How can we quantify and reduce the uncertainty of a watershed-scale pesticide transfer model? A comparison of several approaches

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To cite this version:

Emilie Rouzies, Claire Lauvernet, Bruno Sudret, Arthur Vidard. How can we quantify and reduce the uncertainty of a watershed-scale pesticide transfer model? A comparison of several approaches. UNCECOMP 2021 - 4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering, Jun 2021, Athens, Greece. pp.1-14. hal-03462086

HAL Id: hal-03462086
https://hal.inrae.fr/hal-03462086
Submitted on 1 Dec 2021

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How can we quantify and reduce the uncertainty of a watershed-scale pesticide transfer model? A comparison of several approaches.

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Introduction

Context
Introduction

The PESHMELBA model

Development of the **PESHMELBA** model (Rouzies et al. 2019) to simulate pesticide transfers and fate on small agricultural catchments

- Simulations of heterogeneous landscapes composed of plots, vegetative filter zones, hedges, ditches and rivers
- Modular structure to explore landscape management scenarios
Introduction
The PESHMELBA model

✓ Process-oriented, fully spatialized model
✓ Water transfers on surface and subsurface + pesticide advection, adsorption and degradation
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✓ Process-oriented, fully spatialized model
✓ Water transfers on surface and subsurface + pesticide advection, adsorption and degradation
✓ One module $\equiv$ one process or ensemble of processes on a landscape element
✓ Coupling of modules within the OpenPALM coupler (Buis, Piacentini, and Déclat 2006) turning the structure flexible

⇒ Complex structure may lead to additional difficulties to diagnose model behavior!
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The PESHMELBA model

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✓ Water transfers on surface and subsurface + pesticide advection, adsorption and degradation
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✓ Coupling of modules within the OpenPALM coupler (Buis, Piacentini, and Déclat 2006) turning the structure flexible

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We have a dream that one day PESHMELBA will be used as a decision-making tool to set up management scenarios and to identify an optimal landscape configuration for pesticide transfer mitigation.
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This is our objective...but before, it is necessary to **quantify** and **reduce** the uncertainty associated to PESHMELBA output variables.
We have a dream that one day PESHMELBA will be used as a decision-making tool to set up management scenarios and to identify an optimal landscape configuration for pesticide transfer mitigation.

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PhD objectives

1. Quantify: performing an uncertainty analysis and a sensitivity analysis of the model

2. Reduce: performing data assimilation to integrate different sources of data: soil moisture images, ERT measurements and in-situ data of pesticide concentration
First GSA of PESHMELBA: let’s keep it simple…but realistic! (types of landscape elements, number of parameters, climate conditions…)

Emilie Rouzies (INRAE, France)
Case study

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3 soil types + 2 vegetation types + ... → 145 parameters !!!
First GSA of PESHMELBA: let’s keep it simple...but realistic! (types of landscape elements, number of parameters, climate conditions...)

Which method to address sensitivity of such a process-oriented, spatialized model?

3 soil types + 2 vegetation types + ... ➞ 145 parameters !!!
GSA methods

Notations $Y = f(X_1, X_2, \ldots, X_k)$

**Variance-based Sobol method** (Sobol 1993)

Decomposition of the output variance in conditional variances.

- $S_i = \frac{\nu_i}{\nu(Y)}$ main effect of $i^{th}$ parameter
- $S_{ij} = \frac{\nu_{ij}}{\nu(Y)}$ interaction effect due to the $i^{th}$ and the $j^{th}$ factors
- $S_{Ti} = S_i + \sum S_{ij} + \ldots + \sum S_{1,\ldots,k}$ overall output sensitivity

Sobol indices for Ishigami function

![Sobol indices for Ishigami function](image)
GSA methods

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Classical Sobol sampling $> 75000$ model runs, impossible!
⇒ Sobol indices obtained with Polynomial Chaos Expansion surrogate model (Wiener 1938) from 4000 simulation runs using UQLab (Marelli and Sudret 2014).
GSA methods

Alternative methods

- **HSIC dependence measure** (Da Veiga 2015)
  Main idea: describe the similarity between \( P_Y \) and \( P_{Y|X_i} \) by using a dependence measure \( d \)
  \[
  S^d_i = \mathbb{E}_{X_i}(d(P_Y, P_{Y|X_i}))
  \]
  Chosen dependence measure: Hilbert-Schmidt independence criterion (HSIC) (Gretton et al. 2005)

  \( \Rightarrow \) **Screening method** (De Lozzo and Marrel 2014)
GSA methods

Alternative methods

- **HSIC dependence measure** (Da Veiga 2015)
  Main idea: describe the similarity between $P_Y$ and $P_{Y|X_i}$ by using a dependence measure $d$

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  ⇒ **Screening method** (De Lozzo and Marrel 2014)

- **Random Forest**
✓ **Scalar variables**: informative variables: cumulated water volume and pesticide mass transferred from each HU by subsurface lateral transfers and by surface runoff.
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✓ **Temporal series**: target variables for DA: surface moisture, mean moisture in first 100 cm, water table pest. conc., water flow and pest. conc. at the outlet
Results
Scalar variables - screening

Screening: independance test based on HSIC measure (power of the test $\alpha=1\%$)

After screening:

- Water surface runoff: 43 parameters
- Pesticide surface runoff: 45 parameters

✓ High number of influential parameters remaining after screening: method not discriminant enough? Many physical processes at stake?

✓ Spatial heterogeneities consistent with heterogeneities in physical processes activation
Results
Scalar variables - ranking

Ranking for cumulated pesticide mass transferred in surface runoff
Results
Scalar variables - ranking

Ranking for cumulated pesticide mass transferred in surface runoff

✓ Discrepancies in ranking between the 3 methods
Results
Scalar variables - ranking

Ranking for cumulated pesticide mass transferred in surface runoff

✓ Discrepancies in ranking between the 3 methods
✓ Pesticide transfers at surface result from the interaction of several physical processes.
Random Forest feature importance for surface moisture on HU 4
Random Forest feature importance for surface moisture on HU 4

✓ Uncertainty on influential parameters will be reduced during the DA process
Results

Surface moisture time serie - ranking

Random Forest feature importance for surface moisture on HU 4

✓ Uncertainty on influential parameters will be reduced during the DA process
✓ Variable mainly gaussian along the simulation: valuable info to choose DA method
✓ PESHMELBA specificities turn sensitivity analysis a challenging task \( \implies \) need for adapted tools: Sobol’ indices from PCE, HSIC, Random Forest

✓ Sensitivity analysis provides valuable information about hydrological processes activation and interaction for a given scenario

✓ Uncertainty/Sensitivity analysis are a necessary preliminary task for data assimilation (which parameters could be estimated? which method can be used?)
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✓ Sensitivity analysis provides valuable information about hydrological processes activation and interaction for a given scenario

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To be further explored:
Sensitivity analysis on temporal series may be improved, especially for pesticide concentration series \(\implies\) On-going test of PCA-PCE analysis.
Thanks for your attention