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Authors

Brunetti, Giuseppe

Šimůnek, Jirka

Turco, Michele

et al.

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On the use of global sensitivity analysis for the numerical analysis of permeable pavements

Giuseppe Brunetti^a , Jirka Šimůnek^b, Michele Turco^c and Patrizia Piro^c

^aDepartment of Civil Engineering, Architecture, Land and Environment and Mathematic, University of Brescia, Brescia, Italy; ^bDepartment of Environmental Sciences, University of California, Riverside, CA, USA; ^cDepartment of Civil Engineering, University of Calabria, Rende, Italy

ABSTRACT

The aim of this study is to investigate the use of different global sensitivity analysis techniques in conjunction with a mechanistic model in the numerical analysis of a permeable pavement installed at the University of Calabria. The Morris method and the variance-based E-FAST procedure are applied to investigate the influence of soil hydraulic parameters on the pavement's behavior. The analysis reveals that the Morris method represents a reliable computationally cheap alternative to variance-based procedures for screening important factors and provides the first inspection of the model. The study is completed by a combined GSA-GLUE uncertainty analysis used to evaluate the model accuracy.

Abbreviations: LID: low-impact development; GSA: global sensitivity analysis; E-FAST: extended Fourier amplitude sensitivity test; GLUE: generalized likelihood uncertainty estimation; NSE: Nash-Sutcliffe efficiency; SM: screening methods; OAT: one-factor-at-a-time

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Introduction

The low-impact development (LID) approach aims to restore the natural hydrological cycle of urban catchments by increasing their evapotranspiration and infiltration capacity. Several studies have confirmed the quantitative and qualitative benefits of LIDs on the hydrological cycle (Brattebo and Booth 2003, Davis 2008, Brunetti et al. 2016b). Even though the benefits of LID are significant, widespread adoption at the catchment scale is rather limited. One of the key limiting factors is availability and knowledge of reliable modeling tools among practitioners. This issue is exacerbated by the complexity of various physical processes involved in LIDs (e.g. infiltration, evapotranspiration, root water uptake, solute transport, heat transport, etc.), which requires a combination of high expertise and modeling accuracy. In this view, mechanistic models have proven to be reliable and accurate tools for the numerical analysis of LIDs, as already demonstrated in several studies (e.g. Hilten et al. 2008, Li and Babcock 2015, Brunetti et al. 2016b).

While mechanistic models can offer both accuracy and modeling flexibility, their calibration and computational cost represent a significant limitation in their widespread adoption. In a recent study, Brunetti et al. (2017) proposed the use of a Gaussian emulator to calibrate a two-dimensional mechanistic model of a stormwater filter. This study has demonstrated how the surrogate model can drastically reduce the computational cost while maintaining relatively high accuracy. A reasonable alternative would be to reduce the dimensionality of the optimization problem by fixing unimportant factors. This is usually accomplished by

running a preliminary sensitivity analysis. Thus far, few studies have investigated the use of a statistically rigorous sensitivity analysis. Recently, Brunetti et al. (2016a) used global sensitivity analysis (GSA) to investigate the influence of soil hydraulic properties on the hydraulic behavior of a permeable pavement using the HYDRUS-1D mechanistic model (Šimůnek et al. 2016). The analysis revealed that the wear layer had the highest influence on the hydraulic response of the pavement. However, the GSA required between 90,000 and 110,000 model runs, thus leading to a significant computational cost. In another study, Turco et al. (2017) combined the two-dimensional HYDRUS-1D model with the Morris method (Morris 1991) to screen most important soil hydraulic factors. While results were promising, more research is needed in this direction to test and compare alternative sensitivity analysis techniques and to evaluate their use in combination with mechanistic modeling.

The aim of this study is to investigate the use of different sensitivity analysis techniques in conjunction with a mechanistic model in the numerical analysis of a permeable pavement installed at the University of Calabria (Italy). The problem is addressed in the following way. First, the HYDRUS-1D model is selected to describe the variably saturated hydraulic behavior of the pavement. Next, the Morris method and the extended Fourier amplitude sensitivity test (E-FAST) (Saltelli et al. 1999) are applied and compared to screen the influence of soil hydraulic properties on the likelihood function. Finally, the E-FAST is coupled with the generalized likelihood uncertainty estimation (GLUE) (Beven and Binley 1992) to carry out an uncertainty analysis of soil hydraulic parameters and to investigate the accuracy of the

model in reproducing the hydraulic behavior of the permeable pavement. It must be emphasized that the use of the GSA-GLUE approach for the mechanistic modeling of LIDs represents a novel application in this field. Furthermore, the comparison between a variance-based sensitivity analysis (i.e. E-FAST) and a screening method (SM) (i.e. the Morris method) could provide important information to urban hydrologists regarding their statistical accuracy and computational efficiency.

Methods

Case study description

The University of Calabria is located in the south of Italy, in the vicinity of Cosenza (39°18' N 16°15' E). The climate is Mediterranean with a mean annual temperature of 15.5°C and an average annual precipitation of 881.2 mm. The permeable pavement has an area of approximately 154 m², an average slope of 2% and a total depth of the profile of 0.98 m. Figure 1 shows a schematic of the permeable pavement, consisting of five layers. The surface wear layer consists of a porous concrete block characterized by high permeability. The bedding layer is composed of a mixture of sand, glass sand and zeolite to improve the pollutant removal efficiency of the pavement. Base and sub-base layers were constructed by following the stone gradations suggested by the Interlocking Concrete Pavement Institute. In particular, the ASTM N°57 stone gradation, used for the base layer, is characterized by a porosity of about 30–35%. The ASTM N°2 stone gradation is used in the sub-base layer for its stability and a high volumetric porosity of about 40%. A highly permeable geotextile separates the bedding layer from the underlining base layer. An impervious membrane is placed at the bottom of the profile to prevent water from percolating into deeper horizons. Baseflow is collected in a horizontal drain, which consists of a perforated PVC pipe, and is conducted to a manhole for quantity and quality measurements.

A weather station located directly at the site measures precipitation, wind velocity and direction, air humidity, air temperature, atmospheric pressure and global solar radiation. Rain data are measured by a tipping bucket rain gauge with a resolution of 0.254 mm and an acquisition frequency of 1 min. Climatic data are acquired with a frequency of 5 min. Data are processed and

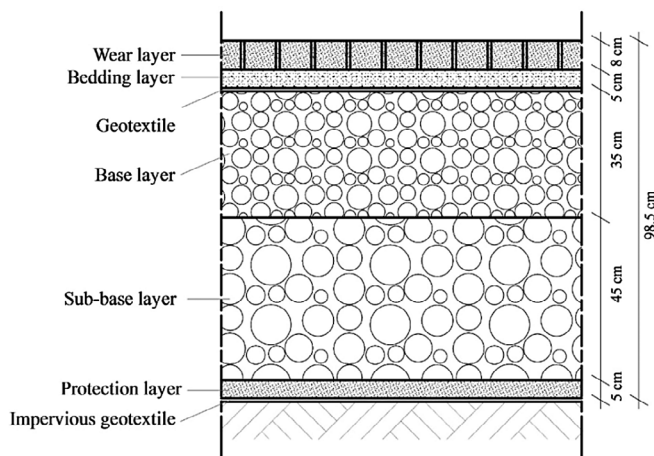


Figure 1. A schematic of the permeable pavement (Brunetti et al. 2016a).

stored in an SQL database. Baseflow is measured by a flux meter, composed of a PVC pipe with a sharp-crested weir and a pressure transducer, which was previously calibrated in the laboratory.

One month-long data-set, which starts on 15 January 2014 and ends on 15 February 2014, is selected for further analysis. The data-set is the same as that used in Brunetti et al. (2016a) and it includes precipitation, climatic data and baseflow. Climatic data are used to calculate hourly reference evapotranspiration using the well-established Penman-Monteith equation (Allen et al. 1998). An albedo of 0.25 is used (Brunetti et al. 2016a). Total precipitation and total reference evapotranspiration for the selected period are 274 mm and 43 mm, respectively. The precipitation and subsurface outflow time series are downsampled to a temporal resolution of 15 min, which is considered a balanced resolution for a monthly numerical simulation. The measured subsurface outflow from the pavement is used to calculate the likelihood values and thus to carry out both the sensitivity and uncertainty analyses. It is worth noting that no surface runoff was observed during the selected period.

Modeling theory

Water flow

The variably-saturated water flow in the permeable pavement is simulated using the HYDRUS-1D model (Šimůnek et al. 2016). The one-dimensional Richards equation describes the unsaturated water flow:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \left(\frac{\partial h}{\partial z} + 1 \right) \right]$$

where θ is the volumetric water content [–], h is the soil water pressure head [L], $K(h)$ is the unsaturated hydraulic conductivity [LT⁻¹], t is time [T] and z is the soil depth [L]. The soil hydraulic properties are described by the van Genuchten–Mualem relations (van Genuchten 1980):

$$\theta = \begin{cases} \frac{\theta_s - \theta_r}{(1 + (\alpha|h|)^n)^m} + \theta_r & \text{if } h \leq 0 \\ \theta_s & \text{if } h > 0 \end{cases}$$

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$K = \begin{cases} K_s S_e^L \left[1 - (1 - S_e^{\frac{1}{m}}) \right]^2 & \text{if } h \leq 0 \\ K_s & \text{if } h > 0 \end{cases}$$

$$m = 1 - \frac{1}{n}$$

where θ_r [–] is the residual water content, θ_s [–] is the saturated water content, K_s [LT⁻¹] is the saturated hydraulic conductivity, n [–] and α [L⁻¹] are two shape parameters, L represents the tortuosity and pore connectivity, and is usually assumed to be 0.5 for many soils, and S_e is the effective saturation [–]. The residual water contents are assumed to be 0.045 and 0.03 for the wear and bedding layers, respectively, and set to 0.0 for both the base

and sub-base layers. The same hydraulic properties are used for the bedding and protection layers, respectively. Despite all these considerations, the model still involves 16 unknown parameters (θ_{s_i} , α_{s_i} , n_{s_i} and K_{s_i} for four soil layers).

Numerical domain and boundary conditions

The vertical domain is discretized into 197 finite elements, refined at the top to accommodate larger pressure head gradients that are likely to occur in the wear layer. An atmospheric boundary condition is applied at the pavement surface using: (a) precipitation and potential evaporation fluxes, (b) a prescribed zero pressure head (i.e. full saturation) during ponding and (c) equilibrium between the pavement surface pressure head and the atmospheric water vapor pressure when the atmospheric evaporative demand cannot be met by the wear layer. The threshold pressured head, which is set to -1000 cm, divides the evaporation process from the pavement surface into two stages: (1) a constant-rate stage when actual evaporation (equal to potential evaporation) is limited only by the supply of energy to the surface and (2) the falling-rate stage when actual evaporation (smaller than potential evaporation) is controlled by water flow towards the pavement surface. Since no vegetation was present on the surface of the pavement, the reference evapotranspiration ET_0 is fully assigned to potential evaporation.

A seepage face boundary condition is specified at the bottom of the protection layer. A seepage face boundary acts as a zero-pressure head boundary when the bottom boundary node is saturated and as a no-flux boundary when it is unsaturated. The initial conditions are specified in terms of the soil water pressure head and assumed to increase linearly with depth, from -90 cm at the top of the flow domain ($z = 0$) to -0.5 cm at the bottom ($z = -98$). The influence of the initial condition on the model's output is assumed to be limited to the first few days of the simulated period and thus does not affect the likelihood.

HYDRUS-1D uses an adaptive time stepping strategy, which automatically adjusts the time step depending on the numerical solution, thus leading to increased computational efficiency. Simulated results are printed with a time-frequency of 15 min to facilitate the comparison with previously downsampled measured data. The mass balance error is calculated for each model run, and simulations affected by mass balance errors above 2% are discarded from the following analysis.

Likelihood function

The Nash-Sutcliffe efficiency (NSE) index is used to measure the agreement between the simulated and modeled hydrographs, and as the likelihood function in the following sensitivity and uncertainty analysis:

$$NSE = 1 - \frac{\sum_{j=1}^T (Q_j^{obs} - Q_j^{mod})^2}{\sum_{j=1}^T (Q_j^{obs} - Q_{mean}^{obs})^2}$$

where Q_j^{obs} is the j th measured value, Q_j^{mod} is the j th simulated value, Q_{mean}^{obs} is the mean value of observed data and T is the number of measured values.

Sensitivity analysis

Morris method

The Morris method (Morris 1991) belongs to the class of screening methods (SM). SMs aim to provide qualitative sensitivity measures for different factors using a relatively small number of model evaluations. In general, the Morris method is a one-factor-at-a-time (OAT) local method, since it computes the elementary effect by changing only one factor at a time. However, it can be viewed as a global method, since it averages several elementary effects computed at different points in the parameter space.

In this study, the modified version of the Morris method proposed by Campolongo et al. (2007) is used to investigate the influence of soil hydraulic properties on the pavement response. Two sensitivity measures, σ and μ^* , are calculated in the Morris method. While the former summarizes the interaction effect, the latter reflects the overall importance of a particular parameter. For a detailed description of the method refer to Morris (1991) and Campolongo et al. (2007). To interpret the results by simultaneously taking into account both sensitivity measures, Morris suggested using their graphical representation in the (μ^*, σ) plane. Considering the intent of the present analysis, which was targeted to investigate the efficiency of the method, the sample size was set to 100, for a total of 1700 numerical simulations.

Extended Fourier amplitude sensitivity testing (E-FAST)

The E-FAST method (Saltelli et al. 1999) belongs to the class of global variance decomposition methods. It does not require any particular assumptions on the model structure, and it provides quantitative sensitivity measures for each factor. In particular, two sensitivity indices are calculated for each parameter, i.e. the main effect S_i and the total effect S_{T_i} . While S_i measures how the i th factor contributes to the output's variance without taking into account the interactions with other parameters, S_{T_i} quantifies the higher-order effects and thus the parameter interactions. A significant difference between S_{T_i} and S_i indicates an important role of an interaction for the parameter considered. $S_{T_i} = 0$ is a condition necessary and sufficient for a factor to be non-influential. In such a case, this parameter can be fixed at any value within its range of uncertainty without affecting the output unconditional variance. For a detailed description of the E-FAST method, please refer to Saltelli et al. (1999).

The E-FAST analysis requires $q \cdot N$ simulations, where q is the number of parameters and N is the sample size. In this study, N is set to 3000 for a total of 48,000 model executions. It is evident that the E-FAST method is more computationally demanding than the Morris method. As a result, it provides quantitative sensitivity measures.

Uncertainty analysis

GSA-GLUE approach

The methodology used to carry out uncertainty analysis consists of a combination of the GLUE method (Beven and Binley 1992) with the E-FAST variance-based sensitivity analysis. The GLUE analysis has been used extensively in the literature for the uncertainty assessment of various hydrological models (Beven and Freer 2001; Montanari 2005). For a detailed description of the

GLUE implementation, please refer to Beven and Binley (1992). The GSA-GLUE approach was first proposed by Ratto et al. (2001). This statistical approach is rather intuitive and straightforward to implement. The sample generated for the variance-based sensitivity analysis is also used in the GLUE framework. In this way, the same sets of model runs provide the statistical base for the calculation of uncertainty bounds. In this study, the sample generated for the E-FAST analysis has been used to carry out the GLUE uncertainty estimation. The confidence intervals at 5% and 95% of significance have been calculated for each soil hydraulic parameter. One of the most critical aspects of the GLUE analysis is the choice of the threshold likelihood value used to identify the so-called *behavioral* solutions. As pointed out by Freni et al. (2008), the threshold value strongly influences the calculated uncertainty bounds. Therefore, care should be taken in selecting the appropriate value. In this study, three values of the threshold likelihood values are investigated: 0.0, 0.1 and 0.2.

Results and discussion

Sensitivity analysis

Results of the sensitivity analysis carried out with the Morris method (left plot) and the E-FAST procedure (right plot) are reported in Figure 2. On first inspection, it is evident how both methods identified a modeling scenario characterized by the high parameter interaction, similar to that reported in Brunetti et al. (2016a). The results of the Morris analysis show that each factor with a high value of μ^* also has a high value of the standard deviation σ , indicating that none of the parameters has a purely linear effect. This is also evident from the scatter plot μ^* - σ , where all points are located around the diagonal. A more careful inspection reveals the presence of two groups of factors: the first one includes the shape parameters α and the second one all remaining factors. However, it must be emphasized that the group separation is rather limited. Since all soil hydraulic parameters exhibited significant values of μ^* and σ , it is not possible to fix these factors and thus reduce the dimensionality of the problem without affecting the quality of the fit.

Findings of the Morris method are, in general, confirmed by the results of the E-FAST analysis. The main effect S_i and the total effect S_{T_i} for each factor are reported in the right plot of Figure 2. In

particular, grey and black bars indicate the total and main effects, respectively. It is evident that all parameters exhibit a significant S_{T_i} and only a limited or negligible S_i . Differences in S_{T_i} - S_i indicate strong interaction effects between factors and a high nonlinearity of the model. Similarly as for the Morris method, the shape parameters α are the most influential, although their ranking is slightly different, with α_4 being slightly more sensitive than α_2 . The saturated hydraulic conductivities of the wear and base layers are the less sensitive parameters, although their total effects were still significant. Since the condition $S_{T_i} = 0$ is never encountered, the model cannot be further simplified.

It is worth noting that the two sensitivity analyses reach similar results and conclusions. Both highlight strong parameter interactions and the nonlinearity of the model, as well as identifying the shape parameters α as the most influential factors. The main difference between the two methods is the computational cost, with the Morris method being computationally cheaper than the E-FAST approach. As a result of this analysis, a number of conclusions can be drawn:

- Both the Morris method and the E-FAST analysis indicate that the model response is mainly driven by parameter interactions, underlining the high nonlinearity of the model.
- The shape parameters α have the highest influence on the model's output in both sensitivity analyses.
- All soil hydraulic parameters exhibit a substantial total effect S_{T_i} and thus it is not possible to reduce the dimensionality of the problem by fixing some parameters.
- Results of the Morris method and the E-FAST analysis are in good agreement, indicating that the former can represent a computationally cheaper alternative to global variance decomposition methods when the main goal of the analysis is to screen important factors.

Uncertainty analysis

The sample generated for the E-FAST analysis is used next to carry out the GLUE uncertainty assessment of soil hydraulic parameters. Figure 3 shows cumulative probability distributions of analyzed soil hydraulic parameters obtained for three

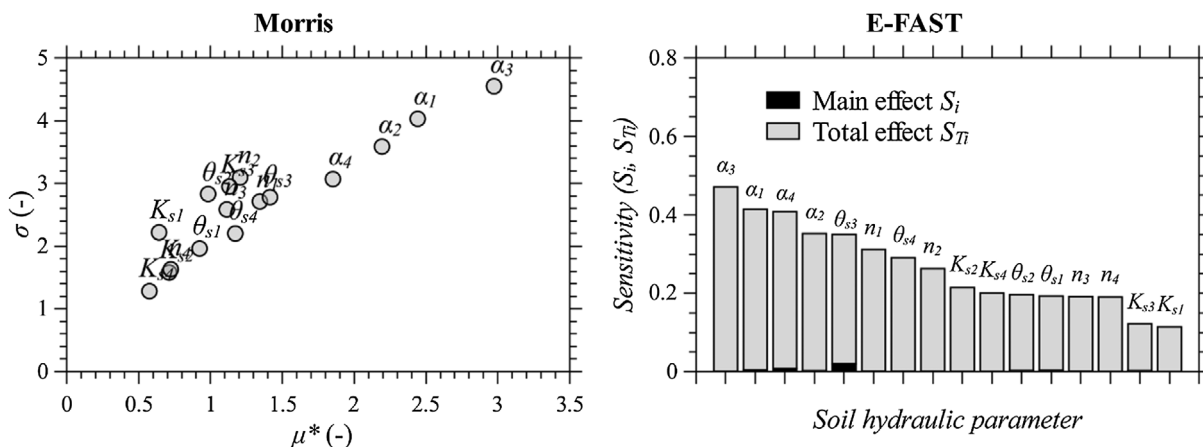


Figure 2. Scatter plots of the Morris sensitivity measures (left plot) and a bar chart of the E-FAST sensitivity indices (right plot) for various soil hydraulic parameters.

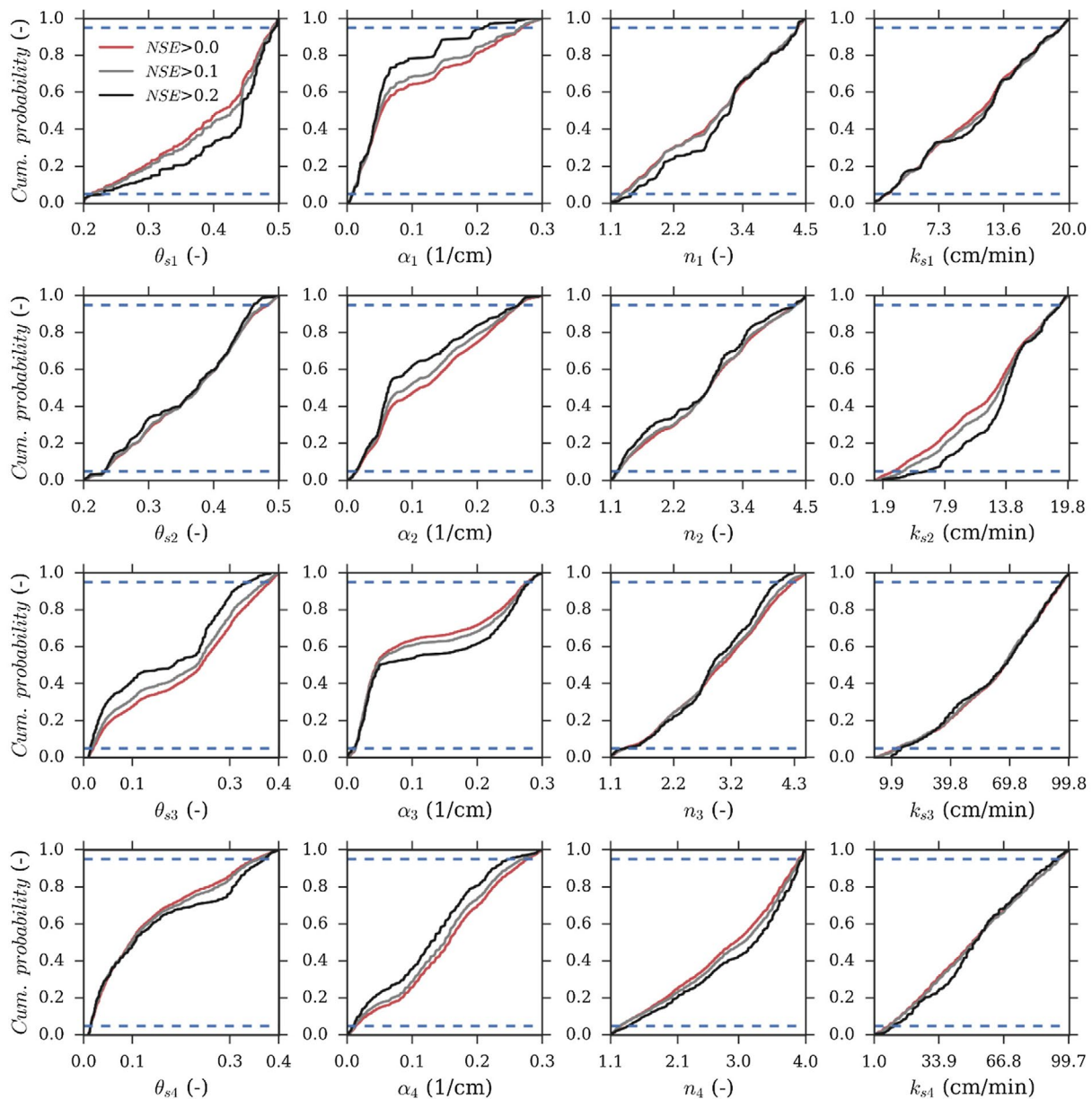


Figure 3. Cumulative likelihood distributions of soil hydraulic parameters calculated using the GSA-GLUE analysis for three different values of the GLUE threshold (i.e. $NSE > 0$, $NSE > 0.1$, $NSE > 0.2$). Dashed blue lines indicate the 5% and 95% confidence intervals.

different values of the NSE GLUE threshold. It is evident how factors exhibit significantly different behaviors. The cumulative distribution for K_{s1} is approximately linear and insensitive to the GLUE threshold, indicating a significant parameter uncertainty and a general lack of identifiability. This confirms the findings of the sensitivity analysis, which highlighted the limited influence of K_{s1} on the likelihood function. This behavior could indicate that the information content of measured variables related to subsurface outflow is not sufficient to identify K_{s1} and that other types of measurements are needed to reduce parameter uncertainty. On the other hand, the influence of the saturated hydraulic conductivity of the wear layer of a strongly unsaturated system, such as the pavement, is expected to be hydraulically limited unless surface pressure heads approach saturation (e.g. surface runoff), a situation that never occurred during the observed period. A similar behavior is encountered

for the saturated hydraulic conductivity K_{s3} , which together with K_{s1} exhibits the lowest total effect S_T in the sensitivity analysis. Conversely, K_{s2} is appreciably sensitive to the GLUE threshold, although parameter uncertainty remains high. These results are in agreement with a recent study by Turco et al. (2017), who analyzed the hydraulic behavior of a permeable pavement at the laboratory scale. Turco et al. (2017) used the Morris method to investigate the influence of four soil hydraulic parameters on subsurface outflow and water contents in the bedding layer. Their results confirmed that K_{s1} had a low impact on outflow, while K_{s2} exhibited a significant influence on it. Furthermore, similarly to our study, the shape parameter α was the most influential parameter.

Cumulative likelihood distributions of the shape parameters n_i are always almost linear and insensitive to the GLUE threshold. Only n_1 shows an appreciable influence for $n_1 < 3.4$. On the other

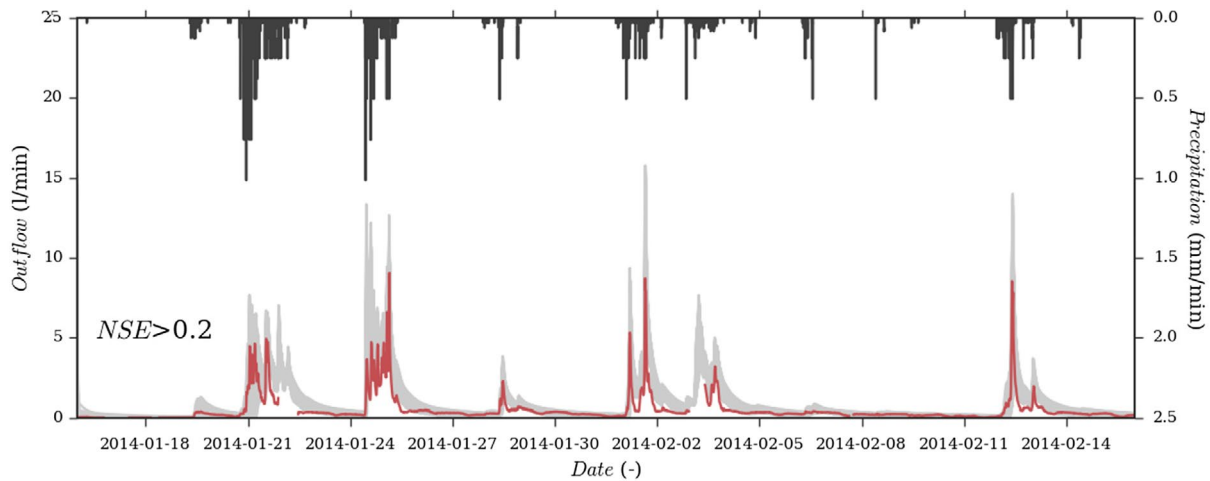


Figure 4. A comparison of measured (red line) and modeled (grey area) outflow from the pavement. The grey area represents the uncertainty band.

hand, the shape parameters α_i are highly sensitive to the GLUE threshold. The cumulative likelihood distribution for α_1 indicates a leptokurtic and positively skewed posterior parameter distribution. While the 5% percentile is insensitive to the GLUE threshold, the 95% percentile changes significantly. In particular, the 95% confidence limit changes from 0.27 to 0.2, thus reducing the parameter uncertainty. This indicates that the model tends to give a more accurate reproduction of the measured hydrograph for low values of α_1 . Again, these results agree with what was found by the earlier GSA, when α_1 was among the most sensitive parameters. In general, the analysis reveals that selected observations allow estimates of the shape parameter of the wear layer to be found with good confidence. A similar situation is observed for α_2 , while some differences are evident for α_3 and α_4 . In particular, the shape parameter of the base layer, α_3 , exhibits a multimodal behavior, with two substantial increases around 0.05 and 0.3. Interestingly, the sensitivity of the saturated water content of the base layer, θ_{s3} , is significant and well matches results of the E-FAST analysis, which ranked θ_{s3} as the fifth most influential parameter.

The cumulative probability distributions obtained using the GSA-GLUE approach are used to calculate confidence intervals and to evaluate the accuracy of the model in reproducing the hydrograph. In particular, the *behavioral* sample obtained with the threshold value $NSE > 0.2$ is used. Figure 4 compares the measured hydrograph (red line in Figure 4) with the modeled uncertainty bands (grey area in Figure 4). The uncertainty bands are obtained by sampling solutions (i.e. set of soil hydraulic parameters) with $NSE > 0.2$. More specifically, *behavioral* solutions are passed to HYDRUS, which is then executed, and for each numerical simulation, subsurface outflow is stored. Measured outflow lies only partially in the uncertainty bands, thus indicating the poor accuracy of the proposed model in reproducing the hydraulic behavior of the pavement. The results confirm the tendency of the model to overestimate the hydrograph, similarly to the report by Brunetti et al. (2016a) for the same pavement modeled using the unimodal van Genuchten function for the soil hydraulic properties. The analysis suggests a general inadequacy of this formulation in describing the water flow in the pavement. However, it must be emphasized that other possible sources of uncertainty (i.e. measurement errors, input uncertainty, etc.) were

not accounted for in the present study and thus a more comprehensive uncertainty analysis is recommended to clearly separate the effects of model input and structural errors.

Conclusions

The main aim of this study was to investigate and compare the use of global sensitivity analysis techniques for the numerical analysis of the hydraulic behavior of permeable pavements. The Morris method and the variance-based E-FAST analysis were used in conjunction with the HYDRUS-1D mechanistic model to investigate the influence of soil hydraulic parameters on the ability of the model to reproduce measured outflow from the pavement. Both methods reached similar conclusions, indicating strong parameter interactions and the nonlinearity of the model. Interestingly, the analysis revealed that the Morris method represents a reliable, computationally cheap alternative to variance-based GSAs, such as E-FAST. It can be used prior to model calibration to screen important and unimportant factors and to provide the first inspection of the model's behavior at a reasonable computational cost. On the other hand, the E-FAST approach must be chosen when the modeler's aim is to obtain quantitative sensitivity measures. Furthermore, at the same computational cost, the combined GSA-GLUE analysis allows one to estimate the parameter uncertainty and to evaluate the accuracy of the model in reproducing the hydraulic behavior of the pavement. However, since the choice of the likelihood threshold strongly influences the estimation of the model predictive uncertainty, leading to wider posterior parameter distributions, the use of the formal Bayesian analysis is suggested. An interesting future development could be to test the use of the Hamiltonian Monte Carlo algorithm combined with the no-u-turn-sampler (Hoffman and Gelman 2011), which guarantees high computational efficiency compared to the traditional Monte Carlo Markov chain algorithm.

Overall, the GLUE uncertainty analysis presented in this study targeted a modeling situation characterized by high parameter uncertainty. As previously stated, further measurements are needed to constrain the model and reduce uncertainty. The type of measurement can be chosen using a model-based

optimal Bayesian experimental design approach. Synthetic modeling scenarios can be used in conjunction with Bayesian techniques (i.e. GSA-GLUE) to quantify the model predictive uncertainty when different types of data are used. The set of data that minimizes the model uncertainty for the variable of interest (e.g. subsurface outflow) can be adopted in a following experimental test. While this and other studies report promising results, there are still other open questions that need to be addressed in the future: in particular, how to reduce parameter uncertainty, how to maximize the information content of measurements and how the uncertainty in LID modeling propagates at the catchment scale. However, by combining accurate modeling tools, reliable measurements and modern statistical techniques, it is possible to answer these questions and boost the adoption of LIDs.

Nomenclature

t	time [T]
z	pavement depth [L]
h	pressure head [L]
S_e	effective saturation [–]
m	retention curve shape parameter [–]
θ_r	residual water content [–]
θ_s	saturated water content [–]
α	retention curve shape parameter [L^{-1}]
n	retention curve shape parameter [–]
K_s	saturated hydraulic conductivity [LT^{-1}]
L	tortuosity [–]
σ	Morris sensitivity measure of the parameter's interaction [–]
μ^*	Morris sensitivity measure of the parameter's main effect [–]
S	E-FAST sensitivity measure of the parameter's main effect [–]
S_T	E-FAST sensitivity measure of the parameter's total effect [–]

Subscripts

i	layer number (1–4)
J	data ID

Disclosure statement

No potential conflict of interest was reported by the authors.

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ORCID

Giuseppe Brunetti  <http://orcid.org/0000-0001-7943-8088>

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