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3D multidisciplinary numerical model of polychlorinated biphenyl dynamics on the Black Sea north-western shelf

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The Black Sea north-western shelf plays a key role in economics of the developing countries such as Ukraine due to food supply, invaluable recreational potential and variety of the relevant maritime shipping routes. On the other hand, a shallow flat shelf is mostly affected by anthropogenic pollution, eutrophication, hypoxia and harmful algae blooms.

The research is focused on modeling the transport and transformation of PCBs (PolyChlorinated Biphenyls) because they are exceedingly toxic and highly resistant to degradation, hence cumulatively affect marine ecosystems. Being lipophilic compounds, PCBs demonstrate the distinguishing sorption/desorption activity taking part in the biogeochemical fluxes via the organic matter particles and sediments. In the framework of the research, the coastal in-situ data on PCB concentration in the water column and sediments are processed, visualized and analyzed. It is concluded that the main sources of PCBs are related to the Danube discharge and resuspension from the shallow-water sediments.

Developed 3D numerical model is aimed at simulation of PCB contamination of the water column and sediment. The model integrates the full physics hydrodynamic block as well as modules, which describe detritus transport and transformation and PCB dynamics. Three state variables are simulated in PCB transport module: concentration in solute, on the settling particles of detritus and in the top layer of sediments. PCB adsorption/desorption on detritus; the reversible PCB fluxes at the water–sediment boundary; destruction of detritus are taken into consideration. Formalization of PCB deposition/resuspension in the sediments is adapted from Van Rijn's model of the suspended sediment transport.

The model was spun up to reconstruct the short term scenario of the instantaneous PCB release from the St. George Arm of Danube. It has been shown that PCB transport on sinking detritus represents the natural buffer mechanism damping the spreading PCB contamination in the Black Sea shelf ecosystem. Special numerical experiments were carried out to evaluate the artificial sorbent efficiency as a possible post-accidental counter-measure.

End-user application is implemented to provide operational PCB forecast in order to support decision making and minimize ecological risks. The graphical user interface allows specifying instantaneous or continuous PCB release scenarios and quick updating the prediction of PCB release trajectory and temporal variability of the mass balance components. It provides visualization of PCB contamination at the sea surface, in the water column and in the upper layer of sediments over time, including the animations of PCB movement.

The integrated ocean-ecosystem-sediment-pollution approach developed is applicable to any coastal area and allows further implementation related to advances in the model representation of natural processes and to improvements of PCB monitoring.