Sensitivity analysis with external stochastic forcings: application to a water and pesticide transfer model

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Context: PESHMELBA

Landscape features speed up or slow down pesticide transfer from the plots to the river.

⇒ The configuration of the catchment can influence the water quality.
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Rencontres Mexico 4-5 déc. 2023, Palaiseau
PESHMELBA, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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Figure: PESHMELBA\textsuperscript{a}, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.


- Not all model parameters can be measured directly
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Figure: PESHMELBA, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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Figure: PESHMELBA\textsuperscript{a}, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

\textsuperscript{a}Emilie Rouzies et al. (June 2019). “From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior”. \textit{In: Science of The Total Environment} 671, pp. 1144–1160. \texttt{DOI: 10.1016/j.scitotenv.2019.03.060.}

- Not all model parameters can be measured directly
- → calibrate these model parameters with terrain observations
- Impact of external uncertainties on the calibration results
Context: model calibration
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\[ M(\theta_0, u_1) \]
Context: model calibration

\[ \dot{\theta} \rightarrow M(\theta_0, u_1) \rightarrow y_{obs} \]
Context: model calibration

\[ \left| \mathcal{M}(\theta_0, u_1) - y_{obs} \right|^2 = J(\theta_0, u_1) \]
Context: model calibration

\[ J(\theta_0) \]

\[ |\mathcal{M}(\theta_0, u_1) - y_{obs}|^2 = J(\theta_0, u_1) \]
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\[ J(\theta_0, u_2) = \left| \mathcal{M}(\theta_0, u_2) - y_{\text{obs}} \right|^2 \]
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\[ |M(\theta_0, u_2) - y_{obs}|^2 = J(\theta_0, u_2) \]
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\[
J(\theta_0) \quad J(\theta_0, u_1) \\
J(\theta_0, u_2)
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\[
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\[ J(\theta_0, u_1) \]

\[ J(\theta_0, u_2) \]

\[ \theta_0 \]

\[ \theta^*_1 \]

\[ \theta^*_2 \]
Context: model calibration

\[ |\mathcal{M}(\theta_0, U(\omega)) - y_{\text{obs}}|^2 = J(\theta_0, U(\omega)) \]
Before passing to calibration: a sensitivity analysis on the cost function can provide the information on the identifiability of the parameters, (Mai 2023).

Context: model calibration

$\theta_0 \xrightarrow{J(\theta_0)} M(\theta_0, U(\omega)) \xrightarrow{|M(\theta_0, U(\omega)) - y_{obs}|^2 = J(\theta_0, U(\omega))} y_{obs}$

$\omega \xrightarrow{U(\omega)} M(\theta_0, U(\omega)) \xrightarrow{|M(\theta_0, U(\omega)) - y_{obs}|^2 = J(\theta_0, U(\omega))} y_{obs}$

$J(\theta_0, u_1) \quad J(\theta_0, u_2)$
1. Introduction: Sensitivity analysis

The variability in $J$ comes from two types of inputs:

1. Parameters ($\theta$): hydrodynamic soil properties.
2. Stochastic ($U(\omega)$): external forcing (rain).

Only the parameters can be controlled by the modeler. What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs? (Dell'Oca 2023)
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**What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs?** (Dell’Oca 2023)
2. Methodology: Sobol’ indices as random variables

\[ J : \mathcal{D} \times \Omega \rightarrow \mathbb{R}, \]
\[ (\theta, \omega) \mapsto J(\theta, U(\omega)), \]
2. Methodology: Sobol’ indices as random variables

The methodology involves estimating Sobol’ indices for random variables.

\[ J : D \times \Omega \rightarrow \mathbb{R}, \]
\[ (\theta, \omega) \mapsto J(\theta, U(\omega)), \]

\[ S_i(\omega) = \frac{\text{Var}_{\theta_i} [E[Y | \theta_i, \omega]]}{\text{Var}[Y | \omega]} \]

Sobol’ indices as random variables,\(^a\).

Estimation of Sobol’ indices with polynomial chaos expansion,\(^a\):

\[ J(\theta) = \sum_{\alpha \in \mathbb{N}^K} c_\alpha \psi_\alpha(\theta) \approx \sum_{\alpha \in A} c_\alpha \psi_\alpha(\theta) \]

\[ \hat{S}_i = \sum_{\alpha \in A : \alpha_i > 0, \alpha_j \neq i = 0} c_\alpha^2 / D, \]

\[ D = \text{Var} \left[ \sum_{\alpha \in A} c_\alpha \psi_\alpha(\theta) \right] = \sum_{\alpha \in A, \alpha \neq 0} c_\alpha^2 \]


\(^a\)Sudret 2008; Marelli and Sudret 2014.
2. Methodology: metamodel validation

The $Q^2$ of the PCE metamodels are calculated on an independent test set for each rain:

We deem the metamodels a correct approximation of the original and proceed to Sobol' indices calculation.
3. Case study: moisture profiles

![Diagram showing moisture profiles over time and cumulated rain.](image-url)
3. Case study: moisture profiles

Rain

$u_A$  $u_B$  other

Different rains on soil moisture

Cumulated rain [mm]

40
30
20
10
0

Time [h]

0 2 4 6

Helios

INRAE

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### 3. Case study: Sobol’ indices under one rain realization

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Unit</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_{s,\text{surf}}$</td>
<td>water content at saturation (surface)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N}$ (0.3375, 0.0338²)</td>
</tr>
<tr>
<td>$\theta_{s,\text{inter}}$</td>
<td>water content at saturation (intermediary)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N}$ (0.3322, 0.0332²)</td>
</tr>
<tr>
<td>$\theta_{s,\text{deep}}$</td>
<td>water content at saturation (deep)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N}$ (0.316, 0.0316²)</td>
</tr>
<tr>
<td>$\theta_{r,\text{deep}}$</td>
<td>residual water content (deep)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N}$ (0.0612, 0.0153²)</td>
</tr>
<tr>
<td>$mn_{\text{deep}}$</td>
<td>Van Genuchten retention curve parameter (deep)</td>
<td>$[-]$</td>
<td>$\mathcal{N}$ (0.1791, 0.0179²)</td>
</tr>
<tr>
<td>$hg_{\text{deep}}$</td>
<td>Van Genuchten retention curve parameter (deep)</td>
<td>$[-]$</td>
<td>$\mathcal{N}$ (−9.69, 0.969²)</td>
</tr>
</tbody>
</table>
4. Results: Sobol’ indices depending on rain

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\theta_{s\text{.surf}}$</th>
<th>$\theta_{s\text{.inter}}$</th>
<th>$\theta_{s\text{.deep}}$</th>
<th>$m_{n\text{.deep}}$</th>
<th>$\theta_{r\text{.deep}}$</th>
<th>$h_{g\text{.deep}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{\mu}(S_i^T)$</td>
<td>0.11</td>
<td>0.17</td>
<td>0.58</td>
<td>0.09</td>
<td>0.10</td>
<td>&lt; 0.01</td>
</tr>
<tr>
<td>$\hat{\sigma}(S_i^T)$</td>
<td>0.04</td>
<td>0.07</td>
<td>0.19</td>
<td>0.11</td>
<td>0.11</td>
<td>&lt; 0.01</td>
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</tbody>
</table>
4. Results: Sobol’ indices depending on rain
5. Conclusion:

1. Sobol’ indices were obtained for 6 input parameters in 200 different rain realizations.
2. the sensitivity analysis disentangles the variability in the parameters $\theta$ from the one in the stochastic forcing $\omega$.
3. the parameter $hg$ was found non-identifiable in all rain realizations.
4. the ranking of the input parameters varies depending on $\omega$

What’s next? :

1. other ways of synthesizing information of $S(\omega)$ ?
2. based on the sensitivity analysis results, implement a robust calibration method
3. study different model outputs, such as transferred pesticide mass.
4. study different stochastic inputs, such as pesticide application dates.


Bibliography II


