



## **A fugacity based approach to simulate pollutant fate and transport after floods**

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Hazardous substances released into the environment during the flood are transported and dispersed in complex environmental systems that include air, plant, soil, water and sediment. Effective environmental models demand holistic modeling 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). The applications range from contaminant leaching to groundwater, runoff to surface water, partitioning in lakes and streams, distribution at regional and even global scale. 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.

We developed a two-dimensional fugacity based model for fate and transport of chemicals during floods. The model has three modules: the first module estimates toxins sources 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 sources are identified on the base of land use for contaminants that are representative of oil products. The second module simulates the flood dynamics by using a parabolic approximation of the two dimensional shallow water equation. The model uses simplified initial and boundaries conditions, such as flooding points and flooding volumes or satellite derived DTMs and land use , avoiding problems with moving drying and wetting fronts, typical of other flooding models. Thanks to its computational efficiency it is possible to run several simulations in order to adjust ICs and BCs, 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 advantage of the fugacity instead of concentration is that, since fugacity is continuous among phase interfaces and concentration is not, it renders the analysis of contaminant transfer between the phases easier.

The two dimensional – depth averaged- mass balance equation is solved numerically by a finite volume technique over a rectangular regular grid.

The model has been applied to the inundation of the SHKODRA region in Albania during January- February and November – December 2010. The maximum water depth was about 8 m and the estimated flooded area was about 14.000 hectares including both urban and agriculture areas; around half of the Shkodra city has been inundated, almost 14.000 persons has been evacuates, and 10 000 homes were under the water level. This flood was the largest occurred in recent centuries in Albania, and caused incalculable damage to the population and environment. The application of the model to the case study allowed to estimate the extend of the potentially contaminated areas for different oil products such as gasoline, diesel or lubricant.