Effect of forcing uncertainty in the sensitivity and calibration of a pesticide transfer model

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The use of pesticides poses major challenges to sustainable agriculture and water quality, necessitating the development of risk assessment tools to better understand and manage these impacts. One such tool is the PESHMELBA model [1] (Pesticides and Hydrology: modeling at the catchment scale), a distributed, physically based model that integrates water and pesticide transfer processes at the catchment level. This model enables the comparison of different landscape management scenarios and their effects on water quality.

Before employing it as a decision-making tool, it is essential to properly quantify its uncertainties, coming from various sources. While parameter uncertainty has been increasingly studied, forcing uncertainties (e.g., rainfall/evapotranspiration forcings, or pesticide application dates and quantities) are often overlooked. The uncertainty in hydrological data used for forcing input directly impacts model simulations and further decision-making [2], but it also has indirect impacts when used in the process of parameter calibration [3]. Ignoring forcing uncertainty can result in biased parameter values or sensitivity indices that are only valid in one forcing condition and cannot be extrapolated to different forcing conditions [4].

We investigate how the uncertainty in forcing data propagates to the model output, particularly how it affects the sensitivity of model outputs to their parameters. Additionally, we examine how forcing uncertainty influences parameter calibration.

First, we perform a global sensitivity analysis (GSA) to identify the main parameters contributing to output uncertainty and focus on their calibration [5]. An operational approach [6] to GSA is employed. This approach considers the different nature in the variability of the forcing inputs and the parameter values, i.e. it distinguishes the stochastic (and thus uncontrollable) variability of the forcings from the variability of the model parameters' possible design values, thus demonstrating how the forcing uncertainty impacts the model's sensitivity to parameter values.

We then assess the advantages of a robust approach to parameter calibration for the PESHMELBA model. As the uncertainty of forcing inputs highly depends on the specific problem and model, we opt for a methodology that does not assume a particular structure of the forcing inputs. Rather, the methodology relies on a sufficiently large set of realizations that represent the forcing uncertainty. To manage the high computational burden of robust calibration methods and ensure the non-intrusiveness in the forcing input space, we employ a polynomial chaos-based metamodel for stochastic simulators based on [7], which approximates the response surface across parameters while emulating the uncertainty of the forcing input.

Two case studies are considered, each with varying model outputs and sources of forcing uncertainty, representing increasing complexity in model processes and scale of application:

- the first case examines the soil moisture profile of a single catchment plot. Here, forcing uncertainty arises from measurement errors and the spatial heterogeneity of a rainfall event.
- the second case focuses on the daily pesticide concentration at the river outlet. In this scenario, forcing uncertainty stems from the lack of knowledge regarding the exact dates

of pesticide treatment. This case study is more complex due to the intricacies of pesticide transfer processes and spatial interactions between catchment plots.

Our GSA results demonstrate that the sensitivity of model outputs to parameters varies across the domain of forcing uncertainty. We find that rainfall uncertainty leads to varying sensitivities of soil moisture to hydrodynamical properties at different horizon depths. Meanwhile, varying pesticide application dates by just a few days impacts the dominant processes of pesticide transfer. This results in a greater influence of parameters governing surface runoff when pesticides are applied prior to heavy rainfall events.

Comparing robust parameter calibration with classical calibration, evaluated on an unseen set of new forcing data, reveals improvements in robustness criteria for moisture profile parameter calibration. However, in complex cases, the difficulty of fitting a stochastic emulator that accurately captures the original model behavior increases rapidly with the growing interactions between forcings and model parameters. This raises questions about the scalability of the presented approach in complex studies.

References:

[1] E. Rouzies, C. Lauvernet, C. Barachet, T. Morel, F. Branger, I. Braud and N. Carluer, "From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior", *Science of The Total Environment*, **671**:1144–1160, 2019. doi: 10.1016/j.scitotenv.2019.03.060

[2] A. Devers, J.-P. Vidal, C. Lauvernet, O. Vannier, and L. Caillouet, "140-year daily ensemble streamflow reconstructions over 661 catchments in France", *Hydrology and Earth System Sciences*, **28**:3457–3474, 2024. doi: 10.5194/hess-28-3457-2024

[3] H. K. McMillans, I. K. Westerberg and T. Krueger, "Hydrological data uncertainty and its implications", *WIREs Water*, **5**:e1319, 2018. doi: 10.1002/wat2.1319

[4] V. Andréassian, N. Le Moine, C. Perrin, M.-H. Ramos, L. Oudin, T. Mathevet, J. Lerat, and L. Berthet, "All that glitters is not gold: the case of calibrating hydrological models", *Hydrological Processes*, **26**:2206–2210, 2012. doi: 10.1002/hyp.9264

[5] J. Mai, "Ten strategies towards successful calibration of environmental models", *Journal of hydrology*, **620**:129414, 2023. doi: 10.1016/j.jhydrol.2023.129414

[6] A. Dell'Oca, "Sensitivity Analysis: An Operational Picture",
Water Resources Research, **59**:e2022WR033780, 2023. doi: 10.1029/2022WR033780

[7] N. Lüthen, S. Marelli and B. Sudret, "A spectral surrogate model for stochastic simulators computed from trajectory samples", *Computer methods in applied mechanics and engineering*, **406**:115875, 2023. doi: 10.1016/j.cma.2022.115875

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