development of wave models. The improvement of atmospheric models quality lead to the improvement of wave models quality and as a result, to the accuracy of issued forecasts. Besides that, with the more profound understanding of ocean and atmosphere physical processes defining the mechanisms of wave interaction with the near-water air, it becomes more and more evident that these interactions are deeper, than it was represented before.

In deep sea wave models the development of waves is mainly controlled by wind. In calculations of wave parameters initial wind information is provided in the form of a sequence of diagnostic and predictive fields of wind vectors. In shallow sea areas where the relation of wave height to its length is less than 0.5 such factors as bottom topography, coastline relief, etc. have the impact on wave development.

Many dozens of models are applied in the world to reproduce wind waves. They can be divided into four groups: a) spectral discrete models; b) spectral parametrical; c) integrated parametrical; 4) others (empirical, eneregy, monochromatic and their various combinations). Discrete models are conditionally subdivided into generations, that differ in the degree of detailing of description of the mechanism of nonlinear interaction in wind wave spectrum. First three generations use theoretically nonstrict procedures of the interaction integral reduction, such as for example in the widely known WAM model. In present time, there are only two fourth generation models in the world with exact mathematical description of the nonlinear interaction mechanism – EXACT-NL and the Russian atmospheric and wave model of “focused” approximation of wave spectrum (PABM).

The most famlous wave models are the discrete WAM model with its modifications applied in the European Center of Medium-term Forecasts (ECMF) and the WAVE WATCH (WW3) model that is used for wave forecats by the US Weather Service.

The majority of deep sea wave models applied now are based on the numerical solution of the radiation equation for a two-dimensional wave spectrum. The equation of transfer describes the distribution of various wave components in the spectrum with various frequencies and distribution vectors with respective group velocities. Energy of these components changes under the influence of wind, dissipation and nonlinear interactions of high order. By means of wave models the full two-dimensional wave spectrum is calculated on each time step and in each knot of grid area. The equation of energy transfer is as follows:

$$\frac{\partial E}{\partial t} + \nabla(C_g E) = S, \qquad (2.4)$$

where $E = E\ (f,\ \theta,\ x,\ t)$ – two-dimensional wave spectrum (spectrum of surface fluctuations) depending on frequency f and direction of waves θ;
$C_g = C_g(\ \mathrm{f},\ \theta)$ – group velocity in deep water;
S – source function, including various processes such as S_{in} – energy income due to wind; S_{nl} – nonlinear transfer of energy due to wave interaction; S_{ds} – dissipation of energy due to breaking wave crests and internal turbulent friction.

The most important from the modeling point of view is the definition of function $S = (S_{in} + S_{nl} + S_{ds})$. If this function is defined precisely the equation can be integrated under certain initial and boundary conditions that makes it possible to calculate spectral characteristics of waves with accuracy depending mainly on accuracy of initial wind fields. When this function is equal to zero the equation 2.4 describes the distribution of dead swell in deep water. In general case this equation has no analytical solution and is realized by numerical methods.

Estimates of various components in the right part of equation 2.4. show their different time-space scales where various evolutionary mechanisms occur defining the behavior of wind wave field. Study of the mechanisms forming the spectrum is now one of the central problems of wind wave modeling.

2.1.3. Forecasting models of waves

As it was already mentioned in chapter 2 one of the most widely applied models in operational routine of wind wave forecasting is WAM model. The model was developed by the international Wave Modeling Group WAMDI and prepared for practical use. WAM model belongs to the third generation models and is based on numerical integration of equation 2.4. Spectrum is approximated by 26 frequencies and 12 vectors with a 30-degree resolution. Integration time step is 15 min. for the regional version of the model and 1 hour – for the global one.

The mathematical problem is solved in spherical variables that allow to use the model as global. The model is classified as a model of the third generation. In present time, WAM model is perhaps the only wave model where the equation of spectral energy balance is realized in a more complete form. This model is used as operational in ECMF. Two versions of the model are used: first – global, gives wave forecasts up to 10 days ahead on a spherical grid with a 3o step; second version is adapted for conditions of the Mediterranean Sea. It works on a 0.50 resolution grid for a period of up to 5 days. The model also allows to make calculations of waves at shallow areas. The model accounts for refraction and bottom friction, and the function of weak nonlinear energy transfer considers the relevant correction due to variations of weak nonlinear interaction of waves in a basin of finite depth.

WAVEWATCH model. WAVEWATCH model was developed in the USA. In fact, it is the evolution of WAM model concerning the parameterization of source function S, although it uses the same approximation of weak nonlinear interaction as WAM model. WAVEWATCH model applies a more perfect numerical scheme of solution of the equation of wave energy balance than WAM model.

SWAN model. SWAN model (Simulating WAves Nearshore) was developed at Delft Technical University (Netherlands) and is focused on calculation of waves in limited water areas, gulfs, lakes and estuaries. The model is based on wave action balance equation. It calculates wave generation by wind, wave refraction due to currents and drop of depths, dissipation due to breaking waves ("white-caps"), and influence of bottom friction. Wind and current fields serve as initial information. Results of calculation are presented as a field of wave heights. In addition, the model produces fields of wave lengths and periods as well as wave vectors.

The equation of wave balance is:

$$\frac{\partial}{\partial t}N+\frac{\partial}{\partial x}c_xN+\frac{\partial}{\partial y}c_yN+\frac{\partial}{\partial \sigma}c_\sigma N+\frac{\partial}{\partial \Theta}c_\Theta N=\frac{S}{\sigma}, \tag{2.5}$$

where N – action density spectrum.

In the left part of equation the first term describes the local velocity of action density variability, the second and the third – action distribution (with respective velocities of distribution c_x and c_y in x and y space), the fourth – change of relative frequency due to change of depth field and current field (with distribution velocity c_σ in σ-space), the fifth – refraction of waves induced by variations of depth and current fields (with distribution velocity c_Θ in Θ-space). The right part of equation - source in terms of energy density, reflecting the effects of generation, dissipation and nonlinear interaction of waves.

SWAN can estimate wave transmission through a (line-) structure such as a breakwater (dam). Such an obstacle will affect the wave field in two ways, first it will reduce the wave height locally all along its length, and second it will cause diffraction around its end(s). The model is not able to account for diffraction. In irregular, short-crested wave fields, however, it seems that the effect of diffraction is small, except in a region less than one or two wavelengths away from the tip of the obstacle. Therefore the model can reasonably account for waves around an obstacle if the directional spectrum of incoming waves is not too narrow. Since obstacles usually have a transversal area that is too small to be resolved by the bottom grid in SWAN, an obstacle is modelled as a line. SWAN can operate in first-, second- and third-generation mode.

2.1.4. Models of oil pollution

Along with hydrodynamic models of state of the marine environment, operational forecasting systems include models of distribution and transformation of oil pollution as a most widespread type of marine pollution.

By now, there is a rather large number of models developed and applied for calculation and forecasting of emergency oil spills. The applied models dependending on the solved tasks vary from simple modeling of pollution plume trajectory (drift or trajectory models) to complex three-dimensional models of transfer and transformation of oil pollution.

The majority of existing models simulate the processes of spreading, advection and diffusion of oil and a standard set of transformation processes that usually includes evaporation, wind wave dispersion of oil in water, emulsification. They use the same or similar (with small variations) semi-empirical relationships obtained on the basis of results of laboratory and field experiments in 1980s [Reed et al., 1999]. As a rule, the models do not consider the processes of dissolution, photooxidation, chemical and biological decomposition of oil hydrocarbons. In addition, three-dimensional models calculate the distribution of oil hydrocarbons in water column and sedimentation.

We will consider the models that now are most widely applied in practice and, in principle, to some extent meet the formulated requirements. It is important to note that not all oil spill models are distributed commercially but free of charge.

The Baltic Sea operational oceanographic system (OOS) includes the model of calculation of oil pollution SEATRACK that was specially developed at Swedish Meteorological and Hydrological Institute (SMHI). The model simulates transfer and transformation of oil pollution in operational mode, gives forecasting parameters of pollution and calculates the “reverse” transfer of pollution for a period of up to 10 days. Together with the use of vessel tracking information system, such calculations allow to identify a polluting vessel for imposing of penalties. Basically, the model is a well developed drift model. Threedimentionality of the model is demonstrated in its ability to calculate the distribution of tracers with neutral buoyancy. Ice cover influence is considered by restricting the area of pollution distribution. Underwater sources are not considered.

For operational calculations of oil pollution transfer and transformation in the North and Norwegian Sea and the western part of the Barents Sea the OSCAR model is used, developed at Norwegian institute SINTEF. The model is coupled with a specially developed model of oil transformation OWM (Oil Weathering Model) which is based on results of numerous experimental studies of different types of oil and oil products. The model simulates the distribution of the dispersion plume in the top layer of water. Ice cover influence is accounted by restricting the area of pollution distribution during its spreading and evaporation. Besides, the solid ice influence on oil transfer is also considered. The model also considers pollution from underwater sources.

There is a notable complex of software products developed in the USA in Applied Science Associates (ASA). The models were widely applied and used for calculations on water areas of the US east coast, Australia, Brazil, etc. The model complex includes a model of oil pollution transfer and transformation OILMAP, a three-dimensional model of oil distribution SIMAP, model of oil pollution from underwater sources OILMAPDEEP and ten more environmental models (www.asascience.com). All ASA models use the interface developed on the basis of ESRI GIS technology. The models can be used in operational mode. Ice cover influence is not considered.

In the coastal waters of Portugal and Spain the model complex MOHID is used for calculation of oil pollution transfer and transformation developed by MARETEC group at Portuguese Technical University and including a three-dimensional hydrodynamic model and a module of oil pollution transfer and transformation. The oil module considers all main processes of oil transformation, including processes of increasing density and viscosity. After coupling with the Spanish weather model the operational system METEOMOHID was formed. The model simulates the distribution of the dispersion plume in the top layer of water. The influence of ice cover and pollution from underwater sources is not considered in the model.

For calculation of oil pollution transfer and transformation in the Black and Azov Seas the OILTOX model was developed in Institute of Problems of Mathematical Machines and Systems of NAS of Ukraine. The model has a good theoretical basis and can be applied in operational mode. The special attention in the model is paid to the process of oil slick vertical dispersion by wind waves. The model is three-dimensional but it considers only the distribution of dispersion plume and oil drop adsorption on suspended organic particles. The influence of ice cover and pollution from underwater sources is not considered in the model.

In Russia the development of operational oil models is not so popular as abroad. The preference is given to well-known foreign developments. Thus, Northwest Hydrometservice uses SEATRACK for oil pollution distribution forecasting, the Murmansk Administration - OSCAR+OWM. An exception here is the operational system VOS-RT applied for the water area of the Sakhalin shelf and based on the Far East Hydromet Research Institute model and the SPILLMOD model developed at State Oceanographic Institute [Ovsiyenko et al., 2005;]. The model considers the transfer and transformation of oil pollution only at sea surface, pollution from underwater sources is not considered in the model. The model has a modification accounting for low temperatures and ice. In addition to that, calculations require the setting of ice cover characteristics – concentration, thickness, characteristic size of ice floes, their arrangement (distance between ice floes), direction and drift speed. Unfortunately, now ice models are not capable to simulate the characteristic size of ice floes and their arrangement. Therefore, such approach being physically reasonable on one hand, on the other remains so far low-suitable at operational calculations of emergency oil spills in freezing seas.

According to observations and results of retrospective modeling [Reed et al., 1999] the speed of oil transfer significantly decreases depending on ice conditions, and the direction of transfer of an oil slick deviates on up to 60° from the predicted transfer direction without ice cover. Therefore, the parameter depending on concentration of ice in neighboring grid knots is introduced in calculations of the spillet speed and transfer direction.

The model of transfer and transformation of oil pollution in the Arctic freezing seas OilMARS developed in Arctic and Antarctic Research Institute (Oil Spill Model for the Arctic Seas) [Stanovoi, et al., 2007] considers the transfer and transformation of oil pollution on the sea surface as a result of emergency continuous/instant oil spills from stable or moving sources, as well as distribution of detected surface oil spills. Now the model operates in the three-dimensional mode simulating the in-water distribution of the dispersion plume and submerged oil. The model is capable to calculate the occurrence and distribution of secondary oil pollution on water surface and seafloor pollution. Besides that, the model accounts for the influence of ice cover concentration and drift on pollutant distribution, as well as oil pollution of the top surface of ice cover and under ice area as a result of drifting ice compression. The model was finalized for operational work and inclusion in OOS of the Arctic Seas [Stanovoi, et al., 2009]. The approach used in the model allows to simulate the behavior of oil during ice compression. When ice concentration is increased up to score 10 the probability of oil occurrence on the ice surface or under ice is equal. Therefore, a random coefficient from 0 to 1 was introduced that defined what part of spillet mass occurs on ice. At the same time, the rest of oil is considered to occur under ice.

Once oil gets on the ice surface it spreads across the surface continuing to evaporate, and is partially absorbed by ice and transferred by the drifting polluted ice floe. To simulate the process of oil spreading on the ice surface and calculate the depth of oil penetration into the ice the semi-empirical parametrizations were used obtained during laboratory and experimental studies. Also, the model considers the case of instant oil discharge on the top ice surface.

For calculation of the process of oil spreading under the ice the semi-empirical equation for a horizontal and rather smooth lower surface of ice is used, i.e. it is assumed that the horizontal size of an oil spill is less than distances between the ice roughnesses limiting oil spreading. As the experimental studies showed, oil transfer against the lower ice surface starts when some critical velocity of water current is achieved. When current velocity is less than critical value, oil moves together with ice. The value of critical velocity is a function of oil density, oil–water surface tension, ice roughness and oil slick thickness. Also, the model considers the possibility of pollution of ice lower surface when oil rises and secondary pollution occurs in the drifting ice zone.

In order to account for ice concentration influence on the processes of oil spreading on water surface, evaporation, vertical dispersion and horizontal diffusion in the OilMARS model it is necessary to limit the area of the spill and increase its thickness, i.e., in principle, this does not differ from the approach applied in OSCAR+OWM.

2.2. Assimilation of observational data in numerical models

The success of an oceanographic forecast for small limited areas of the sea is determined by both perfection of used hydrodynamic model, and quality of the forecast of atmospheric characteristics, initial conditions and boundary conditions at the liquid part of the border. The last factor – setting the forecasting conditions on the liquid part of the border – is a key problem of the oceanographic forecast, which successful solution determines to a great extent the quality of final result. In fact, the hydrodynamic model itself can be upgraded, providing the improvement of calculation quality of hydrodynamic fields. Boundary conditions on the sea surface are set based on some operational atmospheric model that gives forecasts using real time data on atmospheric characteristics. Initial conditions in the investigated basin, taken as a rule from results of the previous forecast, can be “corrected” by observational data using modern methods of assimilation. And quality of conditions on the liquid border is completely determined by another (external) operational oceanographic model which unlike atmospheric models uses limited number of field data, and worsens as a result of inevitable interpolation from the external model grid on the grid used by the main predictive model. Thus, the only way for the developer to improve the oceanographic forecast of the studied sea area – to assimilate in operational mode the highest possible volume of data of observations including satellite information.

Assimilation of observational data in a numerical model is a complex and independent task in operational oceanography. There are various approaches and methods of assimilation of data that will be considered in the following chapter of the textbook.

Chapter 3. HYDROMETEOROOGICAL DATA ASSIMILATION IN OPERATIONAL OCEANOGRAPHY

3.1. The problem concept OF Observation data assimilation

Main purpose of an operational oceanographic system can be defined as production of information on the current state, the future state (forecast), and the past state (retrospective forecasts or re-analysis) of the ocean.

The major source of information about the ocean is observation data. Many different measuring methods are available today. These observations may include fixed point measurements (anchored moorings), marine environment characteristics profiles obtained by a CTD or a spatial distribution map of a variable based on remote sensing data, etc. However any of the marine environment characteristic observations are always fragmentary, i.e. correspond to a specific spatial and temporal location only, and also have certain limitations; for example, Argo drifters transmit measurement data once every 10 days, thought the satellite surface temperature product with high spatial resolution of about 1km is available more often than once a day, but a cloud cover may considerably limit the product coverage. Besides, the observations provide information on specific parameters of a dynamic system, while the rest of the system state remains unknown; therefore no observations can provide a complete understanding of a 4-dimensional state of any dynamic system.

Another popular method of a dynamic system study is mathematical modelling. However, it is important to keep in mind that a model is merely an approximate description of some real object. Moreover, the model equations, which are used to describe a state of any system, are not flawless. The latter are restricted by our limited knowledge of dynamic system driving processes. Furthermore, the equations are written in discrete form and are subjected to resolution limitations. Generally a regional hydrodynamic model have one mile as a minimal horizontal spatial resolution, and 1 meter as vertical resolution, therefore the grid does not allow a number of processes to be resolved, which, therefore, have to be described parametrically. The most common example is turbulent mixing coefficients determination; all modern turbulence closure schemes contain some kind of parameterization with multiple undefined numeric constants.

While one of the mathematical modelling challenges has been described above, there is another, which is not less relevant. Any numerical simulation is very sensitive to a set of initial conditions, which are defined on in accordance with available observation data. As mentioned above, the latter are always fragmentary and may not reflect a real system state. This problem is getting even more complicated when we take in consideration the fact that motion interactions of different spatial and temporal scales are nonlinear. Nonlinear interaction leads a dynamical system driven into unsteady state. This means that any two initially close states of a system are not preserved in time. This leads to increased discrepancy between a model and a real dynamic system state.

A solution to the challenge described above comes as a joint use of observations and mathematical modelling. In particular, the procedure of mathematical model calculations correction with experimental data is the problem of observation data assimilation. The main purpose of observation data assimilation is to improve our understanding of ocean processes, to enhance monitoring and forecasting on various temporal and spatial scales.

The procedure of "assimilation" is an essential component of operational forecasting; it is engaged to improve the predictive quality of numerical models by constantly renewed forecasts which take in consideration the difference between previous projections and recent data. General idea of an assimilation scheme, which is a part of ocean thermo-hydrodynamic model, is presented in figure 3.1.

Modern data assimilation techniques are also used for re-analysis of a dynamic system [Daley R., 1991]. Field re-analysis is a product with specific characteristics: firstly, it represents a three-dimensional reconstruction of the object's state as close to the real state as possible, secondly, it is used as initial conditions of a numerical simulation, and finally it can be used for models tuning.

Data assimilation is used not only for retrospective, short-term and long-term forecasts. It can provide a quality control mechanism for operational observing systems. In some cases, assimilation models can identify questionable observations operationally and possibly reject them, based on a comparison with the corresponding model predictions, and taking into account the statistical distribution of errors. A sequence of incorrect observations can help identify a faulty device, which should be promptly repaired.

The practices of process models and observations combination result in gaining of substantially more insightful observations. Indeed, measurement data in their nature have absolutely specific area of significance, presenting a characteristic function of a system state at precisely that location and time

Figure 3.1 – General algorithm of an assimilation process

where and when observations have been made, due to this fact, observations are always fragmentary. When observations are used in conjunction with process models, information content of data increases significantly, that is because the process of assimilation allows "vision" of spatial and temporal scales at which observation data has its "influence".

These days, an operational system is unthinkable without a data assimilation procedure. This has become possible, primarily due to development of computer networks and supercomputers and availability of high-speed communications, as well as the advent of large arrays of observed information available in near real time: such as satellite observations and automatic buoys. All this requires to develop an appropriate mathematical apparatus and to design robust implementation algorithms.

Key challenges, which are to be solved in implementing of assimilation procedures are listed below:

– data assimilation – is the inverse problem, i.e. a finite number of discrete observations are to serve to describe a continuous field of a function, which contains an infinite number of points ;

– inverse problems are always incorrectly formulated problems. A problem is considered properly formulated when it complies with three conditions: the existence of a solution, uniqueness of the solution and the solution continuous in the observed data in some reasonable domain. The third condition is never fulfilled because of the discrete nature of simulation both in time and in space. Even in the case of assimilation the resultant field from the point of view of the inverse problem solution is not fully the defined. An outcome, in fact, presents a set of fields that exactly match the observations and the modelled result, thus the solution is not unique;

– ocean dynamics is not linear, whereas most of the methods for the inverse problem solution calculation are based on linear approximations;

– any model and the data are incomplete and contain uncertainties;

– majority of data available for assimilation into a numerical model are measured in the ocean surface layer only, for example, data on the sea surface temperature or altimetry information.

A list of different methods to assimilate observation data can be found in literature, for example, in [Daley R., 1991, Wunsch C, 1996], various assimilation schemes with respect to Oceanology applications are discussed in. Here we range the main assimilation techniques, which gained wide acceptance in oceanography, according to the complexity degree of their implementation:

– Cressman analysis, which belongs to "objective analysis", a successive correction method (SCM), relaxation schemes,a nudging method (attracting);

– Kalman filter, a method of Optimal interpolation

– Three-dimensional variational analysis (3D-var)

– Four-dimensional variational analysis (4D-var), Extended Kalman filter.

3.2. Simple Assimilation Schemes

It is essential to introduce the basic concepts and terms used in the mathematical formulation of a data assimilation problem before looking at the functional principles of various assimilation schemes.

The state vector x. Vector containing information about the state of a dynamical system, here can be presented as:

$$x = \begin{bmatrix} \zeta \\ T \\ S \end{bmatrix},$$

it may as well contain information about currents velocity or about any other parameters of the ocean state.

The analysis x_a. The result of an assimilation procedure is usually referred to as the analysis, which represents a state of a dynamic system that is closest to a real state. A “real state” is considered to be real on the basis of available observation data and only in the case when all the dynamical system physical laws are satisfied. In practice the analysis assumes a form of various fields of marine environment characteristics (i.e. temperature, salinity, level, current velocities, etc.).

Preliminary forecast or background state (background) x_b is a predicted state of a dynamical system before calling an assimilation procedure. A model solution can be accepted as a background state as well as and long-term averages – climatic values.

True state x_t is the true state of a dynamical system, which, in practice, can never be known.

Observation vector y. is a vector that contains all the information from observation data.

Increment vector ∂x is is the so-called analysis increment vector, which is defined as the difference between the sought state vector (analysis) x_a and the background state vector x_b.

Here we consider one of the simple assimilation schemes. Let us assume an assimilation procedure as an algorithm in which the analysis is equal to an observed value in the neighbourhood of this particular observation at some particular state (it can be both climate averages and the preliminary forecast value). This approach forms a basis for the Cressman analysis [3].

Consider a one-dimensional discrete field of any sought parameter $x_b(i)$ at the nodes of the model space i, determined by climate averages or the preliminary forecast value, $y(j)$ - the observed values of the same parameter at observation points j = 1, ... m. Modelled state x_a obtained from the analysis of Cressman at each point of the model field i, can be described by the following equation:

$$x_a(i) = x_b(i) + \frac{\sum_{j=1}^{m} w(i,j)\{y(j) - x_b(i)\}}{\sum_{j=1}^{m} w(i,j)}, \quad (3.1)$$

$$w(i,j) = \max\left(0, \frac{r^2 - d_{i,j}^2}{r^2 + d_{i,j}^2}\right), \tag{3.2}$$

where $d_{i,j}$ is the distance between the nodes of the calculated model field i and the observation points j, $w(i,j)$ is a weighting function, which is equal to 1in the case when the points i and j coincide, in this case, the background value is replaced by the observed, r = const is the radius of influence, so that if $w(i,j)$ exceeds r the weight function of this observation is 0.

In figure 3.2 you can see an example of action analysis Cressman. The analysis represents an interpolation between the background state and the observation value in the neighbourhood of each observation, while the value of the weighting function becomes greater the closer it is to the observation point.

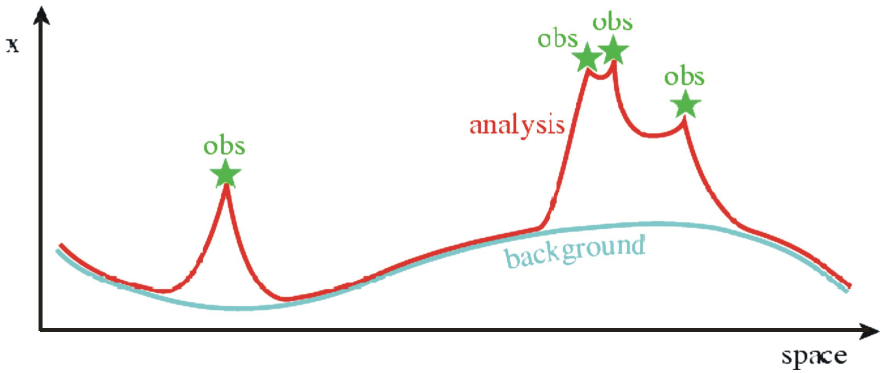

Figure 3.2 – Cressman analysis

Thought there are many variations of the Cressman analysis, the essence remains the same. Each variation of the method has different form of the weight function; for example it can be presented as:

$$w(i,j) = \exp\left(-d_{i,j}^2 / 2r^2\right).$$

A method of successive corrections (SCM) and a nudging method can also be considered within this group [8]. The difference from the Cressman analysis method is that the weighting function at the point of observation cannot be equal to 1. In practice, these methods are not necessarily to be applied for the only one step, but a relaxation scheme can be applied, i.e. a correction of the model fields is made for each of a few iterations, making the analysis of the field smoother.

Of course with a certain model fit good results can be achieved, but there are no reasonable assumptions for the best type of weight function selection. From a practical standpoint any application of the Cressman analysis is not satisfactory according to the following provisions:

– if a preliminary assessment of the model state is of a quite good quality, there is no need to replace it with observation data of a poorer quality ;

– moving away from the point of observation is not clear how the analysis field should tend to the background state, in other words, the question arises as how to determine the form of the weight function ;

– the analysis must conform to the basic physical laws of the system, such as smoothness (continuity) of solutions and interrelation with other variables (hydrostatic and geostrophic balance, behaviour at the border). The Cressman analysis does not guarantee that there are no unphysical phenomena in the solution.

Therefore the Cressman analysis can only be used as a primary tool.

3.3. Probabilistic Approach to Observation Data Assimilation Problem

So, what requirements are necessary to fulfil to obtain the analysis of a satisfactory quality?

– the most crucial is a model that produces a good quality preliminary forecast, i.e. if our model is basically inadequate and does not describe the main features of the system's behaviour, then no assimilation is able to correct it;

– it is assumed that the analysis field belongs to the distance between the real state and the observation data, that is when a sufficiently dense data field is used. In this case the analysis should better fit the data , which we trust more, while the " suspicious" observations (less representative) should obtain much less weight ;

– the analysis field should be smooth, since it is natural for real physical fields. Therefore, the further the point with the data from the node the more the analysis should tend to the background values while changing smoothly within the scale of the predicted parameters typical variability;

– the analysis has to satisfy both the physical laws of the system and the ability to simulate natural anomalies, as the most important part of a forecast is to produce extreme behaviour and catastrophic events.

To summarize: a data assimilation procedure should employ information on observation data, background state and physical laws knowledge of the dynamical system in concideration. It is important to note that any data are an additional source of information, but at the same time they should not be taken as true, a compromise takes place as there are errors in the model and in the observation data, and there is never any certainty, which are true. Consequently, it is necessary to find a method that will minimize the average difference between the analysis and the true state of a dynamical system.

To create a computational algorithm an uncertainty of data has to be mathematically described (for both observations and preliminary forecast). This is possible with the involvement of a probabilistic approach. Assimilation algorithm must be based on formal requirements while the subjective approach should be minimized. In this case, the assimilation procedure can be imposed as an optimization problem.

The existing uncertainty of a preliminary forecast, of the analysis and of observation data have to be presented in order to apply the probabilistic approach to the observation data assimilation problem. The uncertainties are resented by defining errors between these values and the true state.

– *preliminary forecast errors* ε_b, where $\varepsilon_b = x_b - x_t$ is the difference between the background state vector (preliminary forecast) and the true state vector. Note that the errors associated with discretisation are not considered here. Error covariance matrix has a form of:

$$\mathrm{B} = \overline{\left(\varepsilon_b - \overline{\varepsilon_b}\right)\left(\varepsilon_b - \overline{\varepsilon_b}\right)^{\mathrm{T}}},$$

where the superscript T denotes the matrix transposition;

– *observation data error* ε_0, where $\varepsilon_0 = y - H(x_t)$ is the difference between the observation data vector and the true state vector, $H(x)$ is the so called observation operator, which provides a transition from the model space to the observation data space. In practice, the operator H is an operator that interpolates the model grid points to the data observation locations. For observational data error the the observation error covariance matrix takes a form of:

$$\mathrm{R} = \overline{\left(\varepsilon_o - \overline{\varepsilon_o}\right)\left(\varepsilon_o - \overline{\varepsilon_o}\right)^{T}}.$$

R includes instrument errors, the errors of measurement and dis-cretisation errors.

– *analysis error* ε_a, $\varepsilon_a = x_a - x_t$ is the difference between the analysis and the true state of the system. The covariance matrix of error analysis has a form of:

$$\mathrm{A} = \overline{\left(\varepsilon_a - \overline{\varepsilon_a}\right)\left(\varepsilon_a - \overline{\varepsilon_a}\right)^T}.$$

Actually the assimilation problem is to minimize the analysis error.

When the averaged errors are not equal to zero, it indicates the presence of some systematic errors, which can occur in the model itself, in the observation data used and in the assimilation procedure.

3.4. Stochastic and Variational approach for observation data assimilation

Wes shall consider the linear analysis method based on the least squares method. Suppose we have a preliminary forecast vector x_b of n dimension and a observations vector y of dimension m, then the dimension of the error covariance matrix B of a preliminary forecast is equal to $n \times n$, R dimension $m \times m$ and A dimension $n \times n$. Let us make the following assumptions:

– observation operator variability is linear and for all x sufficiently close to x_b $H(x) - H(x_b) = H(x - x_b)$ is true, here H is a linear observation operator, representing a linear procedure for interpolation of the modelled simulation results to the locations of the observation data.

– covariance matrices B and R both are positively definite matrixes.

– preliminary forecast and observation errors are random variables, i.e. $\overline{\varepsilon_b} = \overline{\varepsilon_0} = 0$ and they are uncorrelated $\overline{\varepsilon_b \varepsilon_0^{\mathrm{T}}} = 0$.

Linear analysis suggests that the analysis field is determined by correction vector of a preliminary forecast, which is linearly dependent on the difference between the preliminary forecast and observation data. At the same time an optimal analysis is sought as a closest state to the true state, which, in this case is based on the method of least squares, i.e. on minimization of the analysis error dispersion.

Below we consider two fundamentally different approaches to data assimilation which are stochastic and variational approaches.

Stochastic approach is based on the interpolation equations solution:

$$x_a = x_b + \mathrm{K}\left(y - H\left[x_b\right]\right), \tag{3.3}$$

$$\mathrm{K} = \mathrm{BH}^{\mathrm{T}}\left(\mathrm{HBH}^{\mathrm{T}} + \mathrm{R}\right)^{-1}, \tag{3.4}$$

where K is a linear operator, which inherently represents a matrix of weights. Covariance matrix of errors K for each analysis may be defined as:

$$\mathrm{A} = \left(\mathrm{I} - \mathrm{KH}\right)\mathrm{B}\left(\mathrm{I} - \mathrm{KH}\right)^{-\mathrm{T}} + \mathrm{KRK}^{\mathrm{T}},$$

here I is the identity matrix, and for the least squares method,

$$\mathrm{A} = \left(\mathrm{I} - \mathrm{KH}\right)\mathrm{B}. \tag{3.5}$$

Thus the stochastic approach for the assimilation problem comes down to the matrix K determination.

Variational approach is based on the solution of the variational optimization problem. In this formulation, the analysis is sought as the state vector, in which there is a minimum of cost function J:

$$J(x) = (x - x_b)^{\mathrm{T}}\mathrm{B}^{-1}(x - x_b) + (y - H[x])^{\mathrm{T}}\mathrm{R}^{-1}(y - H[x]) = J_b + J_o, \tag{3.6}$$

The first term of the cost function J_b is associated with the background state, the second J_o with the observation data. The cost function is quadratic and it meets its minimum when the gradient function is equal “0”:

$$\nabla J\left(\mathrm{x_a}\right) = 0 = 2\mathrm{B}^{-1}\left(x_a - x_b\right) - 2\mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\left(y - H\left[x_a\right]\right), \tag{3.7}$$

$$0 = \mathrm{B}^{-1}\left(x_a - x_b\right) - \mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\left(y - H\left[x_a\right]\right) - \mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\left(x_a - x_b\right), \text{ then}$$

$$x_a = x_b + \left(\mathrm{B}^{-1} + \mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\mathrm{H}\right)^{-1}\mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\left(y - H\left[x_a\right]\right). \tag{3.8}$$

Therefore the variational approach for the assimilation problem comes down to finding the minimum of the cost function.

We prove here that both the stochastic and variational approaches to observation data assimilation are equivalent for the least squares method usage. In order to do this, we must prove that

$$x_a - x_b = BH^T(HBH^T+R)^{-1}(y-H[x_b]) = (B^{-1}+H^TR^{-1}H)^{-1}H^TR^{-1}(y-H[x_b]) \quad \Rightarrow$$

$$BH^T\left(HBH^T+R\right)^{-1} = H^TR^{-1}\left(B^{-1}+H^TR^{-1}H\right)^{-1} \Rightarrow$$

$$BH^T\left(B^{-1}+H^TR^{-1}H\right) = H^TR^{-1}\left(HBH^T+R\right). \qquad (*)$$

Transforming the right side (*):

$$H^TR^{-1}(HBH^T+R) = H^TR^{-1}HBH^T + H^TR^{-1}R = H^T + H^TR^{-1}HBH^T = BH^T(B^{-1}+H^TR^{-1}H)$$

which is what we set out to prove.

So, there are two mathematically equivalent algorithms for solution of the observation data assimilation problem :

– stochastic approach based on the direct determination of the weights matrix K;

– variational approach based on the minimization of the cost function .

These algorithms have different mathematical implementation, and their equivalence is violated as soon as the basic hypotheses are not confirmed, such as linearization of observation operator.

The main complication that arises in the implementation of both stochastic and variational algorithms consists in the definition of the covariance matrixes of either background state error B or observations R. They cannot be defined straightforward and, therefore, have to be modelled on the basis of knowledge about physical processes and measurement techniques. Another challenge is that in the modern average oceanographic hydrothermodynamic model dimension is $n = 10^7$, the dimension of the observation data rarely exceeds $m = 10^4$, then the dimension of the preliminary forecast error covariance matrix B will be $n \times n = 10^{14}$, and for $R - m \times m = 10^8$. Inversion of such a high order matrix requires enormous computing resources, which in principle are not achievable on modern computers. When setting the observation error covariance matrix R it is often assumed that the errors are uncorrelated in the observation space, thus, R degenerates into a diagonal matrix that allows it to specify a constant value for each type of observation. For instance, in the first approximation, in the operational model Northern/

Baltic DMI-BSHcmod for assimilation of such observations as profiles of temperature and salinity obtained from buoy stations and measurements made in the course of the ship (ferry boxes), R is equal to the standard deviation of temperature observations and salinity, namely, 0.5 °C and 0.5 ‰. For assimilation of satellite sea surface temperature (SST) R mainly assessed with the use the error SST field product supplied by developers. Determination of a covariance matrix of the background error condition is not less difficult, solutions to this problem will be discussed later in the description of the various methods of data assimilation of observations.

3.4.1. Optimal interpolation method

The method of optimal interpolation (OI) refers to the assimilation of stochastic methods and is simple enough for numerical implementation. The mathematical formulation is described by equations (3.3) and (3.4).

The OI fundamental hypothesis is that for each model variable only some observations are important in determining the increment vector (figure 3.3). Therefore, for each modelled variable *xi* corresponds a small number of observations *pi*, which are selected using statistical criteria (e.g. , the correlation distance). Thus, the covariance error matrix dimension of the background state vector and the of the observation data is reduced to $p_i \times p_i$. In this case, mucg smaller dimension matrix inversion is possible and does not require large computational resources.

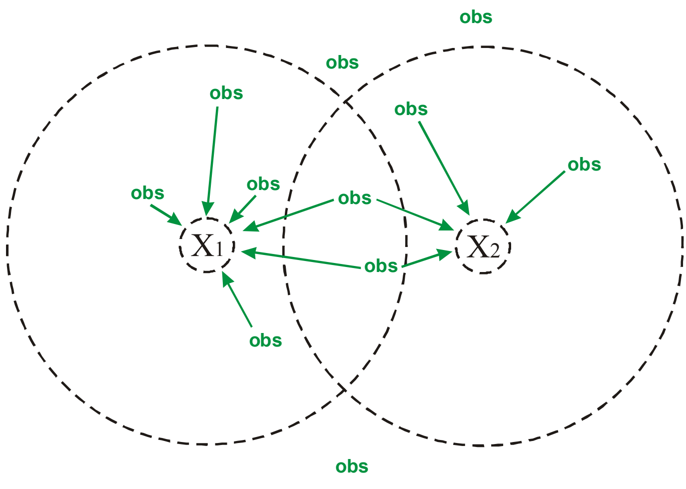

Figure 3.3 – One of the observation data OI schemes [Reed et al., 1999]

In relation to the Baltic Sea, the operational model of the Baltic Sea HIROMB, which is implemented in the Swedish Meteorological and Hydrological Institute (SMHI) uses optimal interpolation method quite successfully [14] for assimilation of satellite sea surface temperature and vertical temperature and salinity in-situ profiles obtained by research vessels expeditions and buoy stations. To identify the correlation radius of SST correlation coefficients between dissimilar points with the rest of the SST field were analysed (figure 3.4). Correlation coefficient of 0.5 was chosen as a criterion, as seen from Figure 3.4 the distance between points in this case rarely exceeds 50 km, thus this value has been taken as the correlation radius of the optimal interpolation algorithm implementation.

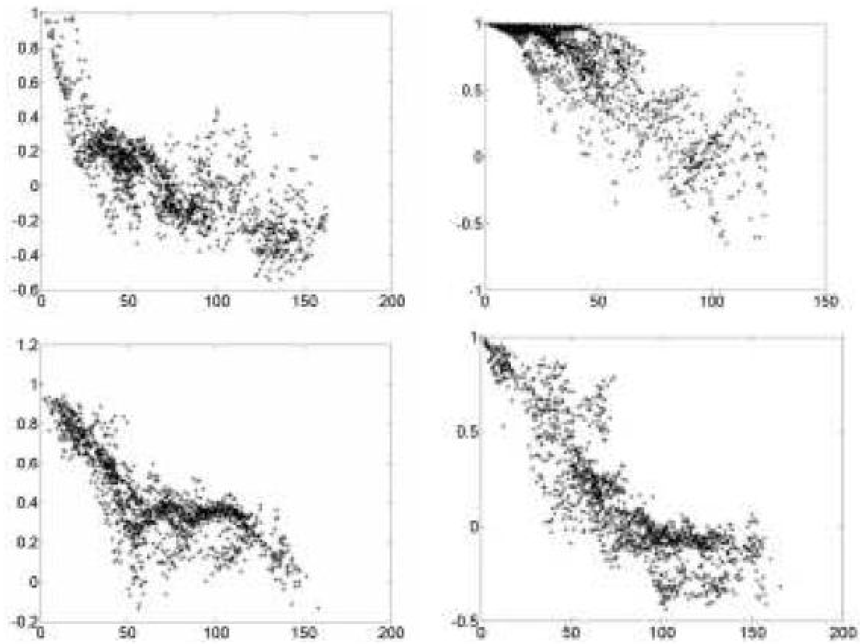

Figure 3.4 – Corelation coefficients between SST in the randomly chosen four points and the observational values in the other points. On the abscissa – distance in km, On the ordinate – dorrelation coefficient value

3.4.2. Three-dimensional variational data assimilation scheme (3D-VAR)

Solution of the assimilation problem with the use of variational method is fulfilled by determination of a certain functional minimum, which describes “closeness” of the model solution and the observation data in a given metric. For implementation of the functional minimization the quadratic cost function mentioned in (3.6) procedure is used. The procedure of the cost function minimisation determines the required increment vectorδX. To find the minimum of the cost function must also define its gradient (3.7). Iterative process redefines the increment vector takes as many operations as needed for the gradient of the cost function to be equal to zero within some prescribed accuracy, which would correspond to finding the extremum of the cost function (its minimum). The result of the assimilation procedure describes a state of a dynamical system (analysis x_a), which is closest to reality, based on the available observation data and modelled preliminary forecast.

Assimilation scheme involves 3D-VAR error covariance calculation for all pairs of variables in the model, as has already been mentioned it is unrealizable on modern computers in principle, because of the need for inversion of background error covariance matrix B. The literature presents many embodiments of the assimilation scheme 3D-VAR, we consider one of the ways to implement 3D-VAR procedure, the problem of high dimensionality of the matrix B, is solved by the transition from the physical space, where all the state vectors are determined, to the virtual space of reduced dimensionality.

We represent the error background state covariance matrix as follows:

$$\mathrm{B} = \mathrm{V}\mathrm{V}^{\mathrm{T}}, \tag{3.9}$$

wherein the cost function is defined using a new control vector v, which is obtained by using a transforming matrix V+, close to the inverse matrix V:

$$\mathrm{v} = \mathrm{V}^{+}\delta\mathrm{x}\,. \tag{3.10}$$

In this formulation, the cost function and its gradient will take the form:

$$J = \frac{1}{2}\mathrm{v}^{\mathrm{T}}\mathrm{v} + \frac{1}{2}\left(\mathrm{HVv} - \mathrm{d}\right)^{\mathrm{T}} \mathrm{R}^{-1}\left(\mathrm{HVv} - \mathrm{d}\right). \tag{3.11}$$

$$\nabla J\left(\mathrm{v}\right) = \mathrm{v} + \mathrm{V}^{\mathrm{T}}\mathrm{H}^{\mathrm{T}}\mathrm{R}^{-1}\left(\mathrm{HVv} - \mathrm{d}\right). \tag{3.12}$$

Thus, the two separate spaces are described, the first is a virtual space of a reduced dimensionality, where control vector v is defined, and the other is a physical space, where the desired increment δx is defined, while the transforming matrix V provides a transition between these spaces.

Transforming the matrix V can be represented in the form of a linear operators sequence:

$$V = V_D V_{uv} V_H V_V, \tag{3.13}$$

where V_D – divergence damping filter; V_{uv} - velocity operator; V_H - horizontal covariance; V_V - vertical covariance.

The described algorithm differs due to the background error matrix split into the horizontal and vertical components. Horizontal covariance is modelled using recursive filter based on the Gaussian function, which require the assignment of the correlation radius for determining. Quantitative estimates of the correlation radius is necessary to obtain on the basis of statistical processing of a large observations number. The vertical component is modelled using empirical orthogonal functions (EOF), describing the vertical variability estimated for the calculation period, which in its turn significantly exceeds the period of forecast . In practice , only the most significant EOFs are used, which number is considerably less than the model state vector size, so the dimension of the arguments of the cost function is also reduced.

V_{uv} velocity operator is responsible for the consistency of the resulting assimilation fields with the rest of the solution, namely , for the amendment of the velocity field, which are induced by the changes due to the density field assimilation. The latter operator V_D is a recursive filter designed to remove divergent zones in velocity fields that occur near the coastline. This is due to the fact that the for the high seas the V_{uv} operator provides a dynamic balance between the increments to the provisional values of speed , level, salinity and temperature. At that the condition of impermeability normal to the shoreline for the velocity component is not satisfied.

3.4.3. Background states covariance error matrix modelling

One of the technical problems of data assimilation algorithms for matrix inversion is the background state with a very large dimension of ~ $10^7 \times 10^7$. One possible way of dimension reduction , as shown above, is the use of principal component analysis or empirical orthogonal functions (EOF). There are implemented for the inverse problem solving where the transition from low-dimensional virtual space to the physical space is fulfilled. In the basics of the EOF the singular value decomposition is applied to the background state covariance error matrix, according to which any matrix L, consisting of real numbers can be represented as:

$$L = U\Sigma V^T, \tag{3.14}$$

wherein U and V — orthogonal matrixes. Elements Σii on the diagonal of Y matrix are called the singular values of the matrix L. Columns of the matrices U and V are called the left and right singular vectors.

If the elements of the matrix Y are in descending order, the rank of the matrix L can be reduced to k, replacing minor eigenvalues with zeros then the expression for the matrix L_k can be rewritten as follows:

$$L_k = U_k \Sigma_k V_k^T, \tag{3.15}$$

here the matrices U_k, Σ_k and V_k are obtained from the corresponding matrices in the singular value decomposition of the matrix L by cutting it off to exactly k first columns. Approximating of the matrix L by a matrix of lower rank, we perform a type of compression of the information contained in L: L matrix of the $n \times n$ size is replaced by smaller matrixes of the size $n \times k$ and $k \times n$ and a diagonal matrix with k elements. In this case the compression is lossy, while the approximation retained only the most essential part of L.

Thus, the meaning of an expansion in orthogonal components is that of a large number of information, primarily the maximal characteristic (singular) numbers and the corresponding eigenvalues (singular) vectors are selected. They describe the main features of the considered initial field, and their contribution to the overall variability of the field is determined by the characteristic number. With increasing numerical order of the eigenvalues the eigenvectors will describe all the less significant (minor) features of the original data.

3.4.4. Four dimensional variational data assimilation (4D-VAR)

4D-VAR presents a use of a 3D-VAR scheme for observation data spread in time. The same mathematical formalism is used here, but comparison of the observation data and model solution is synchronized within a certain period of time, the so-called assimilation window.

At a certain time interval analysis x_a belongs to the initial time, while observations are spaced within some time interval, then y_i, x_i, x_{ti} — are vector of observations , the model state and the true state at a time moment *i*, respectively H_i and R_i — are observation operator and observation error covariance matrix at the time *i*. In turn, the preliminary forecast covariance error matrix B is determined only once at the initial time, ie at the time of the preliminary analysis x_a and forecast x_b.

In the general formulation the 4- dimensional analysis problem is formulated as minimization of the following cost function:

$$J(x)=(x-x_b)^{\mathrm{T}}\mathrm{B}^{-1}(x-x_b)+\sum\nolimits_{\mathrm{i=0}}^{\mathrm{n}}(y-H[x])^{\mathrm{T}}\mathrm{R}^{-1}(y-H[x]). \quad (3.16)$$

For this formulation it is necessary to determine the sequence of state vectors of the model solution x_i, as a sequence of solutions of the model equations:

$$\forall i,\ x_i = M_{0\to i}(x),$$

where in $M_{0\to i}$ is the operator of the model prediction at the initial state until the time *i*, thus 4D-VAR is a nonlinear optimization problem , which is generally difficult to be solved. The first term of the cost function J_b remains the same as in the 3D-VAR, but the definition of the second term J_0 requires *n* iterations of the model calculation from the initial time moment *i* until each observation *i*, and even more when calculating the gradient of the cost function ∇J_0.

Implementation of the 4D-VAR scheme in practice is subjected to the following simplifications :

– modelled forecast can be represented as a result of the intermediate steps of model M_i obtained by numerical integration of the model equations at the initial conditions described by the state vector *x*, then $x_i = M_i M_{i\text{-}1} \ldots M_1 x$;

– the cost function can be regarded as a quadratic, assuming that the operator *M* can be linearized:

$$y_i - H_i M_{0\to i}(x) \approx y_i - H_i M_{0\to i}(x_b) - H_i \mathrm{M}_{0\to i}(x - x_b),$$

where **M** is *M* differential.

Thus, calculation of criterion function and its gradient demands single direct numerical integration from the initial moment to a timepoint of n and single integration of the modified interfaced model representing a set of linearized operators of $\mathbf{M}_i$.

In this statement the algorithm 4D-VAR has the following characteristics:

– creation of the linearized operators of $\mathbf{M}_i$ making interfaced model that presents additional difficulties is required;

– in operational systems there is a need to accumulate observation data for the whole time interval (an assimilation window) whereas in consecutive algorithms (3D-VAR) assimilation can be carried out in process of data delivery;

– it is possible to consider 4D-VAR as optimum algorithm since it provides the best approach to observation data on the chosen time interval even at an imperfect assessment of a covariance error matrix B.

3.4.5. Kalman Filter

One of the basic methods of assimilation of observation data related to stochastic approach is Kalman filter and its derivatives. In simple statement Kalman filter represents the recursive filter and can be applied only to linear systems. The main equations of the Kalman filter were already considered at the proof of stochastic and variation methods equality for data assimilation problem, while in this case the background condition x_b is replaced with predictive x_f, covariance matrixes B and A are replaced with P_f and R_a to emphasize the fact that now the background state is a forecast, and the background vector covariance error matrix of a state evolves in time. The main equations of the Kalman filter appear as:

$$x_f(i) = M_{i-1\to i} x_a, \tag{3.17}$$

$$\mathrm{P}_f(i) = M_{i-1\to i} \mathrm{P}_a M_{i-1\to i}^T + \mathrm{Q}(i), \tag{3.18}$$

$$\mathrm{K}(i) = P_f(i)\mathrm{H}^T(i)\left[\mathrm{H}(i)\mathrm{P}_f(i)\mathrm{H}^T(i) + \mathrm{R}(i)\right], \tag{3.19}$$

$$x_a(i) = x_f(i) + \mathrm{K}(i)\left[y(i) - \mathrm{H}(i)x_f\right], \tag{3.20}$$

$$P_a(i) = \left[\mathrm{I} - \mathrm{K}(i)\mathrm{H}(i)\right]\mathrm{P}_f(i), \tag{3.21}$$

where $Q(i) = M_{i-1\to i} x_t(i-1) - x_t(i)$ is a covariance error matrix model, and the rest symbols remaining as earlier.

Thus, the Kalman filter is a sequential algorithm, for which a solution for the forecast for the interval between the previous and the current period of analysis and background state covariance fields is based on observation data (at the time of analysis).

Forecast model equations are used for extrapolation in time analysis covariance errors, which include the covariance errors of the forecast model itself. The main difference between variational methods and the Kalman filter is that at each subsequent analysis cycle of the Kalman filter the background stat covariance error matrix is forecasted in contrast to the variational methods, where *B* is not evolving.

The use of the Kalman method suggests the following limitations: :

– background state, observations and models error vectors , are independent;

– observation and background state vector errors have a Gaussian distribution ;

– average errors of observations and the background state vector are zero.

Consequently, when the Kalman filter is applied at each time step of the model assimilation a linear operator is acting on the state vector and transforms it into another state vector by adding a vector of Gaussian noise (random factors) .

The correct application of this method is only possible for linear systems , in the case of strong nonlinearity of the model and / or non-Gaussian noise it is possible to obtain estimates of the unknown covariance function by Monte Carlo method (ensemble Kalman filter) and then solve the corresponding equation of the optimal linear filter. One of the methods that are adapted for nonlinear systems is called extended Kalman filter: the nonlinear equations describing the dynamics of the system are linearized with respect to the previous state of the system , an iterative loop allows finding the necessary assessment of the dynamical system (this estimate is not necessarily optimal) .

Summarizing we should point out that recent trends of assimilation systems developments are aimed at joining the advantages of 4D-VAR and Kalman filter algorithms. For short periods for operational systems 4D-Var assimilation is a very effective method of analysis. When using the extended Kalman filter a new estimate of the forecast error covariance is determined for the next analysis by assimilation at each step. Compromise between these algorithms, as well as the use of ensemble forecasting provides the best possible result. Note also that the use of modern methods of observation data assimilation allow to obtain a plurality of side products of high quality. A good example is the reanalysis of a field, which can be used as diagnostic tool to improve the assimilation algorithms and forecasting properties of an operational system.

Chapter 4. OPERATIONAL FORECASTING SYSTEMS FOR THE BALTIC SEA AND THE GULF OF FINLAND

In present, the two models are used for the region of the Baltic Sea: the forecasting atmosphere model HIRLAM, High Resolution Limited Area Model (http://hirlam.org) used as a part of a common operational complex developed by joint efforts of experts of Germany, Sweden, Denmark and the Netherlands, and the three-dimensional sea model HIROMB, High Resolution Operational Model of the Baltic Sea. The version of the atmospheric model HIRLAM has resolution of 11 km. The model area of HIROMB covers the North and the Baltic Seas. Horizontal resolution of the model in the Baltic Sea, the Skagerak and Kattegat Straits is 1 nautical mile, number of layers is 24. The model is coupled with the hydrological HBV model providing the daily flow of the main rivers flowing into the Baltic Sea.

The forecast of the Baltic Sea state within the specified model complex is calculated daily at Swedish Meteorological and Hydrological Institute (SMHI) for the forthcoming 48 hours and is issued every 3 hours. Results of the forecast are available in 5 – 6 hours after the start of calculations in the form of various products, such as flood warnings and forecast along vessel routes. Forecasting hydrophysical fields of top 16 water layers along with fields of wind speed and pressure in the atmospheric boundary layer serve as initial information for one more model of the complex – SeaTrack, intended for monitoring and forecasting of oil pollution distribution over the sea surface. In SMHI the special software (SeaTrackweb) is developed allowing the user to receive through INTERNET forecasts of oil slicks drift in the Baltic Sea. The user has the possibility of direct access to the latest forecasts for 48 hours of wind speeds and currents. Now, almost all countries of the Baltic region, including Russia, are members of HIROMB commcohesion.

One of the first examples of development of elements of operational oceanographic system in the Northwest Region (NR) of Russia is the creation in Russian State Hydrometeorological University together with the specialists of the St. Petersburg Branch of P.P. Shirshov Institute of Oceanology of Russian Academy of Sciences and Arctic and Antarctic Research Institute of a prototype of modern operational forecasting system of the Gulf of Finland state and pollution distribution [Karlin L.N. et al., 2010].

Development of operational forecasting system on the basis of a model complex is very urgent and necessary for the Russian sector of coastal areas of the Baltic Sea where along with frequent natural disasters there is a high risk of technogenic catastrophes causing damage to environment, economy and population of this important region of Russia. The forecast of oil slick behavior in water areas of the Gulf of Finland is especially urgent due to the sharp growth of oil spill emergency probability in the Gulf of Finland in the last decade caused by the increase of shipping and construction of ports and oil terminals (Ust-Luga, Primorsk, Vysotsk). Marine traffic in the Gulf of Finland has been growing very dynamically in the last decade. The volume of oil transported through the gulf has increased from 20 to 104 million tons from 1995 to 2004. Estimates of the Finnish experts show that this volume reached 200 million tons by 2010.

The danger of emergency oil spills repeatedly increases in case of storm surges in the Gulf of Finland and the Neva Bay occurring in time of deep cyclones over the Baltic Sea. In St. Petersburg for its 300-year history there were nearly 300 floods, 48 of which – for the last 25 years. In order to predict the floods and to take measures against possible harm in the region and the St. Petersburg city the research works on hydrology and marine meteorology have been conducted for many years. Operational forecast of this dangerous phenomenon is produced in Hydrometeorological Center of St. Petersburg by the synoptic methods. Hydrodynamic forecast in its current form is applied as an auxiliary that is due to the insufficient accuracy which is mainly the result of inaccuracies of the forecast of input atmospheric parameters. Therefore, the correction of meteorological forecast is a necessary condition of correction of flood forecast and improving its time interval.

4.1. Structure of operational forecasting system GULFOOS

The operational forecasting system based on the three-dimensional hydrodynamic model was developed in a similar way as the famous BOOS system (Baltic Operational Oceanographic System) and is called GULFOOS (the Gulf of Finland Operational Oceanographic System).

The scheme of the operational forecasting system is shown on figure 4.1. It includes the following modules: 1) hydrodynamic GOFM module (the Gulf Of Finland Model), 2) modules of meteorological data, boundary conditions at the entrance to the gulf and river flow, 3) module of model initialization, 4) module of output data, 5) module of assimilation of satellite data on the sea surface temperature (SST).

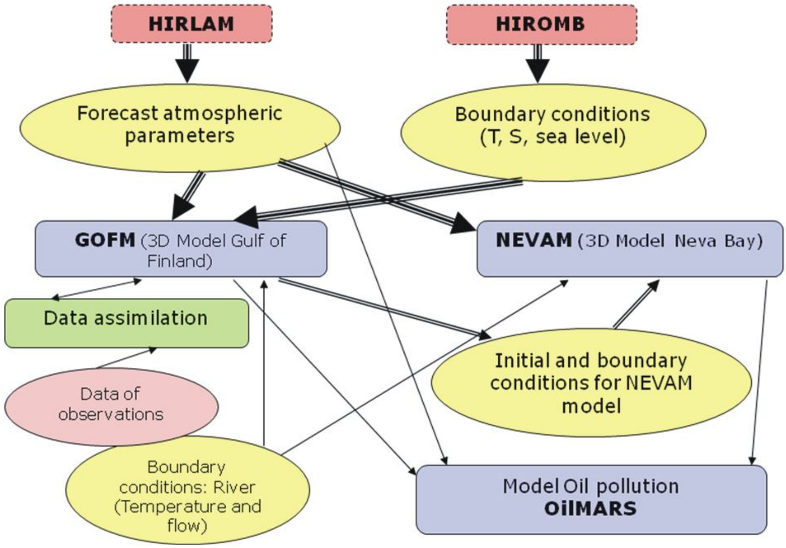

Figure 4.1 – Operational oceanographic forecasting system for the Gulf of Finland GULFOOS. The dotted line shows the planned, but still unrealized part of the system intended for SST assimilation

The hydrodynamic module represents the three-dimensional hydrodynamic model of water circulation and sea ice.

The model of sea circulation is based on complete equations of hydrothermodynamics in the Boussinesq and hydrostatics approximation including the equation of sea water state of Millero and Kremling. Vertical turbulence is described basing on the original *b-l* turbulence model (*b* – kinetic energy of turbulent pulsations, *l* – their spatial scale). The main predicted model variables – current velocity, temperature, salinity and density of water, sea level change.

The model of sea ice describes the dynamics and thermodynamics of snow and ice cover and allows to predict the changes of ice drift speed, its thickness and area. The model is integrated on a spherical grid for the entire Gulf of Finland with 1 nautical mile horizontal step and 1 m vertical resolution.

In the modules of input information (meteorological data, boundary conditions at the entrance to the gulf and river flow) necessary boundary conditions are set. For hydrodynamic forecast of the Gulf of Finland the boundary conditions are: 1) forecast of atmosphere state (near-surface pressure, wind speed, cloud cover, temperature and relative air humidity in near-water surface layer) produced by HIRLAM, 2) forecast of hydrological characteristics (sea level, temperature and salinity of water) at the entrance to the Gulf of Finland which is calculated by HIROMB (HIgh Resolution Operational Model for the Baltic Sea), 3) climatic, average monthly discharges of large rivers flowing into the Gulf of Finland (Neva, Luga, Narva, Kumijoki). In the used version of the GOFM model it is assumed that the difference of rainfall and evaporation is equal to zero.

Forecasts of hydrological characteristics in the Gulf of Finland are produced on the basis of the hydrodynamic module (GOFM model) using the modules of input information. Operational oceanographic system is realized on the computing server of Russian State Hydrometeorological University (RSHU) built on two 4-core Intel Xeon processors. RSHU has been receiving the results of daily 48-hour forecasts from HIRLAM and HIROMB models in real time since March, 2009. Frequency of records of forecasting fields for both models is 1 hour. Results of HIROMB calculations were used as initial conditions at initialization of operational simulations on GOFM (48-hour forecasts) at the first time step (March 10, 2009). For subsequent forecasts the fields obtained 24 hours after the start of the previous forecast are taken as initial conditions. GOFM calculations are fully automated: after they are received the boundary conditions at the entrance to the Gulf of Finland and the atmosphere interface are formatted and interpolated on GOFM model grid, then transferred to the calculation module for producing a forecast which results are then archived. Operational system provides the procedure of assimilation of both satellite and contact measurement information. In case of a tuned procedure of reception and processing of SST satellite data, as shows figure 4.1, these data are used for correction of initial conditions. Launching of several automatic measurement complexes of temperature and salinity vertical distributions in the Russian sector of the Gulf of Finland and organization of reception of these data in real time will allow to expand the procedure of correction of initial conditions including in it the assimilation of these measurements. For assimilation of temperature and salinity profiles it is assumed to use the methods based on variation algorithms.

For visualization of forecasting results the special site http://gulfoos.rshu.ru was created on the RSHU server where the description of forecasting system and the main predicted parameters are presented: temperature, salinity and level (figure 4.2, 4.3a, 4.3b and 4.3c).

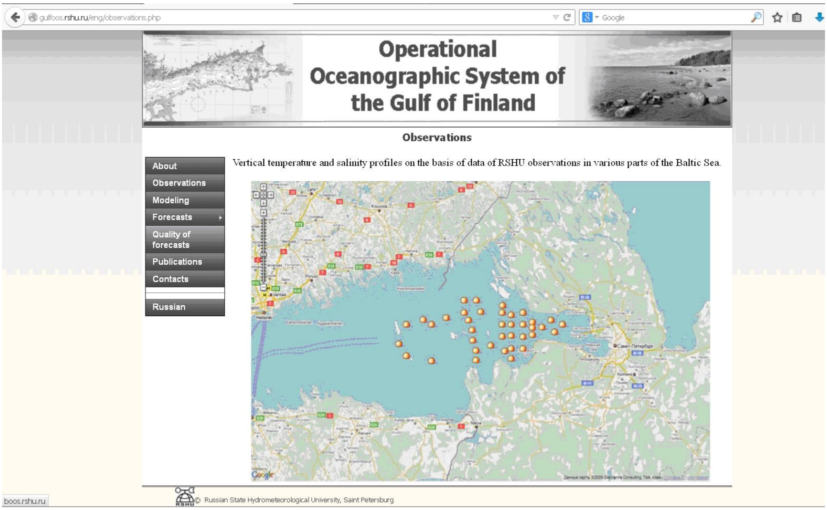

Figure 4.2 – Visualization of forecast results on RSHU server

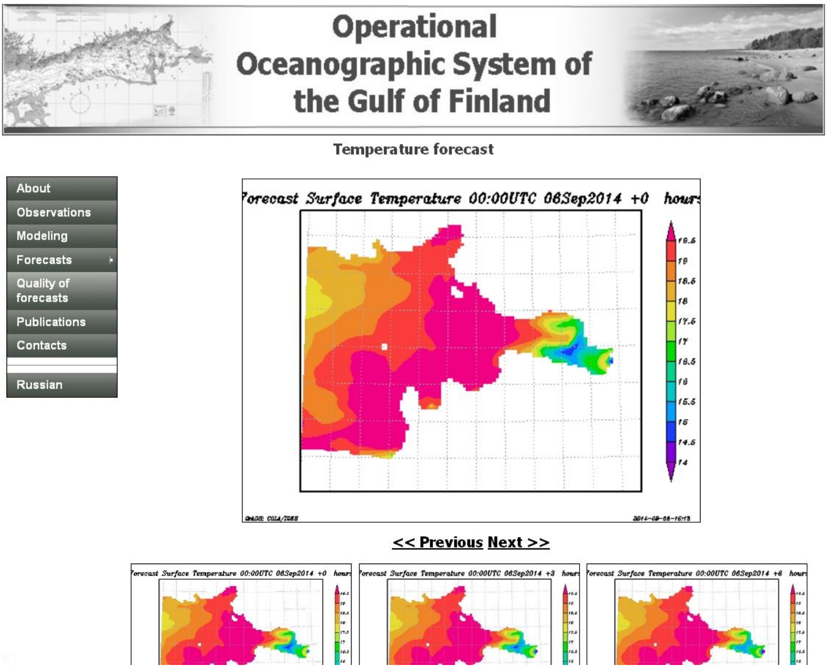

Figure 4.3a – Visualization of forecast results on RSHU server - temperature forecast

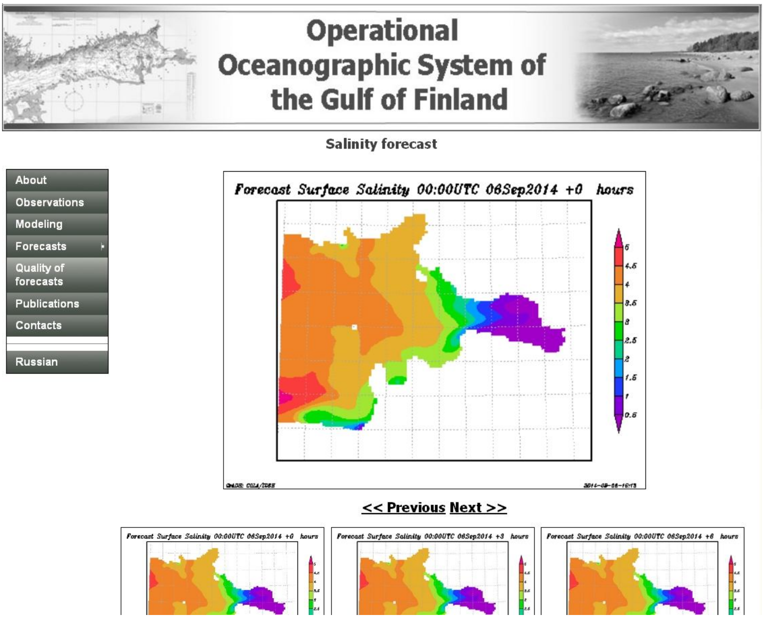

Figure 4.3b – Visualization of forecast results on RSHU server - salinity forecast

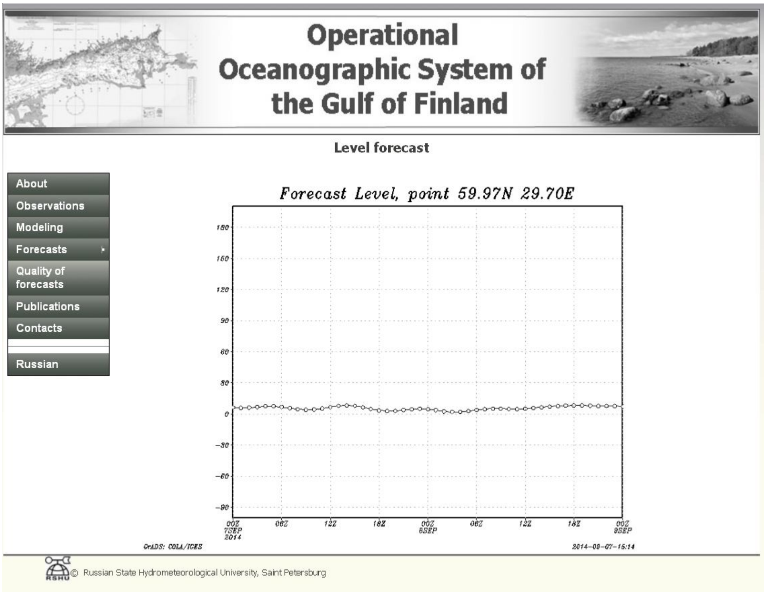

Figure 4.3c – Visualization of forecast results on RSHU server-forecast of sea level

4.2. Operational forecast of oil pollution distribution and transformation in the Gulf of Finland

In order to predict the distribution of oil pollution in the Gulf of Finland the module based on OilMARS model (Oil Spill Model for the Arctic Seas) developed in AARI for calculations of transfer and transformation of oil pollution in the Arctic Seas is coupled with the operational system GULFOOS [Stanovoi, et al., 2007]. The model of transfer and transformation of oil pollution OilMARS is adapted for the Gulf of Finland and represents a separate module which is connected to the Gulf of Finland OOS in case of emergency (a) or registered information on oil spot in the gulf water area (figure 4.4).

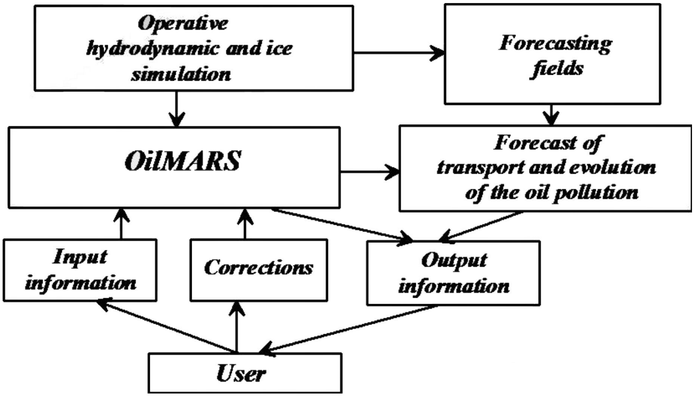

Figure 4.4 – Scheme of operational forecasting model of oil pollution

a) When an emergency oil spill is chosen the spill parameters are entered including the emission coordinates (geographical), emission date and time, oil product type (the user is offered to choose the necessary oil product from a database which contains physical and chemical properties of oil products necessary for calculation), oil product volume onboard the vessel in accident (i.e. the highest possible volume of emission), emission type – continuous or instant. In case of a longterm emission (the most probable case) the initial speed of emission (t/hour) and emission speed for some period (i.e. speed time gradient) are set. Until correction is made the calculation is conducted at a constant speed of emission (two speeds are equal) or at linearly decreasing/increasing speed of emission (speeds are not equal). The model foresees the case when the source of pollution continues to move. Then the source speed in knots and direction is set which are considered constant until the correction. In case of instant emission the emission volume is set. The model foresees the options of calculation of instant emission on water and ice surface.

b) For calculation of oil slick distribution over the sea surface the model has options of known and unknown oil product. In both cases date and time of spot detection and approximate thickness of spots (by default - 10 microns) are entered, in case of calculation of spots of a known oil product a required oil product is additionally entered from the database. Geographical coordinates of points and method of approximation are entered. The user in a dialogue mode enters the initial information necessary for calculation that includes a type of pollution, parameters of emission and simulation.

At operational calculations there are no scenarios of development of both hydrometeorological parameters, and emission parameters, so the procedure of information correction is introduced into the model that can be divided into two parts:

- correction of emission parameters (or assimilation of operational information) made on the basis of operational information from the vessel in accident or on the basis of data of aerial photos and satellite information: change of coordinates of emergency object; termination of emission of oil on water surface (for example, as a result of elimination of a hole in a vessel), change of emission speed, change of speed and direction of the vessel in accident. A possibility of correction of a spot position and emergence of new spots during calculations is also provided.

- correction of calculation parameters including the change of the period of possible correction; forecast period; period of delivery of calculation results; period of calculation and complete termination of calculation when as a result of operational measures for emission elimination further calculation becomes useless.

For adaptation of OilMARS to the water area of the Gulf of Finland it was considered that the gulf represents a shallow and brackish basin with an intensive dynamics of waters, well developed wind waves and low density of water. Besides that, the gulf is the freezing basin having an ice cover for about a half a year.

The OilMARS model works in a three-dimensional option calculating the in-water distribution of dispersion plume and submerged oil [Stanovoi et al., 2012]. The model is capable to count the occurrence and distribution of secondary oil pollution on water surface and seafloor. Besides that, it includes the possibility of accounting for ice cover cohesion and drift impact on pollution distribution, as well as oil occurrence on the ice top surface and under ice as a result of compression of drifting ice.

A longterm emergency oil spill is represented in a form of a large number of small discrete emissions – portions or spillets which with a certain frequency come from a pollution source on water surface depending on emission speed, in general being a time variable. Each spillet has a set of parameters: coordinates, area, density and viscosity of oil, amount of oil on water surface, amount of evaporated oil, etc. All spillet parameters depend on the time this spillet spent on water surface. The approach used in the model makes it possible to consider the spatial heterogeneity of an oil slick, i.e. in each timepoint on water surface there are spillets of different density, viscosity, weight and area.

To calculate the transfer of spillets the Lagrangian approach is applied and the model grid from the model of water circulation (figure 4.5) is used. Spillets are transferred under the influence of wind, currents and waves. Besides that, a random spillet transfer due to horizontal mesoscale turbulence on the sea surface is considered.

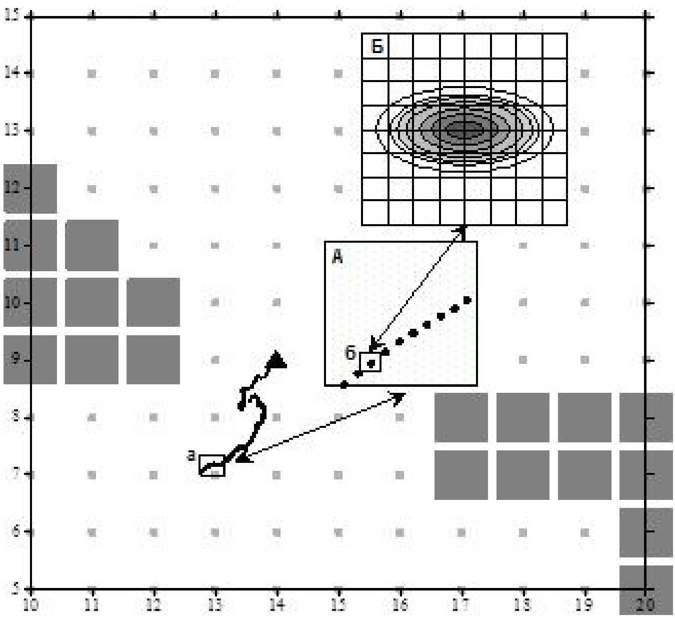

Figure 4.5 – Scheme of application of Lagrangian-Euler approach to the description of transfer and transformation of emergency oil spill. Areas marked with lower case letters correspond to the inserts marked with capital letters. On axes – grid coordinates

For definition of a vector of total currents the results of hydrodynamic model calculations are used. The wind component of spillet transfer is taken equal to 3% of wind speed with a deviation from wind direction on 15 ^{o} clockwise.

Parameters of wind waves are calculated using either a model of wind waves or semi-empirical relationships for developed waves.

In the presence of ice cover according to observations and results of retrospective modeling oil transfer speed significantly decreases depending on ice cohesion, and direction of oil slick transfer deviates on up to 60° of previously calculated transfer direction without ice cover. When a spillet moves to a zone of larger ice cohesion the corresponding spillet area is reduced keeping the same mass.

When oil distribution in ice conditions is calculated it is usually accepted that at ice cohesion higher than 5 oil moves together with ice. But, as showed the results of observation of a real emission oil can move faster than drifting ice. Therefore, it is accepted in the model that at ice cohesion more than 5 a spillet will be transferred with ice drift speed only in case if ice drift speed is higher than spillet transfer speed.

For calculation of oil transformation processes Euler's approach and grids with high spatial resolution are used depending on the initial mass of a spillet. When a spillet is approaching the coast or fast ice the conditions of no-leak and sliding are used. Thus, the site of polluted coastline is registered.

The process of each spillet evolution is presented in two stages: spreading and transformation. To calculate the spreading of oil up to the state of a film in the model a standard approach is used [Reed et al., 1999]. Because of the small spillet volume a process of spreading takes a few hours, during which the light oil fraction evaporates and the volume spillet decreases correspondingly. Also, the cohesion of the ice cover is taken into account. At that diffluent spillet is being transferred over the sea surface. After completion of the spreading calculation the adaptation of the spill is transferred on a rectangular computational grid, taking into account the wind action. Depending on the desired speed of the spill, the initial spillet mass may be different. Therefore, for each spillet specific computational grid is formed, the spatial resolution of the grid depends on the spillet mass.

Further calculation of each spillet transformation is implemented by solving the diffusion equation for non-conservative impurities regarding the oil mass. At each time step (t) the conditions of mass conservation for each spillet are verified.

For the oil evaporation process calculation the pseudo-component method is used in the model, taking into consideration the impact of the viscosity increase due to the emulsion formation. Influence of ice is indirectly taken into account by reducing the spillet area.

When calculating the process of horizontal diffusion the diffusion coefficient is used, this depends on the spatial dimensions of the spill slick. In addition, the calculation formula gains two additional factors that depend on the viscosity changes of the oil and on the cohesion of the ice cover. Also an additional condition limiting the magnitude of the diffusion coefficient is used that is associated with the numerical implementation of the equation.

Calculation of the vertical dispersion of oil in water with wind waves collapse, resulting in an emulsion of “oil in water” and pollution plume in the upper layer of the sea with possible subsequent adsorption of oil droplets suspended in mineral particles, is produced through a widely used in the world method. For weak and moderate winds vertical dispersion contribution to submerged pollution is small enough, but in storm situations at a higher risk of accidental spills, the contribution of the vertical dispersion is greatly increased. So happened in the case of the tanker «Braer» accident, which took place in 1993 near the Shetland Islands, the storm shuffled up to 40% of the spilled oil into the water over the entire thickness of the upper water layer. This oil mass was transferred with currents in the opposite direction to the wind, while only about 15% settled on the bottom.

For the “water in oil” emulsion formation the minimum level of input energy is present, which depends on the wind speed and wave parameters. It is noted that when the wind speed exceeding 12 m/sec occurs oil disperses in water quickly enough and the emulsion “water in oil” is hardly formed. Furthermore, it is necessary for the oil to have a high content of tar and asphaltenes. The model simulates the energy level and the stability index for determining the stability of the emulsion. In the case favourable conditions for an emulsion formation, the calculation of this process is performed. In the model two methods of calculation of emulsion formation are implemented depending on the availability of information about the content of asphaltenes, tars and oil wax.

Crude Oil REBCO (Russian Export Blend Crude Oil), passing through the oil terminals in the north-west Russia, contains a high percentage of asphaltenes and tars. Under certain conditions, the impurities lead to the formation of a stable emulsion “water in oil”.

In the case of light oil fractions evaporation and the emulsions “water in oil” formation the density and viscosity of the oil increase significantly. Furthermore, the density and viscosity of the oil depends on the variability of the water temperature, which is particularly important for the calculation of oil spills in the seas subjected to freezing. To calculate the changes in density and viscosity of the oil semi-empirical relations are commonly used.

As a result, density increase of an oil spill can be a consequence of a quite small change in water temperature or transfer of an oil slick to the area with a lower surface density of water (zone of the river flow influence, the marginal ice zone) for the oil to become heavier than underlying water in the surface layer that leads to sinking of oil.

Immersion depth and the concentration of pollution depend on the density, area and weight of the sunken oil and water density structure. Prolonged spill may have many submerged contaminated clusters with different densitiy of oil, which, depending on the position and capacity of a pycnocline can be located at different depths. The spatial distribution and mixing of the oil contaminated waters are driven by currents and turbulence. The oil pollution may gravitate to the bottom of the shoal heads and banks, or, depending on the spatial inhomogeneity of the density of water can reach the surface, forming a secondary cluster of pollution on the sea surface.

When modelling long lasting spills the density of a given oil (spillet) volume depends on the residence time on the surface of the water and the physical and chemical properties of oil. Due to the spatial variability of the surface density field of water, various spillet can be immersed in water at different times and in different places, any time the density of the spillet exceeds the density of water on the surface of the sea at a point. Because of this submerged oil pollution has multi-core structure.

Submerged pollution is a rather commonplace phenomenon. Measuring the level of petroleum hydrocarbon pollution of the Baltic Sea and the Gulf of Finland, conducted in the 80s showed that the surface of the sea in the form of a film contains less than 4% of pollution, 15% of pollution is contained in sediments and about 80% of pollution was found in water emulsions , colloidal solutions, suspensions, etc.. note that oilcontamination can be detected only by direct methods of measurement (taking water samples to determine the concentration of petroleum hydrocarbons), with remote monitoring via satellites show only cleansing the water from the oil.

For the submerged oil transfer model calculating unit design it was assumed that the concentration of oil and the dynamics of oil transfer do not depend on the state of oil in water (a colloidal solution, emulsion or suspended drops, etc.). It is also assumed that the oil delivered into the water under the action of wind waves (emulsion "oil in water") has a density equal to the density of water in the surface layer at the point where there was a dispersion of oil. To calculate the grid area is formed with a horizontal resolution ($\Delta x3$ and $\Delta y3$), depending on the characteristic spillet dimensions and stability conditions of the calculation scheme. Vertical resolution coincides with the one of the hydrodynamic model.

To calculate the spread of oil pollution in the water the three-dimensional advection - diffusion viscous impurity equation numerical solution is used.

Since the density and viscosity in different hot spots may be different, and it is assumed that they remain constant, the equation of advection and diffusion is solved simultaneously for the concentrations of petroleum hydrocarbons and the products of density times viscosity. Accordingly, the formulations of the sources are also included in the equations in the form of concentration source and of the respective products. For the equation with respect to the concentration:

On the solid boundaries is given by the condition of impermeability, liquid boundaries – free-stream (removal of pollution mass from the computational domain);

At the lower boundary ($z = H$) is given by the condition of consistency-circuiting in the general case or instantaneous flow of petroleum hydrocarbons in the case of deposition of pollution on the bottom;

Similarly, at the upper boundary ($z = 0$) is given by the condition of impermeability in general or instantaneous flow of petroleum hydrocarbons in the case of the formation of secondary pollution of surface water.

It is assumed that secondary contamination spots are located on the water surface with distinguished density and viscosity. After this secondary pollution spot is transported in the space similarly to a spillet of a primary contamination, being exposed to wind waves (vertical dispersion). In case of the clearance of spots in the area with lower density of water, secondary pollution cluster is drowning. In the presence of the ice cover it becomes probable for the clusters of secondary pollution to be transferred under the ice, to account for this a random number $P = [0,1]$ is generated and when $P \leq C_{ice}$ it is believed that secondary pollution was tranfered under the ice.

For the numerical solution of the equation the well-known flow correction scheme FCT (flux-corrected transport) is implemented, which has the best properties of transport without artificial numerical viscosity. To calculate the coefficients of horizontal turbulent diffusion Smagorinsky scheme is used. To calculate the coefficient of vertical turbulent diffusion KPP (K-profile parameterization) scheme is used. The presence of drifting ice or fast ice in the upper boundary of the computational domain is taken into account in the calculations. At each time step (t) verifies the conditions of conservation of mass.

The Gulf of Finland is covered by ice about half of the year. In addition to the impact of cohesion and ice drift on the distribution of oil pollution on the water surface, the pollution of the ice cover can occur as a result of discharge of oil directly on top of the snow and ice cover or under the ice. The approach that is used in the model also takes into account the contamination of an ice cover during compression of ice fields, with the result that some of the oil is on the top surface of the ice («lead pumping») or goes under the ice.

Oil mass that occurs on the upper surface of the ice cover spreads over the surface, continues to evaporate and gets partially absorbed by the snow and ice cover and is being carried by a drifting contaminated ice floe. For calculations of the oil spreading process on the top surface of the ice cover and to calculate the depth of penetration of oil in ice cover a semi-empirical parameterization is used obtained by laboratory and experimental studies.

Oil mass, which is forced under the ice, spreads and accumulates in the cavities and pockets on the lower surface of the ice floe, while some of the oil fills cracks and openings. Moreover, the contamination process depends on the ice roughness and topography of the bottom surface. The more cavities and hollows and the deeper they are, the more oil can be captured in ice and the smaller the size of oil spreading. To calculate the process of spreading of oil under ice using semi-empirical expression obtained for horizontal and relatively smooth bottom surface of the ice limiting the spreading oil, ie it is assumed that the horizontal dimensions of patches of oil are smaller than the distance between the ice cavities. According to experimental studies, the movement of oil relative to the lower surface of the ice begins when a certain critical flow rate of water occurs in respect to ice bottom. When the flow rate is less than the critical then oil moves along with the ice.

When modelling the transfer of oil slicks it is assumed that the position and dimensions of the slick are known (for example, the satellite information). However, the time when the oil pollution appeared on the sea surface, is unknown. Physical and chemical properties of oil (or fuel) may be known or unknown (most likely the case). The model considered both cases, with the calculated advection, vertical dispersion by wind waves; effect of ice cohesion and drift. In the case when the properties of oil are known, the evaporation process (last phase) is calculated in addition and an emulsion formation of a "water in oil" (maximum value) type, if this oil is able to form an emulsion.

Oil spills usually have an elongated shape on satellite images, but it can assume quite a bizarre shape depending on the characteristics and the dynamics of the area. To set the initial shape of the slick reference points (at least 3) coordinate are input to contour the slick. The resulting irregular polygon is uniformly and densely filled with particles (tracers) with the known or unknown properties.

To illustrate oil pollution calculation for different forecast meteorological situations the examples are given. In the examples below the fixed prescribed sources were set with constant velocity of incoming oil on the water surface (30 tons / hour) for 4 - 5 days. Physical and chemical properties of oil correspond to the properties of crude oil REBCO (density 870 kg/m ^{3}; kinematic viscosity of 55.9 cSt; mass fraction of asphaltenes, waxes and tars 12%). Figure 4.6 shows the calculated grid area of the Gulf of Finland and the location of points for which further results of calculations (autumn) are presented. Here and below, on the grid coordinates are given at the axes (grid spacing $\Delta x = \Delta y = 1852$ m - 1 nautical mile).

Figure 4.6 shows an example of an operational forecast simulation results of oil pollution propagation at the point 1. In every picture the position of the "real" spill in shown in black and its forecast distribution for a day is shown in grey.

The figure shows a noticeable disparity of the predicted and the "real" position of the pollution slick. Thus, the forecast position of the spot for a period of 96 hours after the start of the spill, which had been given a day ago, produced a removal of the bulk of the oil to the shore and extensive pollution of the coastline. Calculation of the "real" spill for 96 hours showed that the oil slick had not reached the coast and therefore pollution of the coastline 96 hours after the beginning of the spill did not happen.

As at the time of calculation the given wind speed was 10.5 m/s, under the influence of wind waves a process of vertical dispersion of oil in water and the formation of the emulsion "oil in water" took place. Figure 4.7 shows the distribution of oil pollution of concentration (mg/m^3) at a 3m depth. Here one can clearly see the multi-core structure of submerged oil pollution.

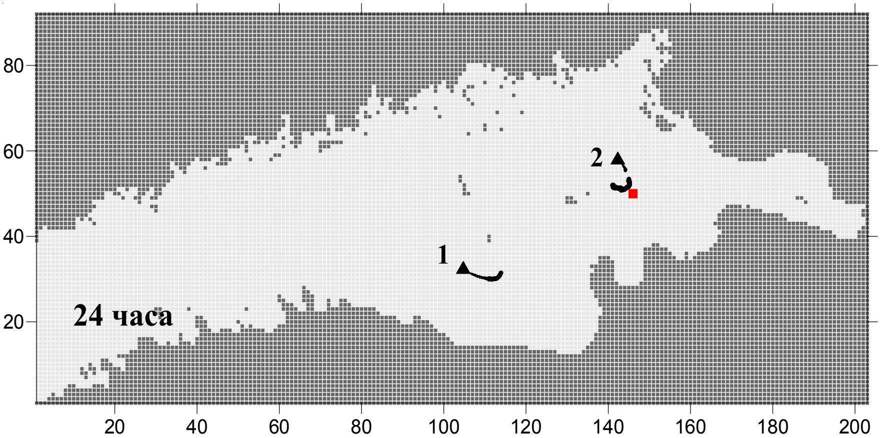

Figure 4.6 – Estimated grid area of the Gulf of Finland, the location of the points and the results of calculation of the oil pollution in 24 hours

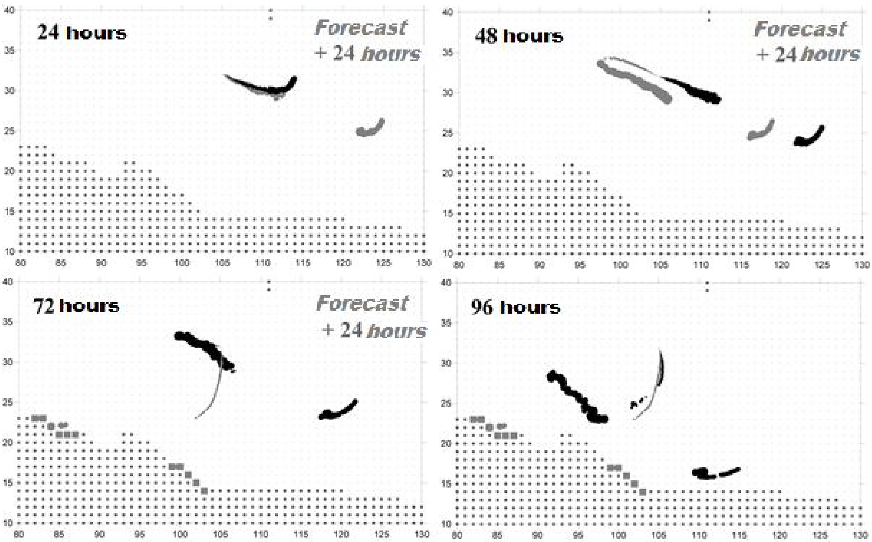

Figure 4.7 – Example of operational forecast calculating of the oil pollution propagation at the point 1. The “real” spill in shown in black and its forecast distribution for a day is shown in grey

According to the results of calculations the concentration of oil pollution decreases with the depth quite rapidly down to the 5m depth where it reaches minimum values.

Point 2 was located in the eastern shallow part of the Gulf. Strong wind combined with spatially inhomogeneous flow field on the surface of water led to a rupture of the slick (see Figure 4.8) and formation of an “oil in water” emulsion in the upper layer of the sea. Features of the spatial inhomogeneity of the density structure of the water led to the formation of secondary pollution spot on the surface because of submerged oil pollution transfer to an area with a higher water density (see figure 4.9).

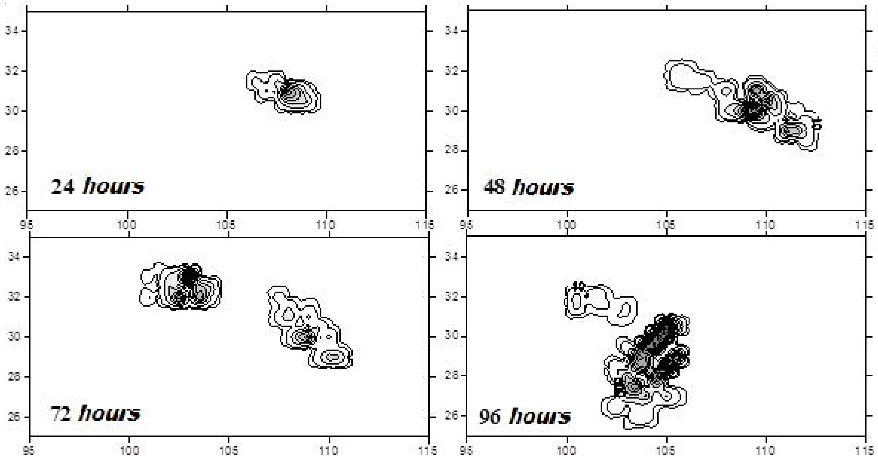

Figure 4.8 – Concentration distribution of oil pollution (mg/m^3) at the 3 m depth

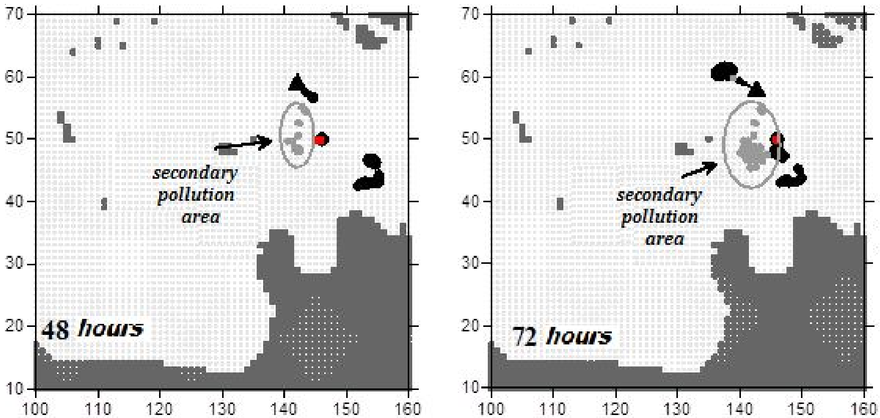

Figure 4.9 – Example of the oil pollution propagation simulation at. Contamination on the surface of the water is in black; secondary pollution is in grey

Oil pollution spread test calculations for the winter (January 2011) were carried out for modelled sources located in the eastern and central parts of the Gulf. In the case the oil spills source located in the eastern part of the bay with ice concentration 8 - 9 points, oil slick occupied a very limited area, the width of the spill was only 100 - 200 m, the thickness of the oil increased up to 5 - 10 mm. The process of evaporation in the conditions of high ice concentration slows down, and the "oil in water" and "water in oil emulsions "formation of did not happen. As a result, such a spill can exist for a long time until compression (diverging) or ice melting.

The modelled source was located in the central part of the bay at the point where the ice concentration was increasing for four days increased from 4 to 8 points (figure 4.10). Increase in ice concentration has a significant influence on the trajectory of the slick spread, while inhomogeneity of the ice field and ice drift velocity leads to rupture of slicks. As was shown by the calculation results, the rate of ice drift in places exceeded spillet own speed, which led to the part of the oil mass transfer together with drifting ice. At the same time, a limitation of the slick area occurred in the vicinity of the source of contamination.

Different tests performed with the OilMARS model showed that the model can be used to predict transport and transformation of oil pollution as a module in operational ocean forecasting system GULFOOS. The quality of the distribution forecast of oil pollution is largely determined by the accuracy of forecasts of hydro-physical characteristics and ice conditions in the Gulf of Finland. It is necessary to carry out the verification of the model OilMARS in order to check the quality of the calculations. In the case of oil spills on the water surface the oil slick position and shape can be fixed by aerial photography or satellite imagery. Concentration of petroleum hydrocarbons in the water column can be determined by carrying out of special measurements in the area of an accident. The same parameters can be fixed in the case of spill propagation when the oil leaks from vessels. Prerequisite for the verification is to track the time, the position and shape of spills, i.e. a regular satellite monitoring of the waters. Satellite imagery use experience has shown that receiving data for the spill location and shape and some data to correct the calculation the model is capable of provision of information about oil masses that were possibly missed in the analysis of images. In the case of forecasts the model is capable of assisting in determination of the slick position in the following pictures. In addition, model calcu-

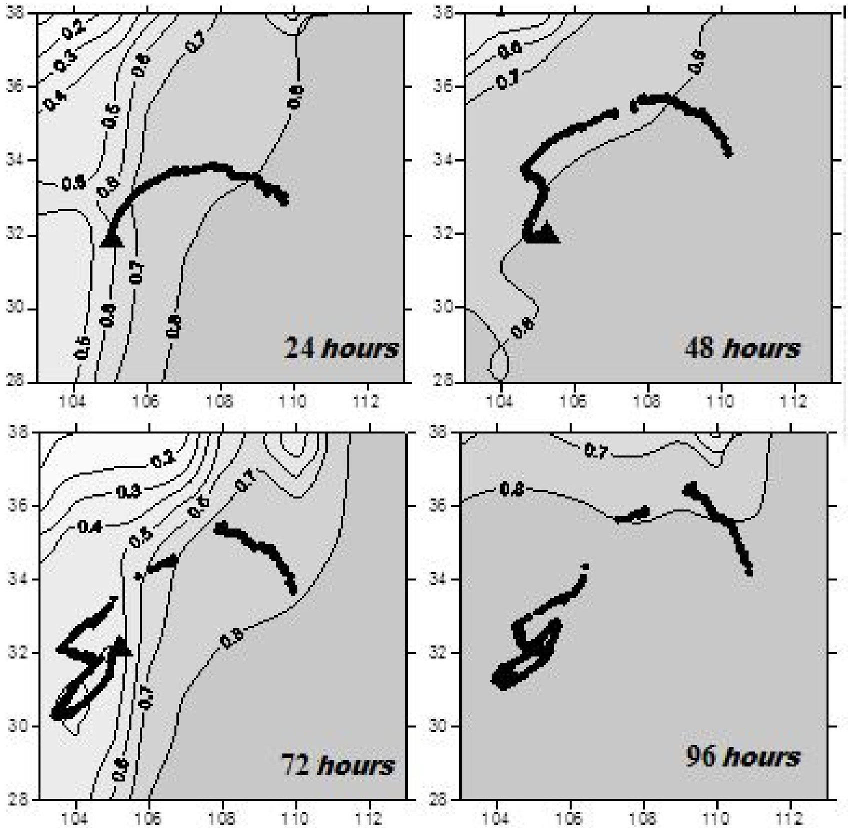

Figure 4.10 – Simulation example of oil pollution propagation in the winter at a point located in the central part of the Gulf of Finland. Isolines represent the concentration of ice (expressed in a decimal numbers)

lations allow us to identify if the detected slick is new or it is a re-discovery of some oil mass from the previous image.

PRACTICAL ASSIGNEMENT

Study of parameter sensitivity of Satellite Sea Surface Temperature (SST) assimilation in to a Three-dimensional variation assimilation scheme in Operational Model of the Gulf of Finland

Objectives of the work:

Find required daily SST for subsequent assimilation with a spatial resolution of ~ 1 × 1 km on a given date on the Web portla SATIN (http://satin.rshu.ru/) (determined by given personal assignment) .

Plot the spatial distribution of satellite SST for the region (the Gulf of Finland) and a provide a comparison with the model results.

Perform an assimilation procedure for satellite SST on the basis of three-dimensional variational assimilation scheme using the proposed software.

Explore the sensitivity of the results to variations in the number of EOF and to the choice of a correlation radius, which determines the horizontal covariance operator .

Analyse the results , pay special attention to the results sensitivity to the number of EOF and correlation radius.

Initial data:

Fields of temperature, salinity and sea level resulting from numerical calculations by three-dimensional model NEMO for the Gulf of Finland for a certain date.

EOF set corresponding to this model solutions.

Technical specification:

UNIX Operating System

Interactive environment FERRET

The assignment guidelines:

Use website SATIN (http://satin.rshu.ru/), designed to search for pre-visualization and remote sensing of the ocean.

Find the “Data Directory” and choose the product “sea surface temperature GHRSST Level 4 MUR Global Foundation Sea Surface Temperature Analysis» - this is the daily SST with a spatial resolution of ~ 1 × 1 km, obtained using optimal interpolation data from several satellites.

To download the SST data using FTP for the required date (depends on personal assignment number) proceed as follows:

– copy the link to a file with the extension *. Bz2 to the clipboard (data are grouped in folders by year and serial numbers of days of the year);

– go to the working directory;

– type the command line: wget «download link»

wget ftp://ftp.solab.rshu.ru/data/allData/JPL-L4UHfnd-GLOB-MUR/2011/140/20110520-JPL-L4UHfnd-GLOB-v01-fv03-MUR.nc.bz2

– open the archive file: bzip2-d «filename”:

bzip2-d 20110520-JPL-L4UHfnd-GLOB-v01-fv03-MUR.nc.bz2

For further work with the file use the interactive environment FERRET.

In the command prompt type:ferret–gif

View the file:

yes? use 20110520-JPL-L4UHfnd-GLOB-v01-fv03-MUR.nc

yes? show data

currently SET data sets:

1> ./ 20110520-JPL-L4UHfnd-GLOB-v01-fv03-MUR.nc (default)

name title	I	J	K	L
ANALYSED_SST analysed sea surface temperatur	1:32768	1:16384	...	1:1
ANALYSIS_ERROR estimated error standard deviat	1:32768	1:16384	...	1:1
MASK sea/land field composite mask	1:32768	1:16384	...	1:1
SEA_ICE_FRACTION sea ice area fraction	1:32768	1:16384	...	1:1

This file contains the required SST (ANALYSED_SST) and observation data error (ANALYSIS_ERROR) on a global grid.

Cut out the Gulf region and perform data visualization:

yes? shade/x=23.5:30.2/y=59.0:60.9 ANALYSED_SST

yes? frame/file=sst.gif

yes? shade/x=23.5:30.2/y=59.0:60.9 ANALYSIS_ERROR

yes? frame/file=sst_error.gif

Plot the spatial distribution of the SST background values (model solution).

Scan the file containing the model solution on the desired date:

yes? use 2013140-model.nc

yes? show data

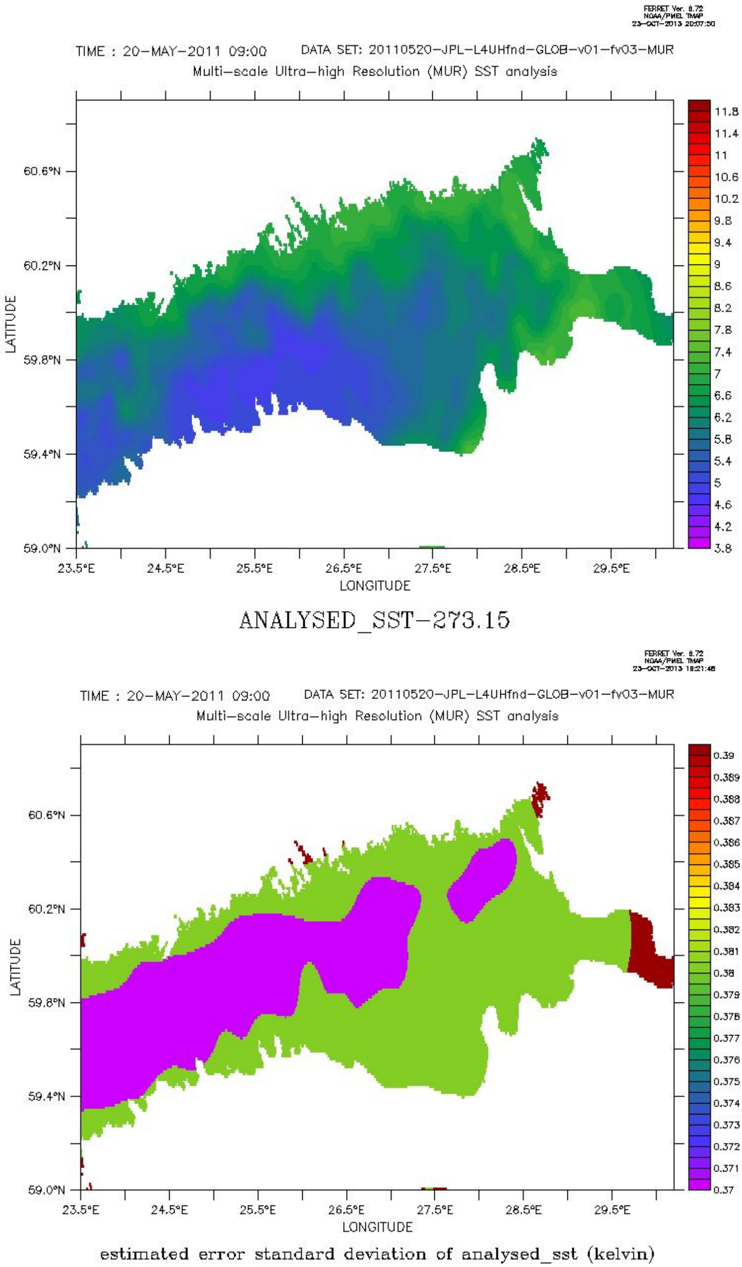

Figure 1 – Spatial distribution of the satellite SST and SST errors

currently SET data sets:

1> ./ 2013140-model.nc (default)

name	*title*	I	J	K	L
NAV_LON	Longitude	1:203	1:89	...	...
NAV_LAT	Latitude	1:203	1:89	...	...
SSH	sea surface height	1:203	1:89	...	1:1
TEM	temperature	1:203	1:89	1:94	1:1
SAL	salinity	1:203	1:89	1:94	1:1

This file contains the model results for the temperature field (TEM), salinity (SAL) and sea level (SSH) on the model grid, described by variables NAV_LON and NAV_LAT.

Perform data visualization (surface water temperature):

yes? shade/k=1/levels=(3.8,12,0.2) TEM

yes? frame/file=modelsst.gif

Perform conversion of SST and observation errors from the global grid to computing model domain grid using script gridSST within the FERRET programme.

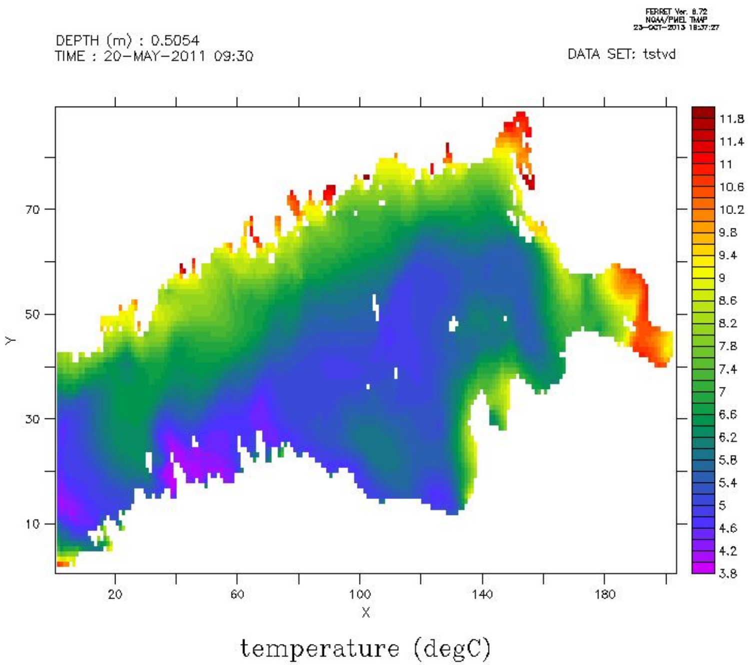

Figure 2 – Spatial distribution of the modeled SST

At the command prompt type: «ferret-script gridSST «name of the input file» «output file name»

Guidelines for working with the 3DVAR observation data assimilation.

Open the settings file for assimilation procedures 3dvar.conf, where you can modify the following parameters:

- the number of EOF (Neof)
- horizontal covariance operator correlation radius (Rcor).

Type at the command prompt: «script 3DVARSST». As a result of the assimilation procedure in the working directory you will find the following files :

- inctem.nc – increment of the sea surface temperature;
- analtem.nc – sea surface temperature after the assimilation procedure.

Visualize the files in a similar way as a file containing the source modelled sea surface temperature.

Repeat the procedure of assimilation, changing settings, thereby study the sensitivity of the assimilation procedure to the number of EOF and correlation radius .

Analyze the results.

SEMINAR TOPICS

1. Structure of Baltic Sea Operational Oceanographic System
2. Black Sea Regional Joint Operational Oceanographic System
3. Mediterranean Operational Oceanographic System
4. Operational Oceanographic System of the European Northwest shelf seas
5. Ireland-Biscay-Iberia Regional Operational Oceanographic System
6. Coastal Ocean Observational and Forecasting System of Cyprus
7. Integrated National System of Information on the Situation in the World Ocean
8. Catalogue of products of ocean monitoring and forecast of MyOcean project

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CONTENTS

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