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NUMERICAL MODELING OF THE FIELDS OF POLYCHLORINATED BIPHENYLS IN THE BLACK SEA

ABSTRACT. A mathematical three-dimensional model was developed by combining a physically complete block of circulation with moduli of transport and transformation of detritus and polychlorinated biphenyls (PCBs). This z-coordinate model has a horizontal resolution of 5 × 5 km, 45 vertical levels, and a step of 5 minutes. The model considers gravitational sedimentation and decomposition of detritus, as well as its deposition and erosion on the bottom. To calculate the transport and transformation of PCBs in the Sea, the model uses three state variables: the concentration of PCBs in solution, in detritus, and in the upper layer of sediment. It also considers sorption, desorption, and reversible flows of PCBs at the bottom.

A 20-day model calculation was performed to simulate a potential accidental release of PCBs in the area of the Danube Delta in spring. The PCBs advection flows dominated and were comparable to the adsorption/desorption flows, while the diffusion fluxes were infinitesimal. Up to 20% of discharged PCBs were adsorbed by detritus in the first two days after the accident. There was a gradual accumulation of PCBs on the bottom; 16 days after the accident, 18% of the PCBs were bound to the sediments. The PCBs transport on detritus serves as a natural buffer mechanism that weakens the spread of PCBs in the sea. The paper analyzes the dynamics of PCB fields formed as a result of the application of an artificial active sorbent to minimize adverse effects on the ecosystem. An end-user oriented software application was developed; it allows forecasting the dynamics of potential releases of PCBs and planning counter-measures. A user-friendly interface allows tracking the field, visualizing the distribution of PCBs in the water column and sediments, and displaying the balance between dissolved and suspended phases.

KEY WORDS: multidisciplinary model, PCB transport, adsorption, desorption, sediments.

INTRODUCTION

Ensuring the safety of the environment requires other measures besides a timely cleanup of hazardous pollutants. A significant reduction of environmental risks has been achieved with the introduction of low-waste technology. However, predicting impact of accidental releases on the existing ecosystem is also very important. Finding solution to these problems is particularly relevant in areas of high population density, regions of active exploitation of marine resources, and recreational areas.

The urgent need to address the problems of ecological and analytical monitoring calls for research on transport and transformation of anthropogenic persistent organic pollutants that, even in low concentrations, adversely affect marine ecosystems. PCBs, some of the most common highly toxic synthetic chemicals, belong to the class of aromatic compounds consisting of two benzene rings connected by the internuclear **C–C** bond (Fig. 1). There, the hydrogen atoms are substituted with the chlorine atoms (1–10) in the ortho-, meta-, or para-positions. Theoretically, there may be 209 PCB congeners with a general formula $S_{12}N_{10-n}Cl_n$, where n = 1 – 10. About a hundred of individual congeners have been detected in the marine environment in real conditions. These compounds have a number of specific features: the global prevalence; extreme resistance to physical, chemical, and biological transformations; bioaccumulation associated with low and high solubility in water and lipids, respectively; and toxicity to living organisms even at low concentrations. Mass production of PCBs occurred in 1929–1986 and then their commercial production was terminated. During this time, the world produced ~2 million tons of PCBs. Such widespread use of PCBs was due to a number of their unique physical and chemical properties: exceptional thermal, physical, and electrical insulating properties; thermal stability; inertness to acids and alkalis; flame resistance; good solubility in fats, oils, and organic solvents; and excellent adhesion. This determined their wide application as hydraulic fluids; coolants and refrigerants; lubricants; components of paints, varnishes, and adhesives; plasticizers and fillers in plastics and elastomers; flame retardants; and solvents dielectrics in transformers and capacitors.

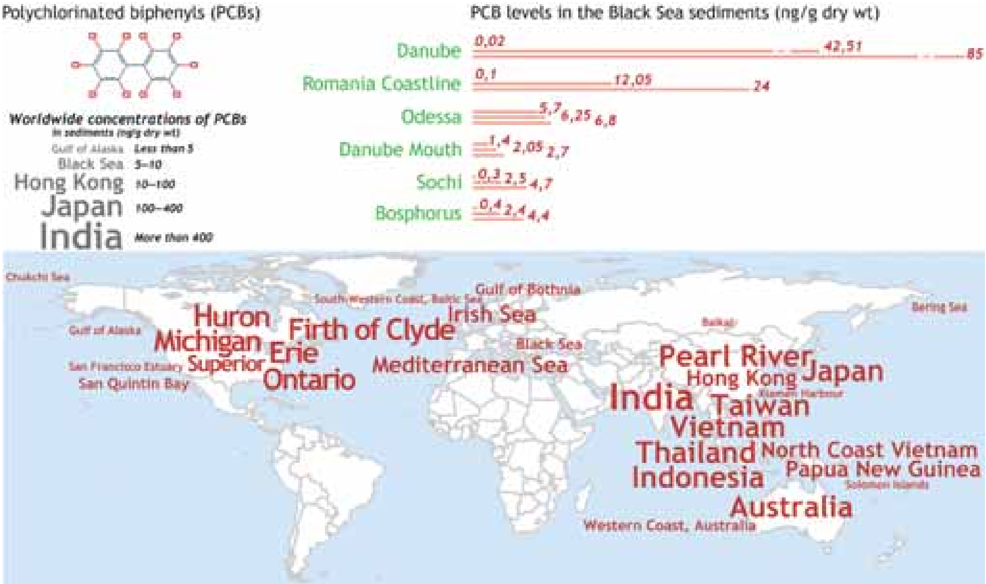

Fig. 1. Global distribution of PCBs

PCBs enter the ocean with river flow, precipitation, and technogenic discharge. The most important physical mechanisms of transport of PCBs in the sea are the advection and turbulent diffusion. The main sources of re-contamination of seawater are the sediments of the coastal and offshore areas of the oceans. It has been estimated [Jonsson, Carman, 2000] that removal of PCBs from the environment would take more than 100 years with a strict prohibition on production.

Experimental data [Orlova, 1994; Maldonado, Bayona, et al., 1999; Zherko, Egorov, et al., 2000; Fillmann, Readman, et al., 2002; Bakan, Ariman, 2004] show a significant PCB pollution of the Black Sea accompanied by intense accumulation of PCBs in biota [Tanabe, Madhusree, et al., 1997]. The map shown in Fig. 1 was compiled after [Burns, Villeneuve, 1983; Fillmann, Readman, et al., 2002; Bakan, Ariman, 2004; Dove, Hill, 2008] to demonstrate the role of the Black Sea sediments in the global distribution of PCBs.

The degree of PCB contamination of the sediments of the Black Sea and of its north-western shelf is between the relatively clean sediments of the Baltic Sea and the highly contaminated sediments of the basins of India and South-East Asia, where in the 1960s, PCB defoliants (*"Agent Orange"*) were actively used [Dioxins and Health, 1994] and now there is rapid industrial development. The spatial distribution of PCBs in the sediments of the Black Sea (Fig. 1) is characterized by great variability. It shows a high degree of contamination of the sediments of the River Danube, the Romanian coast, and the Gulf of Odessa, which monotonically decreases to the coast of Turkey.

Mathematical modeling is one of the most effective methods for studying processes of PCBs transport in the natural environment. Exceptional capacity for PCB adsorption to organic carbon-rich particles, as well as the complex interaction of the processes of accumulation and release at the bottom, makes it impossible to model PCBs as conservative tracers. Despite a fairly large number of laboratory studies and a steadily growing volume of field measurements so far there has not been a comprehensive model that adequately reproduces the spatial and temporal evolution of the PCB fields in the Black Sea. The specifics of our study is a comprehensive consideration of the dynamics of the three-dimensional flow fields and turbulent diffusion with adsorption and desorption of PCBs on detritus particles (suspended fraction of dead organic matter) as a natural sorbent of PCBs. Interaction between PCBs and sediment is also considered in the model. Development of advanced systems for forecasting the state of the marine environment and the consequences of accidental releases of PCBs aimed at scientific support of management decisions to minimize environmental risks is possible only within the framework of the above-described multi-disciplinary approach.

DESCRIPTION OF THE MODEL

A mathematical model [Lyubartseva, Ivanov, et. al., 2012] was used to calculate the three-dimensional fields of PCBs in the north-western shelf of the Black Sea. The Black Sea is a deep (~2 km) semi-closed elliptical basin (Fig. 2) with the zonal and meridional length of 1000 km and 400 km, respectively. Hydrological structure of the Black Sea is mainly determined by freshwater runoff of the major European rivers: the River Danube, the River Dnepr, and water exchange through the Bosporus and Kerch straights. Limited by the isobath of 200 m, the north-western shelf occupies 16% of the sea water and accounts for 0,7% of its volume [Ivanov, Belokopytov, 2011].

The model is built on the assumption (Fig. 3) that the distribution of PCBs in sea is determined by transport mechanisms: advection, turbulent diffusion, and gravity sedimentation of mono-disperse detritus and of PCBs on detritus. In the water column, PCBs is adsorbed on detritus particles to certain saturation. Then, the reverse process (desorption) begins, etc. On the bottom, diffusive exchange of dissolved PCBs with

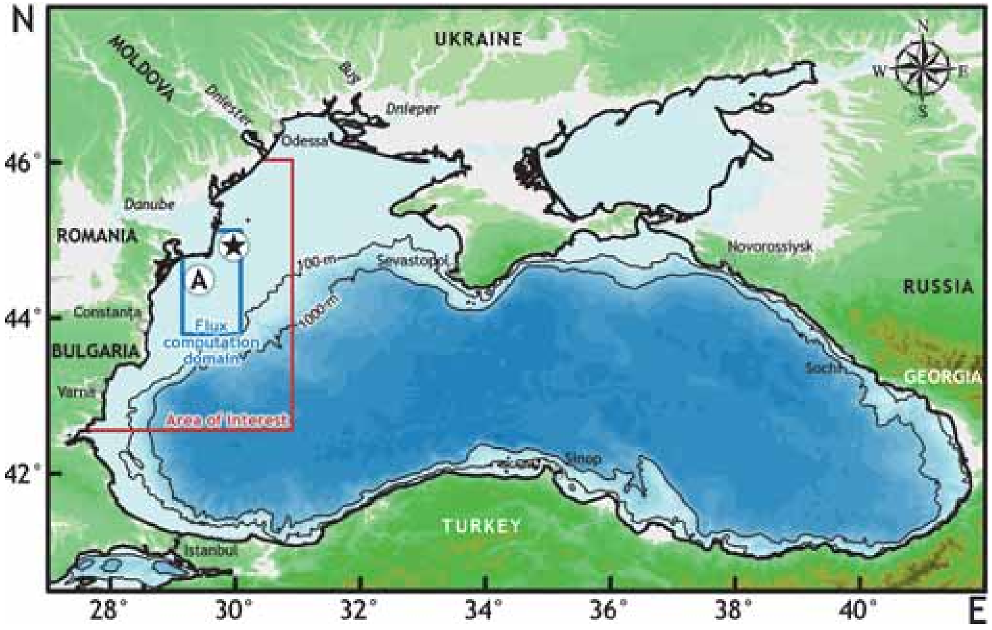

Fig. 2. The Black Sea. The star indicates the PCBs spill point used in the simulation. The obtained Hovmoller diagrams relate to Station A

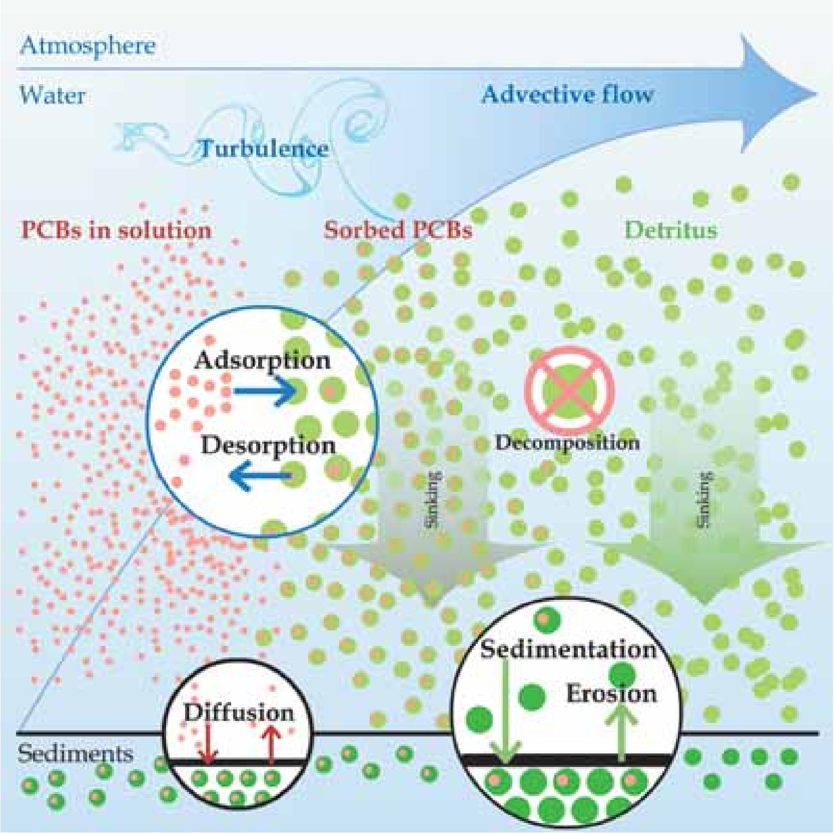

Fig. 3. Schematic representation of the modeled processes

the upper layer of the sediments takes place. The bottom exchange between detritus and PCBs on detritus is regulated by the balance of sedimentation and erosion flows. The decomposition of detritus is the resulting effect of its microbiological degradation, hydrolysis, and transition of the particles to a different size class.

The mathematical model consists of three blocks. In the hydrodynamic block, three-dimensional velocity fields of currents, temperature, and salinity of sea are calculated. These data are used in the detritus transfer and transformation block. The three-dimensional fields of velocity of currents, temperature, salinity, and concentrations of detritus are the input parameters of the PCBs transfer block, where PCB concentration in the solution, the concentration of PCBs on detritus particles, and the concentration of PCBs in the upper layer of sediments are calculated.

The hydrodynamic block utilizes a three-dimensional numerical z-coordinate model [Demyshev, Korotaev, 1992]. This model was developed in the Marine Hydrophysical Institute of the NAS and is used to solve problems associated with operational forecasts of the Black Sea; from the moment of its creation, it has being constantly improved. The model is based on a full set of nonlinear equations of motion and transfer of heat and salt in the Boussinesq approximation, hydrostatics, and incompressibility of seawater.

On the surface, daily fields of tangential friction stress of wind were assigned. The data array was obtained by averaging the 1988–1998 data derived from the surface pressure distribution, in 6-hrs increments. Daily fluxes of heat, precipitation, and evaporation [Belokopytov, 2004] were obtained through actual measurements and were assimilated according to the algorithm [Knysh, Demyshev, et. al., 2002]. On the bottom and solid sidewalls, the impermeability condition for the normal component of velocity and for adhesion for the tangential component; the absence of heat and salt flows were assumed. At the liquid boundary, the Dirichlet condition at the inflow was assigned; the fluxes of pulse, heat, and salt were set for the outflow. The turbulent exchange of pulse and turbulent horizontal diffusion were specified as biharmonic operators. Parameterization was used as the vertical turbulent closure [Pacanowski, Philander, 1981].

In the detritus transfer block, the three-dimensional non-stationary fields of detritus concentration were calculated by the differential equation of the advection – diffusion – reaction type [Bagaiev, 2010]. The model takes into account gravitational sedimentation and decomposition of detritus. On the surface, the natural flow of detritus formed from decomposition of phytoplankton was assumed [Ivanov, Lyubartseva et. al., 1999]. On the bottom, the conditions of sedimentation and erosion that depend on the bottom shear stress were assigned [Ivanov, Fomin, 2008]. On the lateral boundaries, the absence of detritus flows was assumed.

The PCBs transfer block was based on the three-dimensional equations of the advection – diffusion – reaction type that discribe the PCBs concentration in solution, in detritus, and in the upper layer of sediments [Ivanov, Bagaiev, et. al. 2012]. The processes of adsorption and desorption of PCBs deposited on detritus particles were accounted for according to [Margvelashvili, 1999]. On the surface, the absence of the PCBs flow was assumed. On the bottom, the balance conditions of exchange were assumed: diffusion exchange of the soluble component plus the exchange of the PCB-contaminated particles considering their sedimentation and erosion. On the solid lateral boundaries, the condition of the PCBs flow was assigned. On the lateral liquid-solid boundaries, the PCBs flow was assumed, imitating their entry into the sea from the rivers. The initial conditions assume the infinitesimal background concentrations of all state variables.

Model equations were integrated numerically on a uniform horizontal grid [Lebedev, 1964] with a resolution of 5 × 5 km, by 45 unevenly distributed horizons with a 5-minute time step.

MODELING THE SCENARIO OF A POTENTIAL ACCIDENTAL SPILL OF PCBS FROM THE DANUBE MOUTH

The developed model was used to calculate the three-dimensional fields of PCBs, formed as a result of an instantaneous emergency discharge of 4 kg of PCBs from the Danube St. George Girlie in early spring. The northwestern shelf of the Black Sea during this period has high influx of detritus following the blooming of cold-resistant phytoplankton. It was expected that in these conditions, the process of adsorption and desorption of PCBs on detritus will reach its maximal intensity. Besides, this season has a relatively high flow velocity at the bottom, and it is necessary to examine sediment disturbance in the formation of secondary contamination of PCBs in the water column.

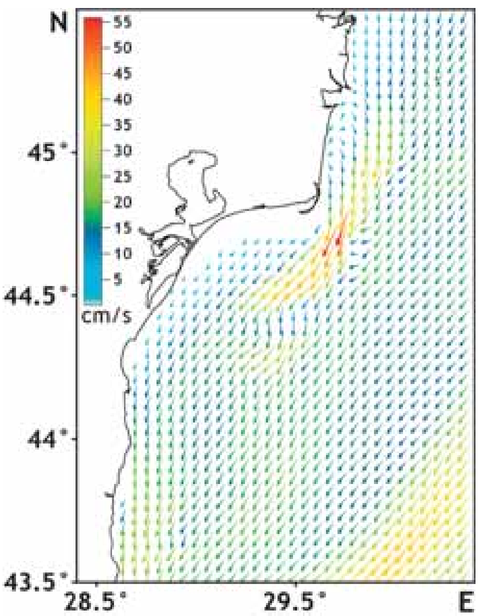

Fig. 4. Spatial distribution of horizontal currents (cm/s) at a depth of 3 m in 10 days after the accident. The results of simulation

The dynamic problem of the PCBs field transport was solved using a 20-day interval.

Due to the prevalence of the north and northeastern winds typical for this season, with speeds of up to 10–15 m/s, the alongshore current, extending in the southwestern direction, formed in the computational domain (Fig. 4). It had the average speed of 20 cm/s. The flow velocity decreased on approaching the shore. The vertical velocity field had a complex structure with a pronounced downwelling and many local areas of sinking water. In the field of surface salinity, there formed a distinct frontal zone with a gradient of 1 PSU/10 km (Practical Salinity Units) due to the freshening influence of rivers.

On the 3rd day after the accident, the PCB and detritus fields at the depth of 3 m were carried to the area of Tulcea (Romania). At a 30 m depth, the field moved slower; there, dissolved PCBs were also adsorbed on detritus. Detritus and PCBs on detritus formed lenses in the bottom layers due to sediment detachment at the water-sediment boundary. Calculations have shown that the incidence of detritus and PCBs in the open sea was limited to a 75 m isobath. In 10 days after the accident (Fig. 5), the considerably diluted pollution fields reached Constanta (Romania). The southern vanguard part of the frontal zone reached Cape Kaliakra (Bulgaria). The boundaries of the fields were somewhat dissolving by diffusion. Analysis of the dynamics of the PCBs concentration fields in the upper layer of the sediments showed that the area was dominated by the classification types of sediments either transporting or accumulating PCB [Jonsson, Gustaffson, 2003]. The sediments of the transporting type, which not only adsorb PCBs, but also release them during detachment, are found near Cape Kaliakra. According to [Panin, Jipa, 1998], this area is under the direct influence of the Danube origin sediment flows and is the most dynamic and active because it comes close to the main current of the Black Sea.

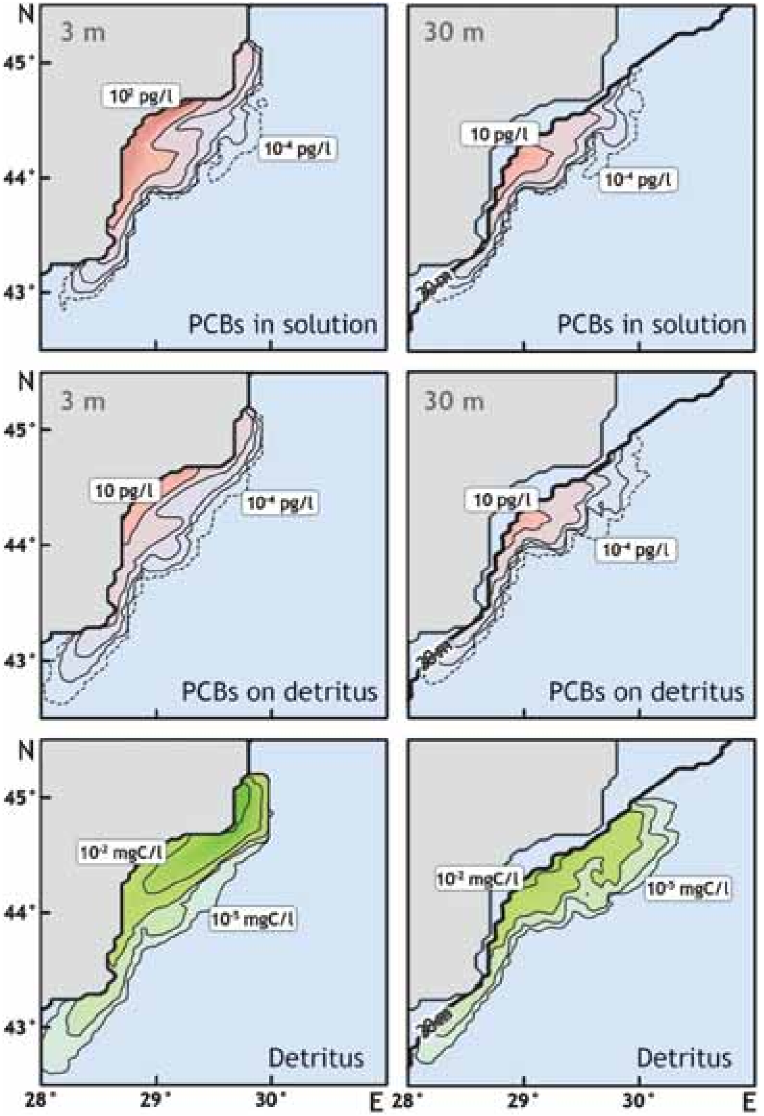

Fig. 5. Spatial distributions of the concentration of PCBs in solution (upper panels); PCBs on detritus (middle panels); detritus (lower panels) at a depth of 3 m (left) and 30 m (right) in 10 days after the accident. The results of simulation

The evolution of the vertical profiles of suspended and dissolved matter at Station A was investigated with the Hovmoller diagrams (Fig. 6). Fig. 6 (*A*) shows that the center of the dissolved PCBs field reaches the Station in 4 days after the accident. The maximal concentration of more than 30 pg/l is located at a depth of 26 m. The intensive adsorption on settling detritus begins. The concentration of PCBs in detritus in the center of pollution reaches 14 pg/l (Fig. 6 (*B*)). The distribution of detritus is patchy (Fig. 6 (*C*)), which is typical for marine ecosystems. The concentration of detritus peaked at 0,01 mg C/l at the same depth (Fig. 6 (*C*)). Contaminated detritus was settling quickly on the bottom, where it was gradually building up (Fig. 6 (*E*)). In 4 days after the accident, the accumulation of PCBs in the sediments was maximal. It is evident that the sediments at Station A belong to the PCB accumulation type. Remaining in water detritus became saturated with PCBs

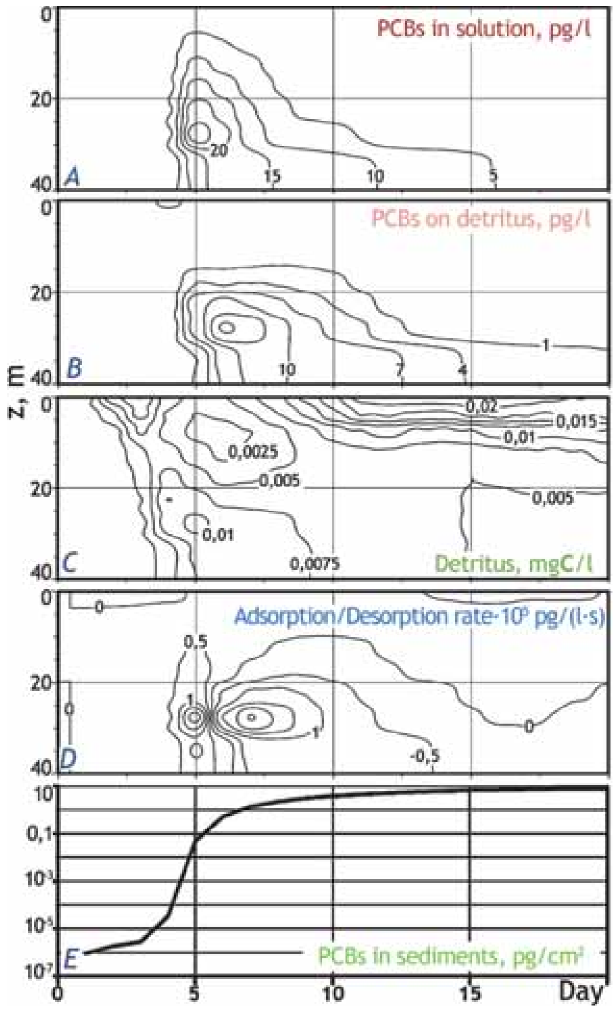

Fig. 6. The Hovmoller diagrams for Station A. (A) concentration of the PCBs in solution; (B) of the PCBs on detritus; (C) detritus concentration; (D) adsorption/desorption rate; (E) the PCB concentration in the top layer of sediments. The results of simulation

and, in 6 days after the accident, the reverse process of desorption took place. The chart (Fig. 6 [*D*]) shows the distribution of the rate of adsorption (positive values) and desorption (negative values). Change in the sign of this value appears as a pronounced dipole at a depth of 26 m. The resulting dipole asymmetry is caused by uneven distribution of detritus in the water column. The calculations have shown that the dissolved PCBs disappeared at this Station 4 days earlier than the PCB-contaminated detritus.

The budget of PCBs (Fig. 7) illustrates the redistribution of the PCBs that have entered after the accident within the entire computational domain. Adsorption dominated during the first two days after the accident, which led to a 20% reduction in the mass of the dissolved PCBs. Desorption began 2 days after the accident. There was a gradual accumulation of the PCBs on the bottom. It has been demonstrated that 16 days after the accident, sediments bounded 18% of the PCBs. It can be concluded that the sinking particles of detritus, as a natural sorbent PCB, form a natural buffer system, which speeds up water purification and binding of PCBs in sediments.

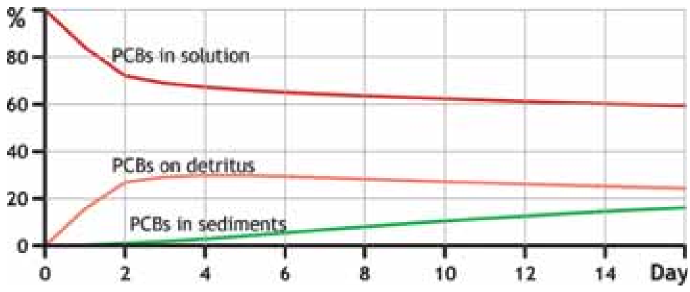

Fig. 7. The PCB budget on the Black Sea northwestern shelf. The results of simulation

To estimate the contribution of different physical mechanisms to the development of the three-dimensional fields of PCBs, the PCBs fluxes were calculated in the closed three-dimensional region bounded by 44,2°–45,1°N and 29,2°–30,1°E, which corresponds to a rectangular area with dimensions of 100 km × 75 km (Fig. 2). The calculations have shown that advection transport and adsorption-desorption of physical and chemical fluxes dominate in this area (Fig. 8). The positive values for advection and diffusion correspond to the influx, while the negative ones – to the efflux. For adsorption, the positive flow means the "transfer" from the dissolved form to detritus. Among the advection flows, the flow through the western boundary dominated, with its maximum of 0,13 g/s on the 6th day after the accident. The adsorption and desorption flows had the following characteristics of the local extremes: $5{,}0 \times 10^{-2}$ g/s on the 6th day and -1.5×10^{-2} g/s on the 10th day. The horizontal turbulent diffusion ($\sim 10^{-18}$–10^{-13} g/s) appeared to be the weakest transport mechanism in the system.

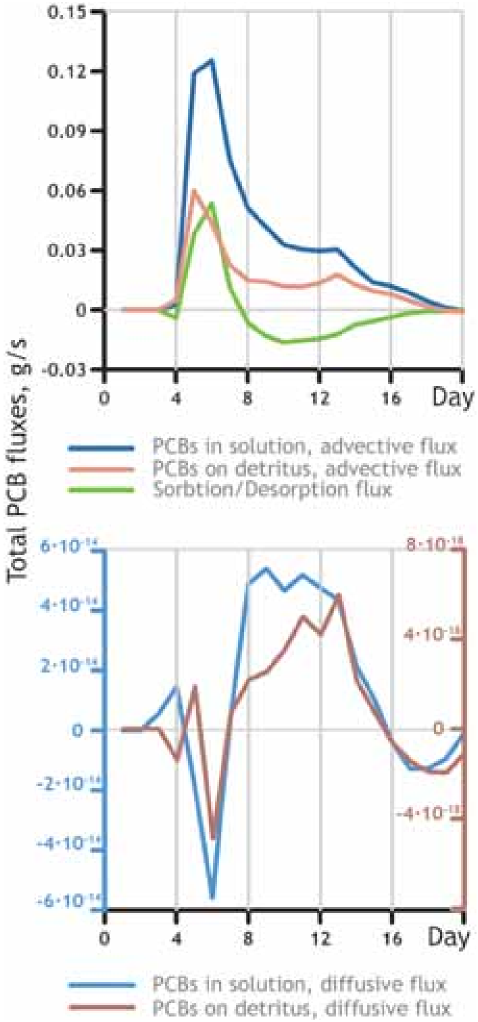

Fig. 8. The total PCB fluxes through the finite domain shown in Fig. 2. The results of simulation

EVALUATION OF EFFICIENCY OF AN ACTIVE SORBENT APPLIED TO CONTROL THE PCBS SPREAD

High sorption capacity of PCBs may be used in integrated post-emergency measures to reduce dispersion of PCBs in the marine environment. The model can evaluate the effectiveness of the use of active sorbents in combating the adverse effects of an accidental release.

For this, the master equations of the model were modified and supplemented with the equations of the advection-diffusion-reaction type for the concentrations of the active sorbent and of PCBs on it [Bagaiev, Lyubartseva, 2011]. Physical and chemical characteristics close to real conditions were assigned [Delle Site, 2001] for the active sorbent. Using test-calculations, a close to optimal strategy of placing the sorbent in the sea was chosen.

A numerical experiment was realized in the following scenario. A hypothetical monitoring service detects an accidental release of PCBs, as described in the previous section. The calculation under the framework of the developed model forecasts the PCBs field trajectory. To minimize negative consequences of the accident, in 5 hours, 120 tons of the active sorbent with the sorption capacity threefold exceeding that of natural detritus were instantaneously dropped into 12 surface boxes located perpendicular to the mean vector of the field movement (Fig. 9).

The calculations have shown that the rate of gravitational sedimentaiton of the artificial sorbent was very important. If the rate is too high, the sorbent settles on the bottom much faster than the speed at which PCBs are adsorbed on its surface. If the rate of sedimentation is too low, the sorbent is removed from the field by strong surface currents before it gets saturated with PCBs. The sedimentation rate of detritus in the model was assumed to be 10^{-3} cm/s; the rate of sedimentation of the active sorbent was $5 \cdot 10^{-3}$ cm/s.

Fig. 9 shows the evolution of the filed of dissolved PCBs at a depth of 3 m without the sorbent (left) and with its application (right). The PCB fields, in violet-blue colors, were delineated by a contour of a 3,10 pg/l concentration of dissolved PCBs. The field of the active sorbent is delineated by the green contour with the concentration of 1 pg/l. In the upper right frame, the black color indicates the line of the active sorbent "injection." On the right series of frames, the sorbent field was drawn on the top of the PCBs filed, because the distribution of the PCBs without and with the sorbent were practically identical. Subtle differences can be seen in the frames corresponding to the 8th day after the accident. The field of concentration of the active sorbent was deforming in the surface water layer due to the dynamically active flow of the alongshore current. By the 6th day, there was a disruption of the active sorbent concentration field. One part of it was carried away in the open sea and the other one was accumulating in the apex area of the coastal zone.

The efficiency of the active sorbent was controlled by the PCBs budget (Fig. 10). By

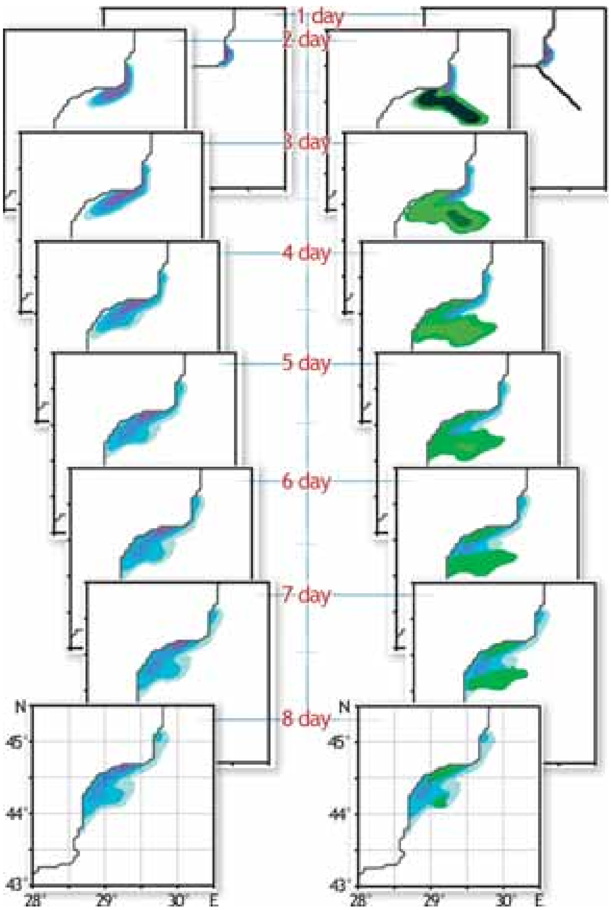

Fig. 9. The PCB-spill evolution at a depth of 3 m, without (left panel) and with (right panel) the active sorbent. The PCB concentration is in blue; the active sorbent concentration is in green. The results of simulation

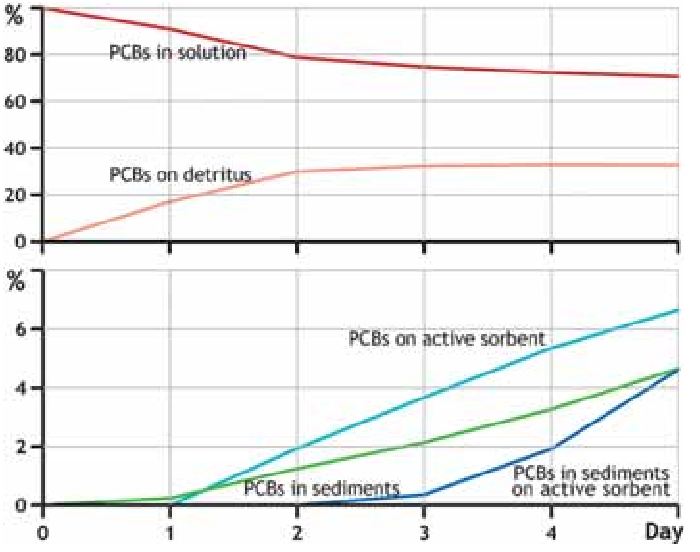

Fig. 10. The PCBs budget in the scenario with the active sorbent. The simulation results

the 5th day after the accident, about 30% of PCBs was adsorbed on detritus particles and only 6% of the PCBs was adsorbed by the active sorbent; 4% of the PCBs was adsorbed by the sediment. The mass of the PCBs adsorbed by the active sorbent was significantly lower than that of the PCBs adsorbed by detritus. However, the active sorbent accumulated PCBs much faster than the top layer of sediment. By the 5th day after the accident, the mass of the PCBs adsorbed by the active sorbent particles was equal to the mass of the PCBs adsorbed by the sediments. In general, it may be stated that the work of the active sorbent in the water column was ineffective because of a too short retaining time of the center of the PCBs contamination in the zone of active sorption. Detritus as a natural PCBs sorbent works much better due to the homogeneous distribution in the water column. Approximately half of the mass of the active sorbent is carried far away at sea, i.e., it is practically useless. The ratio of the areas of the contaminated bottom with and without the sorbent application is about 95%.

However, the numerical experiments showed that, on time scales exceeding 15 days, the active sorbent is more efficient in the PCB containment in the top layer of the sediments compared to detritus. It means that the sorbent should be introduced directly into the upper layer of sediments of the apex near shore areas where it would, due to its high absorptions capacity, actively adsorb contaminants during time-frames of about a month and would block potential re-contamination of the water column.

DEVELOPMENT OF THE END-USER APPLICATION

For efficient decision-making based on the model presented above, an application module with a remote web interface is being developed. A user-friendly system interface (Fig. 11) includes input fields for the date and time of an accident, its duration, the rate of contamination influx, and the coordinates of the discharge. A database of physical-chemical parameters of different congeners and PCB-containing mixtures is being compiled. In the future, this knowledge-based system will allow an end-user to calculate the trajectory of contamination fields, visualize the three-dimensional field of PCBs in solution and on detritus, map the contamination on the bottom, and plan countermeasures.

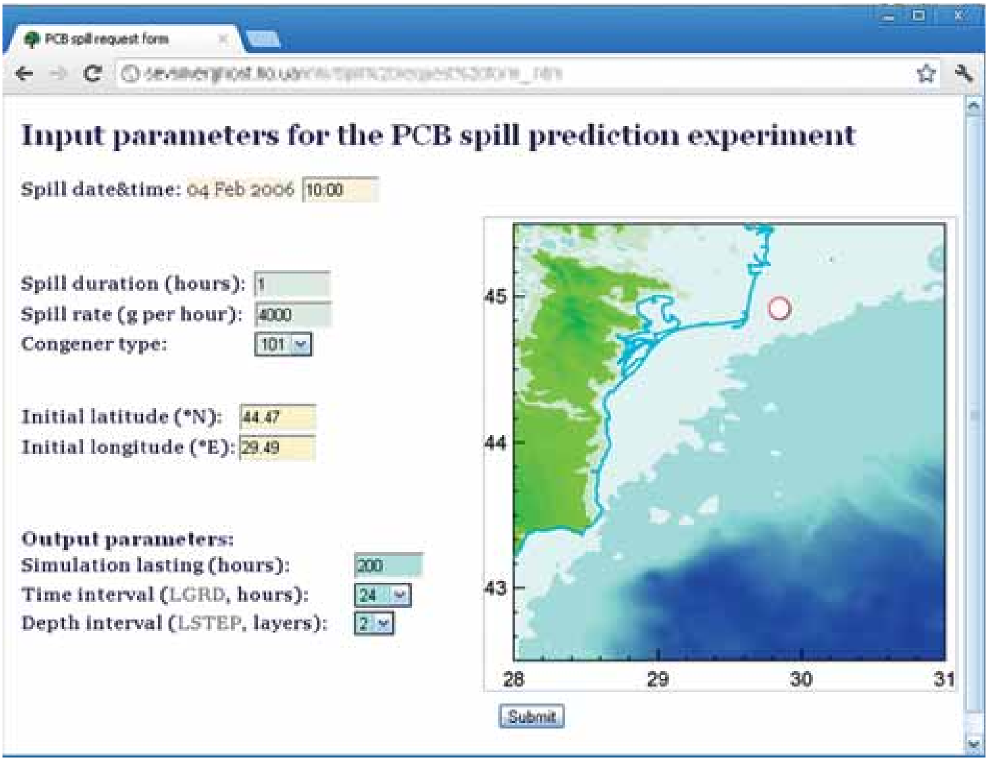

Fig. 11. A web interface for end-users

CONCLUSIONS

1. A 3D interdisciplinary model of the PCBs dynamics has been developed; the model considers physical transport mechanisms, advection and turbulent diffusion, as well as physical and chemical processes of adsorption and desorption on detritus. The model takes into account exchange processes at the boundary water – bottom sediments. The model combined three units: (1) thermo-hydrodynamic, (2) transport and transformation of detritus as a natural PBC sorbent, and (3) PCB transport.

2. The assessment for a 20-day period of the contamination fields after a potential accidental discharge in the Danube River Delta has been conducted. The advection transport of PCBs by the near shore jet current was the dominating mechanism. The adsorption and desorption flows on detritus were comparable with the advection flow. During the first 2 days after the accident, 20% of the mass of PCBs was adsorbed on detritus, indicating the existence of a natural buffer system that speeds up the purification of water and binding of PCBs by bottom sediments.

3. The model allowed assessment of the efficiency of the use of an active sorbent for mitigating negative impacts of an accident. It has been demonstrated that placing the active sorbent into the water column of this dynamically active sea area is inefficient. It is feasible to use it in the top layer of the sediments of the apex areas where it works affectively on time scales of the order of months.

4. To support management decisions using the model, an application module with a remote web interface is in the process of development. In the future, it would allow estimating the trajectory of PCB-contamination fields, visualizing the PCBs fields in solution and on detritus, mapping bottom contamination, and planning environmental protection activities.

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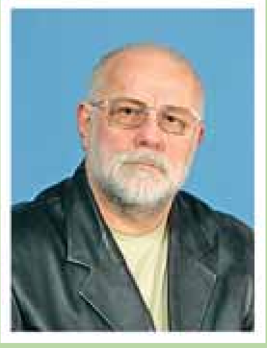

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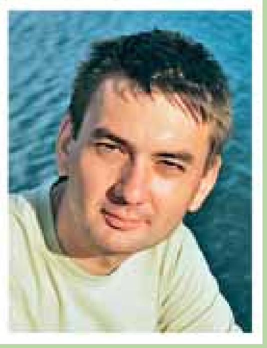

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