**Global Sensitivity Analysis and Stochastic Inverse Modeling to assess behavior of emerging contaminants in soil-water systems**

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**Abstract**

Modeling approaches to assess groundwater quality can be associated with remarkable levels of complexity. This, in turn, could hamper (*a*) unambiguous understanding of relationships among model inputs and outputs of interest as well as (*b*) model calibration. Such elements are critical in a variety of scenarios, including the appraisal of groundwater contamination by Pharmaceuticals, that is documented to threaten the integrity of natural ecosystems and human health. In this broad scenario, emphasis is here devoted to model diagnosis through (moment-based) global sensitivity analyses embedding model, process, and parameter uncertainty. Performing (global) sensitivity analysis in such a context allows (*i*) investigating the sensitivity of model outputs through diverse aspects of uncertainty (i.e., focusing on various statistical moments of the probability density function of the target output) as well as (*ii*) discriminating between contributions to sensitivity due to our lack of knowledge in (*a*) model format and (*b*) parameter values. These results are then employed to guide model calibration in a stochastic context (relying, e.g., on a Bayesian modeling framework through an Acceptance-Rejection Sampling approach). We exemplify the methodology and ensuing workflow upon focusing on the Non-Steroidal Anti-Inflammatory Drug *Diclofenac*, which poses critical concerns due to its continuous release and frequent detection worldwide. Experimental evidences yield controversial results on effective biodegradability of this molecule in groundwater. We leverage on available laboratory-scale batch experiments associated with a soil-water system and embed the resulting model formulation in a stochastic context. We address the way the available information content can be effective in characterizing specific model processes upon (progressively) reducing the complexity of the proposed geochemical model. The resulting mathematical formulations are then employed in a multi-model context to interpret the considered system dynamics conditional to available data. This enables us to quantify the impact of model structure and parametric uncertainty on relevant model outputs, such as the temporal evolution of Diclofenac concentrations.

**Short CV of Alberto Guadagnini**

Vice Rector for Research and full Professor of Hydraulic and Water Engineering at Politecnico di Milano. Director of the Department of Civil and Environmental Engineering at Politecnico di Milano (2017-2022). Adjunct Professor at the Department of Hydrology and Atmospheric Sciences of the University of Arizona (USA). Main research activity is related to qualitative and quantitative aspects of flow and reactive transport in groundwater systems and underground energy resources. Key roles in EU framework projects (FP5-FP7, H2020: Coordinator, Deputy Coordinator, Project leader, Supervisory Board member, and PI of numerous research projects funded by the industrial sector). Chair of the Communication Committee of the International Society for Porous Media (Interpore). Chair of the Committee on Groundwater Hydraulics and Management of the International Association for Hydro-Environment Engineering and Research (IAHR). Chief Executive Editor of the Journal Hydrology and Earth System Sciences (EGU) and Associate Editor of the Journals Water Resources Research (AGU) and PNAS Nexus. Recipient of the Chaire Gutenberg and Prix Gutenberg 2018 (Award by Cercle Gutenberg and Région Grand-Est, France, for research on Climate change and water cycle in Upper Rhine Basin). Elected member of the European Academy of Sciences and Arts (2021).