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Fugacity based modeling for pollutant fate and transport during floods. Preliminary results

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Fugacity based modeling for pollutant fate and transport during floods. Preliminary results

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One of the concerns that arises during floods is whether the wide-spreading of chemical contamination is associated with the flooding. Many potential sources of toxics releases during floods exists in cities or rural area; hydrocarbons fuel storage system, distribution facilities, commercial chemical storage, sewerage system are only few examples. When inundated homes and vehicles can also be source of toxics contaminants such as gasoline/diesel, detergents and sewage.

Hazardous substances released into the environment are transported and dispersed in complex environmental systems that include air, plant, soil, water and sediment. Effective environmental models demand holistic modelling of the transport and transformation of the materials in the multimedia arena. Among these models, fugacity-based models are distribution based models incorporating all environmental compartments and are based on steady–state fluxes of pollutants across compartment interfaces (Mackay "Multimedia Environmental Models" 2001). They satisfy the primary objective of environmental chemistry which is to forecast the concentrations of pollutants in the environments with respect to space and time variables. Multimedia fugacity based-models has been used to assess contaminant distribution at very different spatial and temporal scales. The applications range from contaminant leaching to groundwater, runoff to surface water, partitioning in lakes and streams, distribution at regional and even global scale.

We developped a two-dimensional fugacity based model for fate and transport of chemicals during floods. The model has three modules: the first module estimates toxins emission rates during floods; the second modules is the hydrodynamic model that simulates the water flood and the third module simulate the dynamic distribution of chemicals in the domain during and after the flood.

The chemical emissions rate are estimated based on land use and population for three different classes of contaminants; the classes are representative of contaminants released from agricultural sources, sewage disposal and industrial/commercial emissions. The module for source estimation provides the spatial distribution of the potential emissions rates in the area. Emission rates are forcing input for the third simulation module whenever the pertinent area is inundated.

The second module simulates the flood dynamics by using a parabolic approximation of the two dimensional shallow water equation. The model is properly developed in order to utilize simplified initial and boundary conditions, such as flooding points and flooding voulmes or satellite derived DTMs and land use . Thanks to its computational efficiency it is possible to run several simulations in order to adjust initial and boundary conditions, which are partly unknown, to satellite delineation of the flooded areas which are used as constrain for the 2D dynamic simulation. In this way the result is a dynamically consistent flooded map enriched with important information about hydraulic forcing parameters (i.e. hydraulic depths, flow velocities at every temporal step).

The third module simulates the two-dimensional spatial distribution of pollutants concentration in all the environmental media. The mass balance equation for the chemicals is here derived in term of chemical fugacity instead the classical molar concentration. The advatage of the fugacity instead of concentration is that, since fugacity is continuous among phase interfaces and concentration is not, it renders the analysis of contaminat transfer between the phases easier. The two dimensional – depth averaged- mass balance equation is solved numerically by a finite volume tecnique over a rectangular regular grid.

The model has been applied to the inundation of SHKODRA region in Albania during the January- February 2010. This inundation was produced by two rivers: DRINI and BUNA. The flooded area was about 11.400 hectare including the urban and agriculture areas, almost 7.000 persons was evacuates, and 3.600 homes were under the water and the maximum depth of water was about 1 – 4 m. This flood was the largest occurred in recent centuries in Albania, and caused incalculable damage to the population and environment.

The preliminary results of the model application to the case study is presented; the model allows to estimate the extend of the contaminated areas and the location of the most probable contaminates zones after the flood; furhermore the model can simulate the time for natural restoration. All this infomartion, that are relevant for the post emergency phase, are higly affected by uncertainty; thus a sensitivity analysis of the model has been carried out. The analysys focused on the sensitivity to emission rates, contaminat source location, dynamic of the water flood and mass transport parameters.