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Use of Artificial Intelligence Tools in Modelling of Mercury Cycling

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During the last decades many studies were conducted in order to understand the cycling of mercury in the natural environment. Measurement campaigns and mathematical modelling were used to assess the state of mercury pollution and possible remediation measures. In the frame of EU project MERCYMS, the Mediterranean Sea was studied. The first step in such studies is usually to gather knowledge about Hg species concentration, their transport and biogeochemical transformation processes. As the problem is extremely interdisciplinary and at this stage still not properly defined, one of the possible ways of connecting geophysical and environmental parameters with concentrations of different mercury species and transformation coefficients is the use of machine learning tools. These tools build models inductively, directly from data, and do not need any prior knowledge about the task at hand. Although only results from the Mediterranean are presented, such simple method of building models directly from data is suitable for any environmental problem: all we need is enough high quality experimental data.

The data from deep-sea and coastal measurement campaigns were processed by the WEKA software. The result is a piece-wise linear regression model (regression tree) for each of the observed Hg species: THg (total mercury), RHg (reactive or divalent mercury, Hg2+), DGM (dissolved gaseous mercury), DMHg (dimethyl-mercury) and MMHg (monomethyl-mercury). Although at the first step only oceanographic parameters (temperature, salinity, and depth) were included in the models, the results of regression-tree modelling are promising; the agreement of the measurements and models was for all five species mostly within the factor of two. This is particularly important for the MMHg due to its extreme toxicity and capability of bioaccumulation and biomagnification, and undoubtedly represents a step forward in knowledge about mercury cycling in the environment.

The regression-tree models are being connected with a 3D baroclinic hydrodynamic and transport model PCFLOW3D upgraded with a mercury module (Rajar et al., 2000, 2004). By the use of oceanographic parameters from such a model it is possible to predict Hg concentrations in the Mediterranean Sea. However, the environmental parameters, which are available from measurements, are missing in the PCFLOW3D model and thus the model is being upgraded with the lowest part of the food chain (nutrients, oxygen). It is expected that the coupling of the upgraded PCFLOW3D model with regression-tree models will result in an ecological model, which will be a valuable tool for the evaluation of biogeochemical cycling of mercury in the aquatic environment.

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