Learning uncertain PFAS mechanisms with Finite Volume Neural Network (FINN)

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Per- and polyfluoroalkyl substances (PFAS) are a class of persistent organic substances which appear in various areas of our daily lives. Due to their unique water- and grease repellent properties [1] they find application *e.g.* on rain jackets, pans and in cosmetics [4]. However, they come with drawbacks: PFAS are suspected of having severe effects on human health [3] - aggravated by the fact that PFAS are chemically stable and hardly degrade in nature and humans [2]. Multiple experiments prove the already progressed contamination of groundwater by PFAS [12]. It is necessary to improve understanding of PFAS transport in soil and groundwater to prevent further pollution and to decontaminate polluted areas.

Experiments and modeling are the pillars of understanding environmental processes. Both fields are pushed to their limits when it comes to PFAS: Experiments indicate that only for a few substances relevant transport processes have been studied and modeled in previous research [8]. Two reasons for this issue are apparent. First, only a few of more than 4,000 different PFAS can be measured [9]. Second, it is not yet clear which chemical and biotic processes are involved in the transport and reactions of PFAS in the subsurface [6, 7]. This lack of experimental and process knowledge complicates the formulation of adequate models that represent the full range of transport and reaction processes.

In case of missing process knowledge, machine learning (ML) methods offer the potential to build predictive models based on data alone. However, general ML formulations lack the ability to integrate available fragments of prior information to constrain the model search space to a physically feasible space. A hybrid approach is needed, allowing to gain insights into internal processes while coping with scarce data by leveraging already available process knowledge.

The FINN (finite volume neural network) framework [5] addresses the aforementioned requirements. It is a hybrid neural network that follows the structure of the well-established Finite Volume Method (FVM), incorporating the capacity of a neural network to learn unknown parameters, constitutive relations and/or closures as well as fluxes between control volumes. Owing to this established structure, FINN yields highly interpretable results for learned components. FINN has already been successfully applied to advection-diffusion and diffusion-sorption problems, where *e.g.* sorption isotherms are learned [5, 10]. Extending this, we model the advection-diffusion-sorption problem of reaction and transport of PFAS in FINN.

Since there are many and large blind spots in the knowledge, it is important to stay aware of the uncertainties that persist even after the learning step. Uncertainty quantification (UQ) methods to give sensible estimates thereof are needed. However, due to its complex structure with highly parameterized neural networks molded into an FVM scheme, many out-of-the-box-methods fail in giving realistic estimates for the underlying uncertainty, evoking the need for more tailored UQ approaches. Furthermore, FINN inherits generalization abilities with regard to initial and boundary conditions, something that so-called physics-inspired ML models often struggle with [11]. Since it is common to counteract a generalization problem through inclusion of more data, this is not feasible in the data scarce groundwater applications we model, including PFAS. Thus, we improve PFAS transport and reaction process modeling by building upon the FINN framework. Specifically, process understanding of PFAS in the context of real-world data is further developed by adding uncertainty learning for the unknown components.

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