



Modelling of Mercury Transport and Transformation Processes in Marine Environment

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Mercury (Hg) and its biogeochemical transformation processes are the subject of many research studies for scientists from different fields due to high toxicity of mercury compounds. Particularly in the mono-methylated form (MMHg), mercury can be bioaccumulated and biomagnified in freshwater and marine organisms and as such represents potential danger for the whole food-web and also for human health. Although the use of Hg in industrial processes has been decreasing worldwide, still a few thousand tonnes of Hg are released to the environment every year. The main natural and anthropogenic sources are active and abandoned mercury mines, artisanal gold mining and fossil fuel combustion. Due to its longevity in the elemental form (Hg^0), it can be transported through the air and water and can also be found in very remote areas, therefore it is treated as a global pollutant.

Two different case studies of coupling of hydrodynamic and mercury cycling models in marine environment are presented. Provisional mass balances for the Gulf of Trieste (Northern Adriatic, area about 650 km^2) and the Mediterranean Sea have shown that very different processes are significant in different scales. While in the coastal area the model should be able to deal with the inflow of inorganic Hg with river inflow and methylation in the bottom sediment of the Gulf, the most important process in deep-sea environment is the exchange of elemental mercury with the atmosphere. In both cases the same mathematical model was used.

An existing baroclinic 3-D hydrodynamic model PCFLOW3D has been upgraded with Hg module to simulate transport and transformations of Hg compounds in marine en-

vironment. Typical seasonal velocity fields were calculated first, and measurements of Hg concentrations and environmental parameters were performed. The transport of elemental (Hg^0), divalent (Hg^{2+}) and mono-methyl (MMHg) mercury due to advection and dispersion was calculated for each season together with some of the transformation processes. Sedimentation and resuspension of suspended sediment, exchange with atmosphere and bottom sediment as well as methylation, demethylation, reduction and oxidation were taken into account. Relatively simple transformation equations were used; in each control volume the source term in advection-dispersion equation for each of the Hg species was calculated as

$$\Delta M_i = K_r * M_r,$$

where ΔM_i represents change in mass of reaction product (Hg^0 , Hg^{2+} and MMHg, respectively), K_r are reaction coefficients and M_r is the mass of reactant.

Due to complexity of mercury transformation processes and simplicity of equations the time and space variable reaction coefficients (K_r) had to be determined from in-situ measurements. Several deep-sea castings as well as coastal sampling campaigns were performed during the last four years. Machine learning modelling tools (regression trees) and classical statistical methods have been used to connect the environmental parameters and concentrations of different Hg species.

The simulation results show correct trends in concentrations although not all the transformation processes could be modelled properly at the time. However, the combination of hydrodynamic and transport dispersion models with biogeochemical models and the use of machine learning tools can be a very useful tool in pollutant transport and transformation studies. The latest methods, especially the regression trees, are not sensitive neither to scale nor to the type of environmental compartment and can thus be successfully used to link physical, chemical and / or biological parameters to pollutant concentrations.

The PCFLOW3D model is being further upgraded by coupling with an atmospheric transport and Hg transformation model as well as with bottom sediment transformation processes.

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