The computational technology for estimating average fields of atmospheric contaminant concentrations in remote areas of the Arctic

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Abstract

We have proposed a new formulation of the problem of estimating the spatial structure of the average concentration field of atmospheric contaminant on the base of measurements at one or several monitoring points, without involving information about the sources of the contaminant — the problem of passive location (remote sensing) of the atmosphere by wind. Two new functions are defined: the average effective concentration field and the average effective sources field. The equations for finding these functions are written in the differential and integral forms. As an example, the results of solving the following quasi-two-dimensional problem are presented and discussed — the estimation of the average field of methane concentration in the Kara Sea and in the Barents Sea, on the base single monitoring point measurements made during the summer expedition of 2016 to Bely Island (the northern extremity of the Yamal Peninsula).

Keywords: estimating average fields of atmospheric contaminant, computational technology.

1 Introduction

Understanding and predicting the climate change processes is one of the most important fundamental problems of our time. A key role in understanding the changes in the radiation balance of the planet is played by the possibility of measuring and modeling the spatial distribution of the main optically active components of the atmosphere greenhouse gases and aerosols. At present, the most noticeable changes in the parameters of the climate system are observed in the Arctic region, but at the same time, the study of the distribution of atmospheric contaminants in this region is substantially lower than in the middle latitudes. Difficult access and

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severe climatic conditions make it difficult to conduct research and regular measurements in remote regions of the Arctic Ocean basin.

This paper describes the computational technology of the passive location (remote sensing) of the atmosphere by wind, which combines measuring instruments network with a new method for numerical modeling of the transport of atmospheric contaminants — the method of Fluid Location of the Atmosphere (FLA). The mathematical formulation of the problem that was not used previously is formulated and new equations describing the average fields of atmospheric contaminant concentrations formed by long-range transboundary air mass transfer are written. The developed computational technology allows using data of long-term measurements in a small number of monitoring points, as well as numerical modeling of trajectories of Lagrangian particles and the solution of transport equations, to obtain estimates of the distribution of average contaminant concentrations in the atmosphere at large distances from the monitoring points without using information about the source locations and emissions.

2 Steps of computational technology

The sequence of actions or stages of the implementation of the developed technology is as follows.

1. Measurement and preparation of data. The basic requirement for the formation of the initial series of data — the measurements should be long-term with the maximum diversity of synoptic and meteorological conditions. In a particular case, measurements can only be performed at one monitoring site, and increasing their number will lead to an improvement in the quality of the simulation.

2. The solution of inverse problems for restoring from a measurement data a parameter that obeys the conservation equations. Since in many cases it is not the contaminant concentration is measured, but some function from it, for further modeling it is necessary to find a conservative characteristic. For example, in order to estimate the aerosol content in the atmosphere by remote methods (from surface or from satellite platforms) measurements of the aerosol optical depth are widely used, which requires solving some inverse problems and restoring the concentrations of aerosol particles in the atmosphere.

3. Solution of a set of problems for calculating the back air parcel trajectories for each moment with a known (measured) contaminant characteristic, for each measuring point and for the entire measurement period. As input to solving this problem, it is necessary to have 4D-fields of meteorological parameters throughout the Northern Hemisphere and for the entire measurement period. For this purpose, one can use the reanalysis databases from National Oceanic and Atmospheric Administration USA NOAA-NCEP/NCAR, from European Center for Medium-range Weather Forecasts ECMWF. Another option is the direct modeling of atmospheric dynamics, in other words, the direct calculation of meteorological parameters of the atmosphere with the help of one or another software tool, as well as the assimilation of available meteorological data.

4. Specification of influence zones for each measurement point, simulation zones and control zones with the help of geo-information technology (GIS) tools. The zone of influence is defined as the region from which information about the contaminant comes to the measuring device. The simulation zone is defined as part of the zone of influence, in which the number density of the back trajectories is sufficient for performing the subsequent modeling. In the simulation zone, a numerical solution of the problems will be performed by the FLA method. In contrast to the traditional formulation of the problems for the direct dispersion of pollutants in the atmosphere (in which the modeling domain is given a priori), in solving the problem of passive location of the atmosphere by wind, the modeling zone is determined during the solution of the problem. Control zones are areas that are intersections of the simulations zones of individual measurement stations. Further, in the control zones it will be possible to verify the results of solving the FLA problem on the basis of independent measurement data.

5. Solution of the problem of estimating the average effective field of contaminant concentration in the simulation zone by the FLA method. The iterative procedure of the numerical solution involves three steps: calculation of the effective average concentration field on the set of Euler cells; calculation of the effective average sources/sinks field; redistribution of the contaminant concentration along the trajectories of Lagrangian particles. The number of solved Cauchy problems will be equal to the number of measurements at each monitoring point for the entire analyzed period of time. Spatial resolution of simulation results will depend on the number of measurements and the density of the number of trajectories in the simulation zone.

6. Statistical, spatial analysis and visualization of the solutions. At this stage the distribution function of the initial data is determined and then the problem of calculating the field of the time-averaging errors of the solutions obtained in the previous stage is solved, and also the areas with different degrees of solution reliability are found. With the use of GIS technologies and 4D-field visualization techniques, the problems of analyzing the solutions are solved.

7. Verification of the solutions found. Due to the multistage nature and complexity of the proposed approach, the task of verifying the obtained solutions should be regarded as a fundamentally important step in computational technology.

3 Fluid Location of Atmosphere

The central part of the developed technology is the numerical calculations of the effective average concentration fields based on the data of local measurements and information on the dynamics of the atmosphere — the fifth stage of the proposed technology.

The task of modeling the spatial distribution of the atmospheric contaminant concentration is one of the key issues of atmospheric physics. For solving it in classical formulation, it is necessary to set the equations describing the contaminant transport in the atmosphere, the modeling area, the location and characteristics of the contaminant sources, the initial and boundary conditions. In such formulation, the additional data (in a rigorous mathematical formulation – excess data) of the contaminant concentration measurements usually are used to control the correctness of the solution or may be ignored.

Not long ago, a fundamentally different approach to the use of atmospheric contaminant concentrations measurements, implemented in the back trajectories statistic methods (BTS), was proposed [1, 2, 3]. In all BTS methods, the inverse atmospheric air parcel (the Lagrangian particle) trajectories from the measurement point is calculated for each measurement moments. Each trajectory is associated with the concentration value measured by the instrument. In most BTS methods, it is considered that the contaminant concentration does not change along the trajectories.

The recently proposed [4, 5, 6, 7, 8] Fluid Location of the Atmosphere method (FLA) represents the enhancement of the BTS methods by means of combining the statistical analysis and the solution of the contaminant transport equations along the air parcel trajectories (for Lagrangian particles). The information about the emission and the amount of contaminant in the atmosphere is transferred to the measurement instrument from remote areas due to the airflows, that allows speaking about the passive wind location of the atmosphere.

4 Problem formulation

The essence of the proposed approach is that instead of searching for instantaneous values of the concentration field, some average contaminant concentrations that have formed over a long time T are calculated. For doing that, a definition of two new functions is given and the equations system, which they obey, is written down.

Let us divide the entire region where we are trying to find the concentration distribution, onto a set of the closed, non-intersecting cells of finite volume V, which densely fill the entire space.

Definition 1 The average effective contaminant concentration field $\widetilde{\varphi}_{V,T}$ on the set of calculation cells V for a period of time T is a function:

$$\widetilde{\varphi}_{V,T}(\mathbf{r}) \overset{\text{definition}}{\equiv} \frac{1}{N_{V,T}} \sum_{p=1}^{N_{V,T}} \left(\frac{1}{\tau_{p,V}} \int\limits_{t_{p,V}}^{t_{p,V}+\tau_{p,V}} \varphi(\mathbf{r}_p(t), t)dt \right), \tag{1}$$

where, $N_{V,T}$ – the total number of air particles (of finite dimensions or infinitesimal Lagrangian particles) passing through the computational cell V for a period of time T; $\sum_p$ – means summation over all the particles that have passed through the calculation cell; $t_{p,V}$ – the time of particle p entry into the calculation cell V; $\tau_{p,V}$ – the duration of being the trajectory p in the calculation cell V; $\varphi(\mathbf{r}, t)$ – the contaminant concentration value at the point $\mathbf{r}$ at the moment t; the integration in Equation 1 is performed along the trajectories of the individual particles $\mathbf{r}_p(t)$. The Equation 1 is the definition of the time-average value of the concentration in the calculation cell, calculated with the help of some infinite countable or finite set of Lagrangian trajectories.

Definition 2 The average effective sources field $\widetilde{J}_{V,T}$ on the set of the calculation cells V for a period of time T is a function that depends on the average effective concentration field $\widetilde{\varphi}(\mathbf{r})$:

$$\widetilde{J}_{V,T}\left(\widetilde{\varphi},\mathbf{r}\right) \overset{\text{definition}}{\equiv} \frac{1}{VT}\int\limits_{t_0}^{t_0+T}\left[\iint\limits_{S_V}(\widetilde{\varphi}\,\mathbf{v})\cdot d\boldsymbol{\sigma}\right]dt+\frac{1}{VT}\iiint\limits_{V}\left[\widetilde{\varphi}-\widetilde{\varphi}^{\,0}-\int\limits_{t_0}^{t_0+T}F_E(\widetilde{\varphi},\mathbf{r},t)dt\right]dV, \tag{2}$$

where, T – averaging period; t_0 – the beginning of the averaging period; S_V – area of the surface surrounding the calculation cell V; $d\boldsymbol{\sigma}$ – surface element oriented outside of the cell; $\mathbf{v}(\mathbf{r},t)$ – wind velocity field (considered known); $\widetilde{\varphi}^{\,0}$ – the value of function $\widetilde{\varphi}$ for the previous averaging period $t < t_0$; $F_E(\widetilde{\varphi},\mathbf{r},t)$ – a known function describing in the Eulerian representation physico-chemical processes that change the contaminant concentration.

4.1 The Problem of Fluid Location of the Atmosphere

On a given finite set of calculation cells V, which fill the area of interest; for a known field of wind speeds $\mathbf{v}(\mathbf{r},t)$; for a given data set of the atmospheric contaminant concentration measurements $\varphi_{m,k}$ and for set of trajectories of the Lagrangian particles $\mathbf{r}_p(t)$, passing through the monitoring points $\mathbf{r}_m$ at the moments of measurements $t_{m,k}$, find such a function of the effective average concentration field $\widetilde{\varphi}_{V,T}(\mathbf{r})$, defined by Equation 1, for which the concentration distributions $\varphi(\mathbf{r}_p(t),t)$ along the trajectories obey to the following conservation equations in the Lagrange form with the initial conditions $\varphi_{m,k}$ (Cauchy problem for the Lagrangian particles trajectories):

$$\frac{D\,\varphi(\mathbf{r}_p(t),t)}{Dt}=\widetilde{J}_{V,T}\left(\widetilde{\varphi}_{V,T},\mathbf{r}_p(t)\right)+F_L(\varphi,\mathbf{r}_p(t),t)\ \text{with initial conditions:}\ \varphi(\mathbf{r}_m,t_{m,k})=\varphi_{m,k}\ , \tag{3}$$

where, D/Dt – an operator of the substantial derivative on time $D/Dt = \partial/\partial t + \mathbf{v}\cdot\partial/\partial\mathbf{r}$; $\widetilde{J}_{V,T}$ – average effective sources field; $F_L(\varphi,\mathbf{r},t)$ – a known function describing in the Lagrangian representation physico-chemical processes that change the contaminant concentration.

Differential Equations 3 together with two Definitions 1 and 2 form a closed system of equations. The total number of Cauchy problems is equal to the total number of all measurements at all monitoring points for the entire averaging period.

4.2 System of integral equations

Formally integrating the differential equation in the Cauchy problem (3) along the trajectory of the p th Lagrangian particle from the moment of measuring $t_{m,k}$ to an arbitrary time t, we obtain the integral equation for unknown concentration φ on the trajectory:

$$\varphi(\mathbf{r}_p(t),t)=\varphi_{m,k}+\int\limits_{t_{m,k}}^{t}\left[\widetilde{J}_{V,T}(\widetilde{\varphi}_{V,T},\mathbf{r}_p(t'))+F_L(\varphi,\mathbf{r}_p(t'),t')\right]dt'\ , \tag{4}$$

where $t_{m,k}$ is the starting time of the back trajectory p from the monitoring point $\mathbf{r}_m$, in which the concentration is measured by the device and is equal to $\varphi_{m,k}$.

Using the definition of (1) and the formula (4), we can write the integral equation for the field of average effective concentration $\widetilde{\varphi}_{V,T}$ in the set of the cells V for a period of time T:

$$\widetilde{\varphi}_{V,T}(\mathbf{r}) = \frac{1}{N_{V,T}}\sum_{p=1}^{N_{V,T}}\varphi_{m,k}+\frac{1}{N_{V,T}}\sum_{p=1}^{N_{V,T}}\frac{1}{\tau_{p,V}}\int\limits_{t_{p,V}}^{t_{p,V}+\tau_{p,V}}\left\{\int\limits_{t_{m,k}}^{t}\left[\widetilde{J}_{V,T}(\widetilde{\varphi}_{V,T},\mathbf{r}_p(t'))+F_L(\varphi,\mathbf{r}_p(t'),t')\right]dt'\right\}dt, \tag{5}$$

where $\tau_{p,V}$ is the time of the presence of the trajectory p in the calculated cell V; t' and t are integration variables along the trajectories that have a time sense, and t represents the instants of time when the trajectory p is inside the computed cell V. The function $\widetilde{J}_{V,T}$ on the right-hand side (5) depends on the unknown mean effective concentration field $\widetilde{\varphi}_{V,T}$ and is determined from formula (2). The unknown $\widetilde{\varphi}_{V,T}$ on the right-hand side of the integral in (5) is a function of $\mathbf{r}_p(t')$. In the general case, the function F_L is known and depends on the unknown concentration φ on the trajectories, which obeys the equation (3) or (4).

Thus, the problem is reduced to solving the system of integral equations (4) and (5) with the Definition (2).

4.3 Passive Contaminant

Let us consider a particular case of a "passive" contaminant, when the contribution into the contaminant concentration change due to various physico-chemical processes is negligibly small in comparison with the contribution of external contaminant sources impact $F_L \ll \widetilde{J}_{V,T}$. In this particular case, the following integral equations can be obtained from the Equations (1)-(3), relative to the function of the average effective concentration field $\widetilde{\varphi}_{V,T}(\mathbf{r})$:

$$\widetilde{\varphi}_{V,T}(\mathbf{r}) = \frac{1}{N_{V,T}} \sum_{p=1}^{N_{V,T}} \left\{ \varphi_{m,k} + \frac{1}{\tau_{p,V}} \int\limits_{t_{p,V}}^{t_{p,V}+\tau_{p,V}} \left[\int\limits_{t_{m,k}}^{t} \widetilde{J}_{V,T}\left(\widetilde{\varphi}_{V,T}, \mathbf{r}_p(t')\right) dt' \right] dt \right\}. \tag{6}$$

5 Example of the average effective methane concentration field recovering

Below is the result of solving a quasi-two-dimensional FLA problem (Equation 6) based on monitoring data at one point. As initial information, the results of methane concentration measurements in surface air were used. The measurements were made in July-August 2016 on Bely Island (Kara Sea) using a gas analyzer Picarro G-2401 [9]. The back trajectory calculations of four days duration were carried out using software HYSPLIT4 [10]. For the results presented, the spatial resolution corresponding to the cell sizes of the Euler grid was $1^\circ \times 0.5^\circ$.

The figure 1 presents examples of the back trajectories calculations for a starting height of 500 m for June and July 2016. The black dot marks the monitoring point on Bely Island, and the blue dots are the places from where the air flows started (in a direct time), which reached the monitoring point in 96 hours. It can be seen from the figure that the trajectories bring the signal to the point of measurement from areas distant from it by several thousand kilometers.

Thus, the area covered by the trajectories is a 4-day zone of influence on the monitoring point on the Bely Island in July and August 2016. It can be seen from the figure that the zone of influence covers a considerable area within the Arctic Circle, including the North Pole. In general, the zone of influence extends above the sea surface, the islands of the Northern Earth, Archipelago of Svalbard, the Frantz Josef Land Archipelago and, to a much lesser extent, over the northern territories of Eurasia. Attention is drawn to the asymmetry of the zone of influence relative to the position of the monitoring point. In July and August the nature of air flows is significantly different. In the zone of influence in August there is practically no eastern transfer.

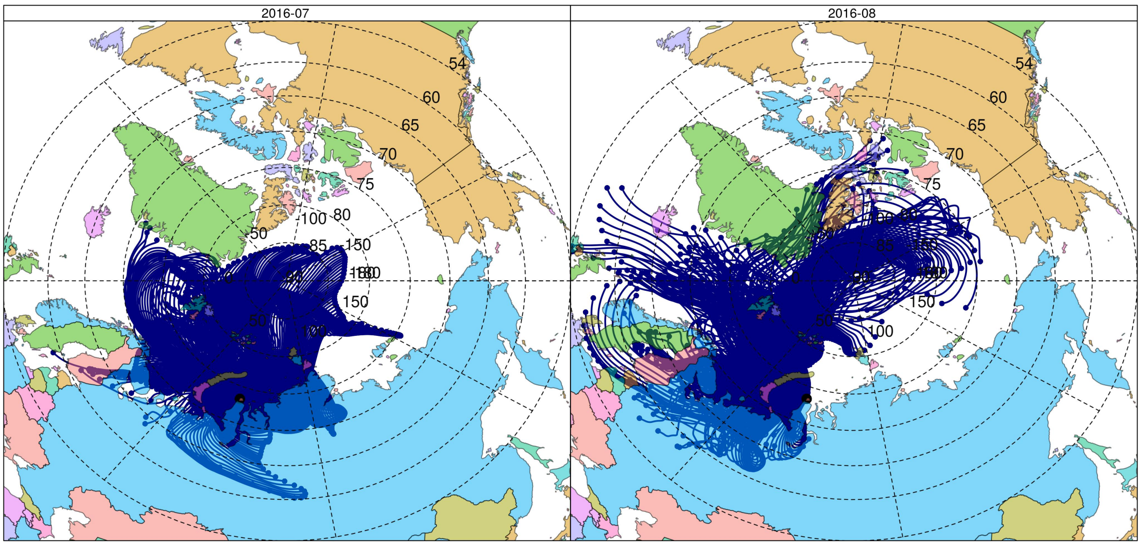

Figure 1: Back trajectories (duration – 96 hours, starting height – 500 m) for monitoring station on Bely Island for July and August 2016.

The figure 2 shows the results of calculating the average effective methane concentration field normalized to the average concentration for the indicated period at the monitoring station on Bely Island - 1323.84 $\mu g/m^3$ (1.924 ppm).

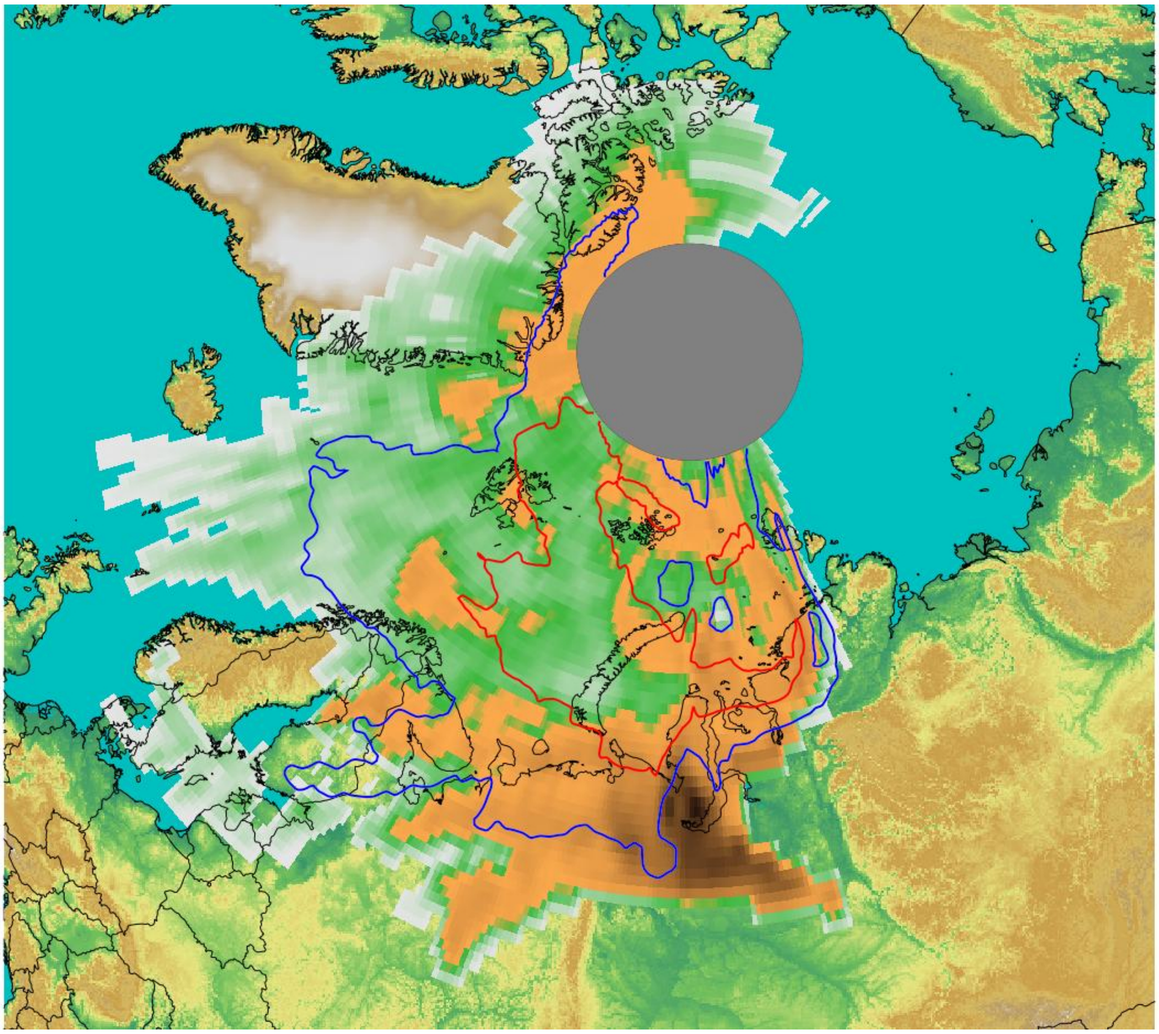

Figure 2: The average effective field of normalized methane concentration $\widetilde{\varphi}(\mathbf{r})$ in the region of Kara and Barents seas in July-August 2016.

White and light green tones correspond to concentrations lower than the average concentration of methane at the monitoring station, and light brown and black - to higher ones. The region of the North Pole located outside the calculation area is shaded in gray. In addition, the boundaries of states are shown, as well as the coastline of continents and islands. An orthographic projection was used with a touch of the geoid surface at the monitoring point at Bely Island: $lat_0 = 73.325°N$; $lon_0 = 70.057°E$. The isolines of the density of the back trajectories are highlighted in blue and red. Within these isolines, more than 10 and 50 trajectories pass through each computed cell, respectively.

Prior to the calculations, it was assumed that increased levels of methane should be observed over the continent, but not above the seas, as the chemical reaction of methane with chlorine above the sea surface should provide a known atmospheric sink of methane. Indeed, the simulation results show that the increased content of methane is mainly observed over the continent and in the region of the coast. An unexpected result is the presence of extensive areas in some parts of the sea surface, where elevated concentrations of methane are also recorded. Now it is not clear, are these areas above the sea surface the result of some methane sources action in these regions, or it are the result of a random concurrence of meteorological conditions occurred over a short period of measurements in the summer of 2016. Probably, this fact can be clarified after getting the long-term data of greenhouse gas measurements in this region.

6 Conclusion

It is proposed a fundamentally new formulation of the problem of estimating the spatial structure of the average concentration field of atmospheric contaminant on the base of measurements at one or several monitoring points, without involving information on the sources — the problem of passive location (remote sensing) of the atmosphere by wind or Fluid Location of the Atmosphere.

The theoretical foundations of the problem of the Fluid Location of the Atmosphere are considered. Two new functions are defined: the average effective concentration field and the average effective sources field. In the differential and integral representations, the equations for finding these functions are written. The proposed approach has pretensions that on the basis of a joint statistical analysis of measurements and numerical solution of the transport equations: 1) to find a statistical estimate of the distribution of the average contaminant concentration; 2) to identify possible locations of contaminant sources; 3) to estimate the average emission of the contaminant into the atmosphere.

In the quasi-two-dimensional approximation for the case of a passive contaminant, the estimates of the average effective methane concentration in the Kara and Barents Seas regions are presented based on measurements on Bely Island in July and August 2016.

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