Accepted Manuscript

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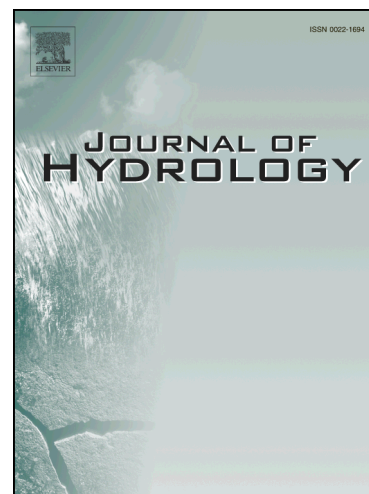Please cite this article as: Brunetti, G., Šimůnek, J., Piro, P., A comprehensive numerical analysis of the hydraulic behavior of a permeable pavement, *Journal of Hydrology* (2016), doi: http://dx.doi.org/10.1016/j.jhydrol. 2016.07.030

A comprehensive numerical analysis of the hydraulic behavior of a permeable pavement

Giuseppe Brunetti[a], Jiř Šimůnek[b], and Patrizia Piro[a]*

[a] Department of Civil Engineering, University of Calabria, Rende, CS 87036, Italy

[b] Department of Environmental Sciences, University of California, Riverside, CA 92521, USA

[*]Corresponding author: giusep.bru@gmail.com

ABSTRACT

The increasing frequency of flooding events in urban catchments related to an increase in impervious surfaces highlights the inadequacy of traditional urban drainage systems. Low Impact Development (LID) techniques have proven to be a viable and effective alternative by reducing stormwater runoff and increasing the infiltration and evapotranspiration capacity of urban areas. However, the lack of adequate modeling tools represents a barrier in designing and constructing such systems. This paper investigates the suitability of a mechanistic model, HYDRUS-1D, to correctly describe the hydraulic behavior of permeable pavement installed at the University of Calabria. Two different scenarios of describing the hydraulic behavior of the permeable pavement system were analyzed: the first one uses a single-porosity model for all layers of the permeable pavement; the second one uses a dual-porosity model for the base and sub-base layers. Measured and modeled month-long hydrographs were compared using the Nash-Sutcliffe efficiency (*NSE*) index. A Global Sensitivity Analysis (GSA) followed by a Monte Carlo filtering highlighted the influence of the wear layer on the hydraulic behavior of the pavement and identified the ranges of parameters generating *behavioral* solutions. Reduced ranges were then used in the calibration procedure conducted with the metaheuristic Particle swarm optimization (PSO) algorithm for the estimation of hydraulic parameters. The best fit value for the first scenario was *NSE* = 0.43; for the second scenario, it was *NSE* = 0.81, indicating that the dual-porosity approach is more appropriate for describing the variably-saturated flow in the base and sub-base layers. Estimated parameters were validated using an independent, month-long set of measurements, resulting in *NSE* values of

27 0.43 and 0.86 for the first and second scenarios, respectively. The improvement in correspondence

28 between measured and modeled hydrographs confirmed the reliability of the combination of GSA

29 and PSO in dealing with highly dimensional optimization problems. Obtained results have

30 demonstrated that PSO, due to its easiness of implementation and effectiveness, can represent a new

31 and viable alternative to traditional optimization algorithms for the inverse estimation of

32 unsaturated hydraulic properties. Finally, the results confirmed the suitability and the accuracy of

33 HYDRUS-1D in correctly describing the hydraulic behavior of permeable pavements.

34

35 **Keywords**: permeable pavement; urban drainage; infiltration; sensitivity analysis; global

36 optimization; particle swarm

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65

66   **INTRODUCTION**

67   Progressing urbanization, connected with the demographic growth of the last decades, has

68   led to an increase in impervious surfaces in urban catchments at the expense of natural areas. This

69   long-term process has resulted in the alteration of the natural hydrological cycle by reducing the

70   infiltration and evaporation capacity of urban catchments, increasing surface runoff, and reducing

71   groundwater recharge. While some studies highlighted a decrease of recharge as a result of an

72   increase of impervious surfaces, other studies identified an increase in recharge due to the leakage

73   of water from an urban infrastructure, such as sewer and water supply systems. The effect of

74   urbanization on groundwater recharge is discussed in detail by Price (2011).

75   Another important factor is that the frequency of extreme rainfall events, characterized by

76   high intensity and short duration, is expected to increase in the near future as a consequence of

77   climate change (Kundzewicz et al., 2006; Min et al., 2011). For example, a recent study of Wasko

78   and Sharma (2015) identified a strong correlation between intense precipitation peaks and high

79   temperatures. They concluded that the expected global warming could lead to an increase of short-

80   duration floods. The correlation between atmospheric temperature and extreme rainfall intensities

81   was also confirmed in other studies (e.g., Westra et al., 2014). This will be accompanied by a more

82   frequent occurrence of flooding events in urban areas (Carbone et al., 2015b).

83   The traditional approach to urban drainage systems focuses on collecting stormwater in

84   piped networks and transporting it off-site as quickly as possible. The increasing frequency of

85   flooding events proves that a new design paradigm for drainage systems is needed. This approach

86   must aim to restore the natural hydrological cycle of urban catchments by increasing their

87   evapotranspiration and infiltration capacity. In recent years, Low Impact Development (LID), an

88   innovative approach to land development, has gained increasing popularity. LID is a 'green'

89   approach for stormwater management that seeks to mimic the natural hydrology of a site using

90   decentralized micro-scale control measures (Coffman, 2002). LID practices consist of bioretention

91   cells, infiltration wells/trenches, stormwater wetlands, wet ponds, level spreaders, permeable

92   pavements, swales, green roofs, vegetated filter/buffer strips, sand filters, smaller culverts, and

93   water harvesting systems. Several studies have evaluated the benefits of LIDs. For example,

94   Newcomer et al. (2014) used a numerical model to demonstrate the benefits of LIDs, in particular of

95   an infiltration trench, on recharge and local groundwater resources for future climate scenarios. In

96   another paper, Berardi et al. (2014) demonstrated how green roofs may contribute to the

97   development of more sustainable buildings and cities. Environmental benefits included ecological

98   preservation, mitigation of air and water pollution, enhancement of urban hydrology, a decrease of

99   urban heat island effects, a reduction of energy consumption, etc. Furthermore, green roofs were

100 able to significantly reduce storm-water runoff and retain rainfall volume with retention efficiencies

101 ranging from 40% to 80% (Bengtsson et al., 2004); bioretention cells were shown to reduce average

102 peak flows by at least 45% during a series of rainfall events in Maryland and North Carolina (Davis,

103 2008). Even though the results of available studies are encouraging, more research is needed to

104 precisely assess the impact of LIDs on the hydrological cycle.

105   Most impervious surfaces in urban catchments consists of roofs, roads, parking lots and road

106 shoulders. The development of any large impervious surface commonly leads to multiple impacts

107 on stream systems. These impacts include higher peak stream flows, which cause channel incision,

108 bank erosion, and increased sediment transport (Trimble, 1997; Whipple et al., 1981). Another

109 consequence of these impervious surfaces is the reduction of infiltration, which lowers groundwater

110 recharge (Rose and Peters, 2001) and potentially also stream base flow (DeWalle et al., 2000;

111 Simmons and Reynolds, 1982). Permeable pavements represent one solution to the problem of

112 increased stormwater runoff and decreased stream water quality. They consist of a surface concrete

113 layer, a filter layer made of sand and other materials, a stony base, and sub-base layers. Permeable

114 pavements offer great advantages in terms of runoff reduction (Collins et al., 2008), water retention,

115 and water quality (Brattebo and Booth, 2003).

116   In spite of many well-known benefits of permeable pavements and other LID practices, the

117 transition to sustainable urban drainage systems is very slow. One of the key limiting factors in the

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118   widespread adoption of such systems is the lack of adequate analytical and modeling tools (Elliot

119   and Trowsdale, 2007). The availability of an effective LID modeling software could encourage a

120   wider adoption of LID principles. Although several stormwater models can be applied to the LID

121   analysis (Elliot and Trowsdale, 2007), most of them do not incorporate accurate descriptions of

122   hydrological processes involved, which leads to inaccurate predictions. Moreover, existing tools do

123   not incorporate automatic parameter optimization techniques and sensitivity analysis routines,

124   which have proven to be fundamental when the model includes multiple parameters. In recent years,

125   researchers have focused their attention on applying and developing physically-based models for

126   the LID analysis (Carbone et al., 2015a), however more research is still needed in this direction.

127   For example, the HYDRUS software suite (Šimůnek et al., 2008) has been widely used in

128   the literature for the description of the hydraulic behavior of green roofs (Hilten et al., 2008; Li and

129   Babcock, 2015; Newcomer et al., 2014; Palla et al., 2009), with excellent agreement between

130   numerical simulations and experimental data. Newcomer et al. (2014) investigated the effects of

131   LIDs on recharge. In their study, the HYDRUS-2D software was used to simulate flow from an

132   infiltration trench and an irrigated lawn installed at the San Francisco State University. While the

133   model was calibrated by comparing the simulated and measured recharge, only few details were

134   given about the calibration procedure. The calibrated model was then used to simulate the behavior

135   of LIDs for future precipitation scenarios. Hilten et al. (2008) used HYDRUS-1D to study the

136   effectiveness of green roofs in mitigating stormwater. Simulations were run using HYDRUS-1D for

137   a 24-h design storm to determine peak flow, retention, and detention time for runoff. Li and

138   Babcock (2015) used HYDRUS-2D to model the hydrologic response of a pilot green roof system.

139   The root-mean-square error deviation (RMSD) between the modeled water contents and field

140   measurements ranged between 0.38 and 1.74%. This suggests that the use of mechanistic models,

141   such as HYDRUS, represents one of the most valuable alternatives to empirical and conceptual

142   models for the LID analysis.

143   Among all LID practices, permeable pavements are those that lack modeling tools able to

144   describe their hydraulic behavior most. The heterogeneity of materials that compose a permeable

145   pavement, together with the high infiltration rates (Brattebo and Booth, 2003), which may lead to

146   preferential flow and especially in the base and sub-base layers, pose complex problems in the

147   numerical modeling of these systems. Very few modeling tools exist in the literature for permeable

148   pavements. One of them is included in the Storm Water Management Model (SWMM) (Gironás et

149   al., 2010). However, results obtained by SWMM have proven to be inaccurate, especially in the

150   description of the effects of base and sub-base layers on the infiltration processes (Zhang and Guo,

151   2015). HYDRUS has also been used for the description of variably-saturated flow in permeable

152   pavements. Illgen et al. (2007) used HYDRUS-2D for the numerical analysis of a permeable

153   pavement and calibrated the model against experimental data collected at a laboratory test facility.

154   The calibrated model was then used to simulate different scenarios not investigated during the

155   laboratory campaign. The Illgen et al. (2007) study provided only limited details about the

156   calibration of soil hydraulic parameters and their uncertainty and sensitivity. The occurrence of

157   preferential flow in the permeable pavement was also not investigated. Moreover, the model was

158   used to simulate a laboratory test facility, the behavior of which can differ from a field scale

159   experimental facility. On the other hand, Carbone et al. (2014) used HYDRUS-1D to model a

160   permeable pavement at the field scale. The HYDRUS-1D model was calibrated against four

161   different rainfall events with optimal results. In this study, the permeable pavement was modeled as

162   a single homogeneous layer and the differences between hydraulic properties of different layers

163   were neglected. Furthermore, the numerical simulations were event-based. In both studies,

164   calibration of soil hydraulic properties was carried out manually without taking advantage of more

165   recent global optimization algorithms. This indicates that research in this direction is limited, with

166   only inconclusive results that need to be further investigated.

167   The lack of studies that provide a comprehensive description of the hydraulic behavior of a

168   permeable pavement at the field scale and that propose a general methodology for the estimation of

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169 its hydraulic parameters suggests that research is particularly needed in the development and

170 identification of accurate modeling tools for the analysis of LID practices, especially for permeable

171 pavements. The aim of this study is to investigate the suitability of the HYDRUS mechanistic

172 model to correctly describe unsaturated flow in typical permeable pavement, installed at the

173 experimental site of the University of Calabria. Multiple uniform and nonequilibrium flow models

174 included in HYDRUS-1D, such as single- and dual-porosity models, are used to describe the

175 hydraulic behavior of the permeable pavement. The problem is addressed in the following way.

176 First, a Global Sensitivity Analysis (GSA) is carried out to prioritize hydraulic parameters and

177 identify those that are non-influential. Results of the GSA, combined with a Monte Carlo filtering

178 approach, are used to investigate the parameter space and identify *behavioral* regions. These

179 regions are then used in the calibration process conducted with the Particle Swarm Optimization

180 (PSO) algorithm. The use of PSO for the determination of unsaturated hydraulic properties

181 represents a new important application of this method. Finally, the calibrated model is validated on

182 an independent set of measurements.

183

184 **MATERIALS AND METHODS**

185 *Site Description*

186 The University of Calabria is located in the south of Italy, in the vicinity of Cosenza (39°18′

187 N 16°15′ E). The climate is Mediterranean with a mean annual temperature of 15.5 °C and an

188 average annual precipitation of 881.2 mm. The permeable pavement is part of the "Urban Hydraulic

189 Park," which also includes an extensive green roof, a bioretention system, and a sedimentation tank

190 connected with a treatment unit. The permeable pavement has an area of 154 m^2, an average slope

191 of 2%, and a total depth of the profile of 0.98 m. Figure 1 shows a schematic of the permeable

192 pavement, consisting of 5 layers.

193   The surface wear layer consists of porous concrete blocks characterized by high

194   permeability. Base, sub-base and bedding layers were constructed by following the suggestions of

195   the Interlocking Concrete Pavement Institute (ICPI), which recommends certain ASTM stone

196   gradations. The ASTM numbers and corresponding gradations can be found in ASTM D 448,

197   *Standard Classification for Sizes of Aggregate for Road and Bridge Construction*. The ASTM

198   N^o57, used for the base layer, is characterized by a porosity of about 30-35%. The ASTM N^o2 is

199   used in the sub-base layer for its stability and a high volumetric porosity of about 40%. The ASTM

200   N^o8 is used for the bedding layer and the protection layer and has a porosity of about 20% of

201   volume. The bedding layer is composed of a mixture of sand, glass sand, and zeolite to improve the

202   pollutant removal efficiency of the permeable pavement for typical contaminants of stormwater

203   runoff. A high permeability geotextile with a fiber area weight of 60 g/m^2 is placed at the interface

204   between the bedding layer and the base layer to prevent sand from migrating into the bottom layers.

205   An impervious membrane is placed at the bottom of the profile to prevent water from percolating

206   into deeper horizons. The protection layer which is composed of coarse sand is placed between the

207   sub-base layer and the impervious membrane. The baseflow is collected in a horizontal drain, which

208   consists of a perforated PVC pipe, and is conducted to a manhole for quantity and quality

209   measurements.

210   A weather station located directly at the site measures precipitation, wind velocity and

211   direction, air humidity, air temperature, atmospheric pressure, and global solar radiation. Rain data

212   are measured by a tipping bucket rain gauge with a resolution of 0.254 mm and an acquisition

213   frequency of one minute. Climatic data are acquired with a frequency of five minutes. Data are

214   processed and stored in the SQL database.

215   Two flux meters, composed of a PVC pipe with a sharp-crested weir and a pressure

216   transducer, measure baseflow and runoff from the permeable pavement. The pressure transducer

217   (Ge Druck PTX1830) measures the water level inside the PVC pipe and has a range of

218   measurement of 75 cm with an accuracy of 0.1 % of the full scale. The pressure transducers were

219 calibrated in the laboratory by using a hydrostatic water column, linking the electric current

220 intensity with the water level inside the column. The exponential head-discharge equations for the

221 two PVC flux meters were obtained by fitting the experimental data with a coefficient of

222 determination R^2=0.999 for both devices. Runoff and baseflow data were acquired with a time

223 resolution of 1 minute and stored in the SQL database. No measurements of pressure heads or

224 volumetric water contents inside the pavement were taken.

225   Two month-long data sets were selected for further analysis (Fig. 2). The first data set,

226 which started on 2014-01-15 and ended on 2014-02-15, was used for parameter optimization and

227 sensitivity analysis. Total precipitation and total potential evapotranspiration for the first data set

228 were 274 mm and 43 mm, respectively. The second data set, which started on 2014-03-01 and

229 ended on 2014-03-31, was used for model validation. Total precipitation and total potential

230 evapotranspiration for the second data set were 175 mm and 81 mm, respectively. The second data

231 set was selected so that it had significantly different meteorological data than during the first period.

232 The optimization set is characterized by multiple rain events with few dry periods. The validation

233 set has fewer rain events, which are concentrated at the beginning and end of the time period and

234 separated by a relatively long dry period between. Surface runoff was not observed during these

235 time periods.

236   Potential evaporation was calculated using the Penman-Monteith equation (Allen et al.,

237 1998). The permeable pavement was installed in 2013 and has been constantly exposed to

238 atmospheric conditions and traffic since then that has altered the surface roughness and color. For

239 these reasons, an albedo of 0.25 was used as suggested by Levinson and Akbari (2002) for

240 weathered gray cement.

241

242 ***Theory***

243   Water flow simulations were conducted using the HYDRUS-1D software (Šimůnek et al.,

244 2008). HYDRUS-1D is a one-dimensional finite element model for simulating the movement of

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245 water, heat, and multiple solutes in variably-saturated porous media. HYDRUS-1D implements

246 multiple uniform (single-porosity) and nonequilibrium (dual-porosity and dual-permeability) water

247 flow models (Šimůnek and van Genuchten, 2008). In this study, two different conceptual models

248 were used to represent flow in the permeable pavement (Table 1).

249 Scenario I assumed that water flow in all five soil layers of the permeable pavement can be

250 described using the classical single-porosity approach (SPM). Unsaturated water flow is then

251 described using the one-dimensional Richards equation:

252
$$\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] \tag{1}$$

253 where θ is the volumetric water content [-], h is the soil water pressure head [L], $K(h)$ is the

254 unsaturated hydraulic conductivity [LT^{-1}], t is time [T], and z is the soil depth [L]. The soil

255 hydraulic properties are described by the van Genuchten – Mualem relation (van Genuchten, 1980):

256
$$\theta = \begin{cases} \dfrac{\theta_s - \theta_r}{(1+(\alpha|h|)^n)^m} + \theta_r & \text{if } h \le 0 \\ \theta_s & \text{if } h > 0 \end{cases} \tag{2}$$

257
$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

258
$$K = \begin{cases} K_s S_e^L\left[(1-(1-S_e^{\frac{1}{m}})^m\right]^2 & \text{if } h \le 0 \\ K_s & \text{if } h > 0 \end{cases} \tag{3}$$

259
$$m = 1 - \frac{1}{n}$$

260 where θ_r [-] is the residual water content, θ_s [-] is the saturated water content, K_s [LT^{-1}] is the

261 saturated hydraulic conductivity, n is a pore-size distribution index [-], α is a parameter related to

262 the inverse of the air-entry pressure [L^{-1}], L indicates the tortuosity and is usually assumed to be 0.5

263 for many soils, and S_e is the effective saturation [-]. In order to simplify the model (to lower the

264 number of unknown parameters), the residual water content of all layers was fixed. In particular, the

265 residual water content for the wear and bedding layers was assumed to be 0.045 and 0.03,

266 respectively, while the residual water content for both the base and sub-base layers was assumed to

267 be 0.0, considering that they were composed of crushed stones. Furthermore, considering that the

268 bedding layer and the protection layer had the same stone gradation, ASTM $N^o 8$, the same set of

269 parameters was used for both. Despite of all these considerations, this scenario still involves 16

270 parameters (θ_s, α, n, and K_s for 4 soil layers).

271   Scenario II assumes a single-porosity model for the wear layer, the bedding layer, and the

272 protection layer, and a dual-porosity model for the base and sub-base layers. This configuration was

273 selected in order to consider the occurrence of preferential flow in the coarse layers of the

274 pavement.

275   The base and sub-base layers are composed of crushed stones, with particle size diameters

276 ranging from 2.5 to 37 mm in the base layer and from 20 to 75 mm in the sub-base layer. Crushed

277 stones were washed before installation in order to remove fine particles. This narrow gradation

278 provides a high volume of voids and increases the water storage and infiltration capacities of these

279 two layers. From a physical point of view, the structure of the base and sub-base materials closely

280 resembles fractured aquifers (Barenblatt et al., 1960). Fractured aquifers are represented by a blocky

281 matrix system intercepted by fractures. Open and well-connected fractures represent high

282 permeability pathways that are many orders of magnitude more permeable than the porous rock

283 matrix. At the same time, one of the characteristics of a fractured aquifer is that the fractures occupy

284 a much smaller volume than the pores of the rock matrix. Traditionally, fractured porous media are

285 thus represented by two separate flow domains: the high permeability (mobile) domain, the network

286 of connected fractures characterized by advective flow, and the low permeability (immobile)

287 domain, dominated by diffusion. The rock matrix also provides storage capacity because of its

288 significantly larger volume than the fracture system. Typical breakthrough curves for a fractured

289 aquifer are characterized by early breakthrough and long tailing (Geiger et al., 2010). This is due to

290 the fact that the matrix has a delayed response to pressure head changes that occur in the

11

291 surrounding fractures. The resulting pressure difference induces matrix-fracture interflow. This flow

292 takes place after initial fracture flow and before the matrix and fracture pressures equilibrate (Bai et

293 al., 1994). Several studies have demonstrated the long tailing from permeable pavements in

294 discharge hydrographs (e.g., Brattebo and Booth, 2003; Fassman and Blackbourn, 2010) and

295 attributed this effect to the storage and flow through the base and sub-base layers.

296   The classical approach to model water flow in fractured porous media is the so-called "dual-

297 porosity" or "mobile-immobile water" (MIM) approach (Barenblatt et al., 1960; van Genuchten and

298 Wierenga, 1976; Warren and Root, 1963). This approach assumes that flow occurs only in the

299 mobile fracture domain, for which an effective permeability must be known, while water in the

300 matrix domain is immobile. Both domains are connected by a simple first-order transfer function,

301 which accounts for the exchange of fluid across the boundary of the two domains.

302   In the dual-porosity approach, the liquid phase is divided into two domains:

303 $$\theta = \theta_f + \theta_m \qquad (4)$$

304 where subscript f refers to the (mobile) fracture system, and subscript m refers to the immobile

305 matrix domain. The dual-porosity water flow formulation is based on a modified Richards equation

306 for flow in fractures and a mass balance equation for moisture dynamics in the matrix:

307 $$\frac{\partial \theta_f}{\partial z} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}+1\right)\right]-\Gamma_w \qquad (5)$$

308 $$\frac{\partial \theta_m}{\partial t} = \Gamma_w \qquad (6)$$

309 where Γ_w is the mass transfer between two domains, which is assumed to be proportional to the

310 difference in effective saturations of the two regions (Šimůnek and van Genuchten, 2008; Simunek

311 et al., 2003):

312 $$\Gamma_w = \omega \cdot (S_e^m - S_e^{im}) \qquad (7)$$

313 where ω is a first-order coefficient [T^{-1}]. Compared to assuming a pressure head based driving force

314 for the mass transfer, the dual-porosity model based on (7) requires significantly less parameters

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315   since one does not need to know the retention function (and corresponding parameters) for the

316   matrix region explicitly, but only its residual and saturated water contents (Simunek et al., 2003).

317   The residual water content for the mobile domain of both the base and sub-base layers is assumed to

318   be 0.0 (Simunek et al., 2003). The tortuosity factor, L, is again assumed to be 0.5 for all layers.

319   Scenario II thus includes 20 parameters (additionally also ω and θ_s of the immobile domain for the

320   base and subbase layers).

321

322   *Numerical Domain and Boundary Conditions*

323   The numerical domain representing the stratigraphy of the permeable pavement was divided

324   in 5 layers. The bedding layer and the protection layer had the same properties since they were

325   constructed using the same ASTM N°8 stone gradation. A relatively fine, finite element mesh with

326   a constant element size of 0.5 cm was used in order to minimize mass balance errors and avoid non-

327   convergent runs during sensitivity analysis and parameter optimization. An atmospheric boundary

328   condition was applied at the pavement surface using (a) precipitation and potential evaporation

329   fluxes, (b) a prescribed zero pressure head (saturation) during ponding, and (c) equilibrium between

330   the pavement surface water content and atmospheric water vapor when atmospheric evaporative

331   demand could not be met by the wear layer. A seepage face boundary condition was specified at the

332   bottom of the protection layer. A seepage face boundary acts as a zero pressure head boundary

333   when the bottom boundary node is saturated and as a no-flux boundary when it is unsaturated. The

334   initial conditions were specified in terms of the soil water pressure head and were set to linearly

335   increase with depth, from -90 cm at the top of the flow domain ($z = 0$) to -0.5 cm at the bottom ($z =$

336   -98). The surface layers are assumed to be drier than the bottom layers since they are directly

337   exposed to evaporation.

338

339   *Objective Function*

13

340   The Nash-Sutcliffe Efficiency (NSE) index (Nash and Sutcliffe, 1970) is used for evaluating

341   the agreement between hydrographs:

$$NSE = 1 - \left[\frac{\sum_{i=1}^{T} (Q_i^{obs} - Q_i^{mod})^2}{\sum_{i=1}^{T} (Q_i^{obs} - Q_{mean}^{obs})^2} \right]$$

342   (8)

343   where Q_i^{obs} is the ith measured value, Q_i^{mod} is the ith simulated value, and Q_{mean}^{obs} is the mean value

344   of observed data. The NSE coefficient ranges between $-\infty$ and 1.0, is equal to 1 in case of a perfect

345   agreement, and, generally, values between 0.0 and 1.0 are considered acceptable (Moriasi et al.,

346   2007). The NSE has been used because it is often reported to be the best measure for evaluating the

347   overall fit of a hydrograph (Sevat et al., 1991).

348

349   *Global Sensitivity Analysis*

350   Most existing environmental models include a high number of parameters. This aspect

351   creates a major problem in their application, as the parameter estimation becomes a high-

352   dimensional and mostly nonlinear problem. To solve this problem, several optimization algorithms

353   were developed (Beven and Binley, 1992; Duan et al., 1992; Poli et al., 2007; Vrugt et al., 2003).

354   Moreover, environmental optimization studies are often affected by the equifinality problem

355   (Beven, 2006) when multiple sets of parameters can produce similar results. This problem is

356   exacerbated when the number of parameters is significant and only limited information about their

357   interactions and their effects on the output is available. However, it is not always necessary to

358   include all model parameters in the optimization process because some of them could be measured

359   or estimated, and some may have negligible effects on the output of the model for a particular

360   application. A sensitivity analysis (SA) can identify the most influential parameters and their

361   interactions and how these parameters affect the output (Saltelli et al., 2005).

362   The principal steps of a SA are: Factors Prioritization (FP), Factors Fixing (FF), Variance

363   Cutting (VC), and Factors Mapping (FM) (Saltelli and Tarantola, 2004). The aim of FP is to

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identify factors that one should measure in order to obtain the greatest reduction in the uncertainty of the output. Conversely, FF identifies factors that are non-influential. By applying these two settings, the modeler is able to reduce the dimension of the optimization problem and have a complete appreciation of the parameters' influences and interactions.

Most SAs performed in the literature of environmental sciences are the so-called 'one-at-a-time' (OAT) sensitivity analyses, performed by changing the value of parameters one-at-a-time while keeping the others constant (Cheviron and Coquet, 2009; Houska et al., 2013; Rezaei et al., 2015). However, when the model includes interactions between parameters, results of the OAT analysis are inaccurate because parameter interactions can be identified only by changing multiple parameters simultaneously. For this reason, when the property of a model is a priori unknown, a Global Sensitivity Analysis (GSA) is always preferred (Saltelli and Annoni, 2010). Practitioners call this analysis a model-free setting.

One of the most widespread algorithms for the GSA is the variance-based Sobol' method (Sobol', 2001). Variance-based methods aim to quantify the amount of variance that each parameter contributes to the unconditional variance of the model output. For the Sobol' method, these amounts are represented by Sobol's sensitivity indices (SI's). These indices give quantitative information about the variance associated with a single parameter or related to interactions of multiple parameters. For a more complete explanation about the Sobol' method, please refer to Sobol' (2001).

Sobol's sensitivity indices are expressed as follows:

$$First\ Order \quad S_i = \frac{V_i}{V} \tag{9}$$

$$Second\ Order \quad S_{ij} = \frac{V_{ij}}{V} \tag{10}$$

$$Total \quad S_T = S_i + \sum_{j \neq i} S_{ij} + ... \tag{11}$$

15

387 where V_i is the variance associated with the ith parameter and V is the total variance. The first-order

388 index, S_i, is denoted in the literature as the "main effect". This index can be described as the fraction

389 of the model output variance that would disappear when parameter X_i is fixed. When the model is

390 additive, i.e., when it does not include interactions between input factors, then the first-order index

391 is sufficient for decomposing the model's variance. For additive models, the following relation is

392 valid:

393
$$\sum_i S_i = 1 \tag{12}$$

394   Even when the model includes interactions between parameters, the first-order index

395 remains the measure to use for FP (Saltelli and Tarantola, 2004). On the other hand, the total effect

396 index, S_T, gives information about a non-additive part of the model. A significant difference

397 between S_T and S_i indicates an important role of an interaction for the parameter considered.

398 Essentially, the total effect index, S_{Ti}, gives a fraction of the total variance that would be left when

399 all factors but X_i were fixed. $S_{Ti} = 0$ is a condition necessary and sufficient for X_i to be non-

400 influential. Therefore, X_i can be fixed at any value within its range of uncertainty without affecting

401 the output unconditional variance. The total effect is the measure to use for FF.

402   Considering that environmental models are generally highly nonlinear, it is almost

403 impossible to calculate the variances using analytical integrals. Hence, Monte Carlo integrals are

404 often applied, which are based on sampling the parameter space in q samples. Obviously, the

405 accuracy in the estimation of integrals becomes more accurate as the number of samples increases,

406 which also increases the computational cost of the SA. For an accurate description of the calculation

407 of Sobol's indices please refer to Saltelli (2010).

408   Basically, the calculation of Sobol's indices requires $q \cdot (2p+1)$ model evaluations, where p is

409 the number of input factors. However, Saltelli (2002) introduced a method that requires only

410 $q \cdot (p+2)$ model evaluations. To sample the parameters' space we used Sobol's quasi-random

411 sampling technique (Sobol', 2001).

16

412   One of the most important aspects of the GSA is the choice of the number of samples, q. An

413   increase in the number of samples will increase the accuracy of Sobol's indices. However, a high q

414   implies a higher number of model evaluations. The number of samples is case-sensitive; it depends

415   on the structure of the model and on the type of simulations performed. A convergence analysis of

416   Sobol's indices is the recommended procedure for estimating q. However, this approach is time

417   consuming because it needs to repeat the GSA several times by increasing the number of samples

418   until the variability of indices between two consecutive analyses is below a threshold value for all

419   parameters.

420   In a recent study, Nossent et al. (2011) gave a comprehensive description of the influence of

421   q on the accuracy of a GSA for an environmental model that included 26 parameters. Nossent et al.

422   (2011) reported that for most parameters, less than 5000 samples were sufficient to reach a stable

423   solution. An extensive review of the GSA in hydrological models is reported in Song et al. (2015).

424   Here, we report the number of model runs for each GSA performed, together with the type of GSA,

425   the number of parameters of the model, and the objective function used. For the GSA based on

426   Sobol's method, the number of model runs rarely exceeds 100,000. Due to considerations discussed

427   above, a value of q=5000 was chosen in our study. Table 2 summarizes the characteristics of the

428   GSA for the two scenarios considered.

429   In order to assess the accuracy of estimations of the sensitivity indices, the bootstrap

430   confidence intervals (BCIs) (Efron and Tibshirani, 1986) were estimated. The basic idea of the

431   bootstrapping is that, in absence of any other information about the distribution, the sample contains

432   all the available information about the underlying distribution. In our particular case, we were

433   interested in computing the uncertainty of estimated sensitivity indices. However, since their

434   distribution is unknown it is not possible to compute the confidence intervals analytically. The

435   rationale of the bootstrap method is to replace the unknown distribution with its empirical

436   distribution and to compute the sensitivity indices using a Monte Carlo simulation approach where

437   samples are generated by resampling the original sample used for the sensitivity analysis. In our

17

438   case, the q samples used for the model evaluation were sampled 1000 times with replacement,

439   whereby Sobol's indices were calculated for each resampling. In this way, 95% confidence intervals

440   are constructed by using the percentile method and the moment method (Archer et al., 1997).

441   The sensitivity analysis was conducted using the programming language Python and in

442   particular, the Sensitivity Analysis Library (SALib) (Usher et al., 2015). An elaborated script

443   overwrites the input file containing the parameters for different materials at each iteration. The

444   script then executes HYDRUS-1D, which usually runs less than one second. If the HYDRUS-1D

445   run is not finished after 15 seconds, it is considered non-convergent; the script then terminates the

446   process and attributes a large negative value to the objective function. The same negative value is

447   attributed when the length of the modeled hydrograph is shorter than one month, which indicates

448   that the run was unsuccessful. Values of the objective function are stored in a one-dimensional array

449   for the subsequent computation of sensitivity indices. Table 3 reports the initial range of all

450   evaluated parameters in the two scenarios. The initial conditions were not included in the GSA

451   because their effects on the hydrograph for a month-long simulation are assumed to be limited to

452   only the first few days.

453

454   *Monte Carlo Filtering*

455   In the context of an optimization framework, results of the GSA can be used to extract

456   useful information about the problem structure. The GSA preliminarily identifies the subset of input

457   factors that drive most of the variation in the model output; to establish their optimal values, these

458   sensitive parameters can be further investigated by using a Monte Carlo filtering approach. Filtering

459   techniques are used to explore the parameter space pertaining to the single or multiple optima. This

460   is particularly relevant when dealing with mechanistic models that almost always contain ill-defined

461   parameters and are thus referred to as over-parameterized models (Draper and Smith, 1981).

462   The Monte Carlo filtering is often coupled with the regionalized sensitivity analysis (RSA)

463   (Hornberger and Spear, 1981). The RSA generally requires two tasks: (a) a qualitative description

464   of the system behavior, and (b) a binary classification of the model output that divides solutions into

465   two behavioral and non-behavioral groups. However, the main drawback of the RSA is that no

466   higher-order analysis is performed and thus interactions between parameters are not investigated. In

467   the GSA, a complete description of main effects and interactions is given. The GSA has been

468   combined effectively with the GLUE analysis (Beven and Binley, 1992) in the context of the

469   parameter optimization (Ratto et al., 2001). In Ratto et al. (2001), the sample generated for the

470   GLUE analysis is also used for the computation of variance-based sensitivity indices.

471   In this study, the GSA is coupled with a basic Monte Carlo filtering. The aim of this step is

472   to identify *behavioral* regions in the parameter space and to reduce the uncertainty in the following

473   parameter estimation step by using the same sample and runs of the GSA. For each parameter set

474   used in the GSA, a value of the objective function is calculated. Potential solutions are divided into

475   two groups: *behavioral*, solutions with *NSE* >0.0, and *non-behavioral*, solutions with *NSE* ≤ 0.0.

476   Two different types of analysis were performed on the filtered sample: a) Kernel density estimation

477   and b) correlation analysis.

478

479   *Kernel Density Estimation (KDE)*

480   The KDE plots have been used to identify regions with a high density of *behavioral*

481   solutions. The KDE is a non-parametric estimator of the probability density function (PDF) of a

482   random variable (Silverman, 1981). A kernel is a special type of PDF with an added property that it

483   must be even. The KDE bi-variate plots have been used because they give a smooth qualitative

484   representation of PDFs in a bi-dimensional space. The uni-variate KDE has also been computed for

485   each parameter. The KDE plots have been calculated using a Gaussian kernel and the Scott

486   procedure for the determination of a bandwidth (Scott, 1992).

487

488   *Correlation Analysis*

489   The correlation analysis helps to identify particular interaction structures between

490   parameters. Detecting high values of correlation coefficients suggests a way to reduce the input

491   factor space. In particular, when the coefficient is positive, the couple of parameters acts in the

492   model as a quotient/difference, and when it is negative, the parameters act as a product/sum.

493

494   *Particle Swarm Optimization*

495   Inverse modeling is a procedure to estimate unknown parameters of the model from

496   experimental data. One of the major reasons to apply inverse modeling is to estimate parameters

497   that cannot be directly measured for various reasons. Numerous applications of inverse modeling

498   for the estimation of soil hydraulic properties exist in the literature (Abbaspour et al., 2004;

499   Hopmans et al., 2002; Vrugt et al., 2008, 2004). The gradient methods (Marquardt, 1963) have been

500   used most widely among hydrologists and soil scientists. However, these methods are sensitive to

501   the initial values of optimized parameters, and the algorithm often remains trapped in local minima,

502   especially when the response surface exhibits a multimodal behavior. These considerations inspired

503   researchers to develop and use global optimization techniques such as the annealing-simplex

504   method (Pan and Wu, 1998), genetic algorithms (Ines and Droogers, 2002), shuffled complex

505   methods (Vrugt et al., 2003), and ant-colony optimization (Abbaspour et al., 2001), among many

506   others.

507   In this paper, a global search method based on Particle Swarm Optimization (PSO)

508   (Kennedy and Eberhart, 1995) is used. PSO has been used in multiple studies involving inverse

509   modeling with complex environmental models (Gill et al., 2006; Jiang et al., 2010; Zambrano-

510   Bigiarini and Rojas, 2013). However, so far it has not been used for the determination of

511   unsaturated hydraulic properties. PSO is a relatively new algorithm for evolutionary computation

512   methodology, but its performance has proven to be comparable to various other, more established

513   methodologies (Kennedy and Spears, 1998; Shi and Eberhart, 1999). One of the main advantages of

514   PSO is the easiness of its implementation (Liang et al., 2006). PSO is characterized by an algorithm

20

515 based on a social-psychological metaphor involving individuals that interact with each other in a

516 social world. PSO was inspired by the behavior of schools of fish or flocks of birds as they seek

517 food or other resources. In PSO, collections of "particles" explore the search space, looking for a

518 global or near-global optimum. Particles in PSO keep track of their best positions thus far obtained

519 in the search space and the best positions obtained by their neighboring particles. The global best

520 position is what all particles tend to follow. A detailed description of the PSO algorithm is given in

521 Shi and Eberhart (1998).

522   The most important parameters in the PSO are: c_1, c_2, and w. c_1 and c_2 are constant

523 parameters known as the cognitive and social parameters, respectively, and w is the inertia-weight,

524 which plays a key role in the optimization process by providing balance between exploration and

525 exploitation. A large w facilitates a global search while a small one facilitates a local search. The w

526 parameter is very similar to the "temperature" parameter in the simulated annealing algorithm.

527 While several strategies have been used in the literature for the inertia weight, in this study, a

528 constant value of w has been used (Shi and Eberhart, 1998).

529   In PSO, each particle is influenced by its σ nearest neighbors. The arrangement of neighbors

530 that influence a particle is called the *topology* of the swarm. Different types of neighborhoods are

531 reported in the literature (Akat and Gazi, 2008). In this study, the *all* topology is used, in which the

532 neighborhood encompasses the entire swarm. The PSO parameters used in this study for both

533 scenarios are reported in Table 4 and are as suggested by Pedersen (2010).

534   A modified version of the PySwarm Python Library was used for the PSO analysis. Similar

535 to the GSA, a Python script has been written for the optimization process. The script overwrites the

536 input file of HYDRUS-1D containing the hydraulic parameters for the different layers, runs the

537 executable module, and retrieves the value of the objective function. A large negative value of *NSE*

538 is attributed to non-convergent runs, as defined above.

539

540   **RESULTS AND DISCUSSION**

541   *Sensitivity Analysis – Scenario I*

542   As discussed above, the basic outcome of Sobol's SA are the first-order (S_1) and total (S_T)

543   sensitivity indices. Table 5 presents these two indices and their relative bootstrap confidence

544   intervals (BCI). In the left part of Table 5 (S_1), it can be seen that only two parameters exhibit a

545   significant direct influence on the output's variance, the pore-size distribution index n_1 and the air-

546   entry pressure parameter a_1 . The third most influential parameter, the saturated hydraulic

547   conductivity K_{s1}, has the effect, which is only half of the second most influential parameter, a_1. Ten

548   parameters have a first-order index lower than 1%, which indicates that their main effect on the

549   output variance is negligible. Table 5 also shows that the sum of all first-order indices is less than 1,

550   which means that the model is non-additive. Only 56% of variance is attributable to the first-order

551   effects, which indicates that interactions between parameters play a fundamental role.

552   The right part of Table 5 (S_T) shows that almost 75% of variance in simulated outflow is

553   caused by n_1, either by the variation of the parameter itself (30%) or by interactions with other

554   parameters. Together with a_1 (51%) and K_{s1} (42%), it is the most influential parameter for simulated

555   flow. It can be noted that the saturated hydraulic conductivity, K_{s1}, has a relatively low main effect

556   but a relatively high total effect. That indicates that this parameter has a limited direct effect on the

557   variance of the objective function, but it has an effect in interactions with other parameters.

558   The effect of the sub-base layer on the output is less significant, while the wear layer

559   strongly conditions the output. That behavior is in agreement with results reported in the literature.

560   Illgen et al. (2007), in his laboratory campaign, confirmed that the wear layer has the major

561   influence on the infiltration capacity of the permeable pavement, while the base and sub-base layers

562   have a minor impact and act as a storage tank. The total index is always greater than zero, which

563   implies that all parameters influence the output variance either directly or by their interactions, and

564   thus no parameter can be fixed without affecting the uncertainty of the output.

565   Scatter plots for the plain Monte Carlo runs for the two most sensitive parameters, a_1 and n_1,

566   are displayed in Figure 3. The scatter plots show that there is no clear pattern of factors driving bad

567   solutions. Particular trends in the solutions were further identified by the regression lines. They

568   indicate that there is a trend for parameter a_1, with admissible solutions in the left part of the plot.

569   On the other hand, the distribution of values for parameter n_1 is flat, and thus no conclusions can be

570   made about the position of a denser region of *behavioral* solutions in the high-dimensional space.

571

572   *Monte Carlo Filtering – Scenario I*

573   A Monte Carlo Filtering procedure was applied to the runs of the GSA. The threshold value

574   of $NSE = 0.0$ produced a filtered sample composed of 1,452 *behavioral* solutions. Figure 4 shows

575   the univariate and bivariate KDE plots and the correlation plots for the wear layer.

576   The maximum Pearson correlation coefficient (in absolute values) was 0.42 between

577   parameters a_1 and n_1. It is also evident from Figure 4 that a moderate negative correlation is present

578   for parameters θ_{s1}-a_1, and a positive correlation for parameters θ_{s1}-n_1, while for the other

579   parameters, the correlation is negligible. The univariate KDEs for parameters θ_{s1}, n_1, and K_{s1}

580   indicate a platykurtic distribution of *behavioral* solutions characterized by multimodality. Parameter

581   a_1 exhibits a leptokurtic distribution, for which a denser region of good solutions is clearly

582   identifiable in the range of 0.001-0.1.

583   This behavior is more clear in the bivariate KDE plots. The bivariate KDE for a_1-n_1

584   highlights the presence of a denser region for values of n_1 in the range 2.5-4.5, a behavior that was

585   not evident from the univariate KDE. The comparison between univariate and bivariate plots

586   reveals that the latter gives a much more comprehensive description of the response surface. This

587   aspect is exacerbated when the model is governed by interactions between parameters, which is

588   clearly highlighted by Sobol's indices. In such a case, the high-dimensional inspection of the

589   parameter space provides significant information.

590   The saturated hydraulic conductivity, K_{s1}, for which the univariate KDE indicates a

591   multimodal behavior, exhibits a denser region in the range of 10.0-20.0; this region is clearly

592   identifiable in the bivariate plot of K_1-n_1.

593

594   *Sensitivity Analysis – Scenario II*

595   Results of the GSA for Scenario II are reported in Table 6. Also for Scenario II, parameters

596   a_1 and n_1 exhibit the highest main effects on the output's variance (about 35%). For Scenario II, the

597   differences are even more evident than for Scenario I. Parameters n_1 and a_1 have a first-order index

598   of 30% and 5%, respectively, while all remaining parameters remain well under 5%. Nine

599   parameters have a first-order index lower than 1%. The main effects represent 53% of the output

600   variance, which clearly indicates both that the model output is again (similarly as for Scenario I)

601   partially driven by interactions between parameters, and that the model is non-additive.

602   The right part of Table 6 (S_T) shows that the output variance is largely influenced by n_1,

603   either directly (30%) or by interactions with other parameters (64%). Similar to Scenario I,

604   parameters a_1 and n_1 are the most influential parameters, and the model's output is mainly driven by

605   the wear layer. Four of the first eight most influential parameters are related to the wear layer. The

606   main difference between Scenarios I and II is the influence of the base and sub-base layers on the

607   model's output. This is evident from Figure 5, in which the average S_T for each layer is reported for

608   both scenarios. For both scenarios, modeling results are most sensitive to the wear layer, which

609   strongly influences the output's variance. However in Scenario II, the influence of the wear layer is

610   partially reduced and redistributed to other layers. It is evident that the adoption of the dual-porosity

611   model for the unsaturated hydraulic properties significantly affects the influence of the base and

612   sub-base layers on the model's output. The dynamics of sensitivity indices between the two

613   scenarios suggest that the physical description of unsaturated flow in the sub-base layer is an

614   important element in numerical simulations.

615   Similar to scenario I, all parameters influence the model's output, either by the variation of

616   the parameters themselves or by their mutual interactions. The condition for FF is never achieved

617   for all parameters.

618 Scatter plots for the plain Monte Carlo runs for the two most sensitive parameters, a_1 and n_1,

619 are displayed in Figure 6. It can be seen that there is again no clear pattern of factors driving bad

620 solutions. The regression lines indicate that there is a slight trend, which is higher for parameter a_1,

621 to have admissible solutions in the left part of the plot. The optimum appears flat, however.

622

623 *Monte Carlo Filtering – Scenario II*

624 A Monte Carlo Filtering procedure was again applied to the runs of the GSA. The filtered

625 sample now consisted of 28,107 *behavioral* solutions. The filtered sample of *behavioral* solutions

626 for Scenario II was considerably larger than for Scenario I. This indicates that the implementation

627 of the dual-porosity model leads to higher values of the objective function.

628 Figure 7 shows the univariate and bivariate KDE plots as well as the correlation plots for

629 parameters of the wear layer. It is evident that no clear correlation exists between various

630 parameters (Fig. 7), except for a negative correlation trend between parameters a_1 and n_1, but only

631 with a small magnitude. The maximum correlation coefficient, in absolute values, was -0.531

632 between parameters a_4 and n_4.

633 The univariate KDE for parameters θ_{s1}-K_{s1} indicates a platykurtic distribution of *behavioral*

634 solutions without a clear identification of a denser region across the parameter space. On the other

635 hand, for parameters a_1 and n_1, the univariate KDEs indicate a more leptokurtic distributions,

636 especially for n_1, for which a denser region of solutions between 1.1-2.8 is identifiable.

637 The bivariate KDEs give a better description of the location of *behavioral* regions in the

638 bidimensional parameter space than the univariate KDEs. The bivariate KDE for the two most

639 sensitive parameters, a_1 and n_1, indicate the presence of a denser region in the range of n_1=(1.1,

640 2.8), and a_1=(0.01,0.15). The bivariate plots, θ_{s1}- a_1 and θ_{s1}- n_1, indicate the presence of a denser

641 region in the range of θ_{s1}=(0.25, 0.40), a region that was not clearly indicated by the univariate plot

642 for θ_{s1}. The saturated hydraulic conductivity, K_{s1}, exhibits a multimodal behavior characterized by

643   several potential regions of interest. A potential *behavioral* region may be identified in the range of

644   K_{s1}=(7.0, 15.0).

645

646   *Particle Swarm Optimization*

647   The results and conclusions from the coupled GSA-Monte Carlo filtering analysis were used

648   to reduce the ranges of parameters for the PSO. The reduction was applied only for parameters that

649   exhibited well identifiable *behavioral* regions in multivariate plots. The original ranges were kept

650   for parameters that displayed high multimodality, in order to avoid the convergence of PSO to the

651   local optimum. Table 7 reports the new ranges for all parameters.

652   Figure 8 compares measured and modeled hydrographs for the two scenarios. The PSO for

653   Scenarios I and II resulted in *NSE* values of 0.43 and 0.81, respectively. Both *NSE* values of the

654   objective function are higher than zero and thus admissible (Moriasi et al., 2007). However, the

655   implementation of the dual-porosity model for the base and sub-base layers in Scenario II provides

656   a more accurate description of the hydraulic behavior of the permeable pavement. In particular, the

657   dual-porosity model is able to accurately reproduce the fast hydraulic response of the permeable

658   pavement and the long-tailing behavior of the measured hydrograph. The modeled hydrograph for

659   Scenario I appears less accurate in reproducing the dynamics of the observed hydrograph, especially

660   the fast response of the pavements to precipitation.

661   Optimized parameters for the two scenarios are reported in Table 8. Significant differences

662   emerge between the two scenarios in terms of estimated values of the saturated water contents, θ_{s1}

663   and a_1; differences between estimated values of the saturated hydraulic conductivities, K_{s1} and n_1,

664   are less pronounced. For layer 2, while estimated values of saturated water contents are very

665   similar, huge differences arise between estimated pore-size distribution indices, n_2, which for

666   Scenario I is less than half of its value for Scenario II. Also, K_{s2} is considerably lower for Scenario

667   II than for Scenario I. Estimated vaues of dual-porosity parameters confirm the assumptions made

668   about the fractured nature of the base and subbase layers. While the saturated water content for the

26

669   mobile domain is very low, the porous matrix possesses a high storage capacity as indicated by the

670   large value of the immobile saturated water content. In particular, the overall porosity of the base

671   layer is about 40% and 30% for the subbase layer. The result for the base layer is slightly higher

672   than the prescriptions of ICPI, which recommends a porosity of 30-35%. The estimated porosity for

673   the subbase layer is 30%, which is lower than the prescribed porosity of about 40%. This difference

674   can be related to the simplifications made in the mobile-immobile dual porosity model for the

675   description of preferential flow and uncertainties related to the effective graduation of the stone

676   material used. However, the significant increase in the accuracy between the single-porosity model

677   and the dual-porosity model suggests that the hydraulic behavior of the base and subbase layers is

678   strongly affected by fast preferential flows in interconnected fractures and the accumulation of

679   water in the rock matrix. This behavior is in agreement with results reported in the literature. For

680   example, Illgen et al. (2007) reported that the water contents in the base and sub-base layers only

681   marginally increased during rainfall events, and that the lower layers act as a storage tank.

682   Both scenarios exhibit low values of porosity for the base and sub-base layers. For scenario

683   II, the total porosity is divided between the mobile and immobile domains. Flow is restricted only to

684   highly conductive and interconnected fractures, which represent a relatively small part of the

685   domain, while the immobile domain provides the storage capacity. While Scenario II assumes

686   overlapping and interacting continua, Scenario I assumes a single continuum approach for all

687   layers. When the optimized value of porosity is very low, such as for the sub-base layer, it is

688   necessary to interpret the optimized values differently than for typical Richards' type flow. In such

689   case, especially for flow in crushed stones, the model tends to approximate a combination of film

690   flow and fingering that likely occur in this layer. This hydraulic behavior is similar to the one

691   reported, for example, by Hodnet and Bell (1990) for unsaturated flow in a medium composed

692   largely of chalk cobbles. In their study, Tokunaga and Wan (1997) analyzed the influence of film

693   flow on unsaturated flow in fractures. High velocities of film flow measured in their study

694   suggested that film flow contributed significantly to preferential flow in fractured rocks. Our model,

695 based on a macroscopic description of this fast unsaturated flow, shares some similarities with the

696 active fracture model proposed by Liu et al. (1998). This approach divides the pore space into two

697 parts, active and inactive. Flow and transport occurs only within the active pore space, with the

698 inactive part simply bypassed. Liu et al. (1998) further assumed that van Genuchten (1980) relations

699 are approximately valid for the active pore space. In a separate study, Liu et al. (2003) reports

700 values of porosity between 0.01 and 0.03 for the pore space used with the active fracture model.

701

702   *Confidence Regions*

703   Since parameter estimation involves a variety of possible errors, including measurement

704 errors, model errors, and numerical errors, an uncertainty analysis of the optimized parameters

705 constitutes an important part of parameter estimation. In order to evaluate the uncertainty associated

706 with the estimated parameters, a confidence region around the best solutions optimized with PSO

707 were calculated using HYDRUS-1D. HYDRUS-1D uses the linear approximation method to

708 identify the confidence region around estimated parameters β, resulting in ellipsoid contours

709 centered at β.

710   Although restrictive and only approximately valid for nonlinear problems, an uncertainty

711 analysis provides a means to compare confidence intervals between parameters, thereby indicating

712 which parameters should be independently measured or estimated. Confidence intervals have been

713 calculated using the Student's t distribution with a confidence level of 95%. It is evident from Table

714 9 that confidence intervals are narrower for Scenario II, and that the most uncertain parameters are

715 the saturated hydraulic conductivities for different layers.

716

717   *Model Validation*

718   In order to evaluate the reliability of the estimated parameters, the model has been validated

719 on another independent set of experimental data. Figure 10**Error! Bookmark not defined.** shows a

720   comparison between measured and modeled hydrographs for the two scenarios during the validation

721   period.

722   The value of the objective functions are $NSE = 0.43$ for Scenario I and $NSE = 0.86$ for

723   Scenario II. For Scenario I, the value of the objective function remains the same, which confirms

724   the reliability of the calibrated model. Although the simulated hydrograph provides an overall

725   sufficiently accurate description of the hydraulic behavior of the pavement, it is less accurate during

726   rainfall events, which may be a time period of main interest. For Scenario II, the value of the

727   objective function actually increased and reached the value $NSE = 0.86$, which is very high and

728   reflects the accuracy of the modeled hydrograph. Also the description of the hydraulic behavior of

729   the pavement during rainfall events is optimal. This capability of the calibrated model is important

730   when dealing with the analysis of combined traditional drainage systems and LID techniques. A

731   correct description of the hydrograph during precipitation gives information about the lag time and

732   the intensity of peak flow, which are fundamental for both a comprehensive hydraulic analysis of

733   drainage systems, and for the evaluation of benefits of LIDs implementation. The initial part of the

734   hydrograph appears to be underestimated, which may be related to the influence of the unknown

735   initial conditions. The model was not able to reproduce outflow induced by the precipitation event

736   on March 15. This may be related to an overestimation of potential evaporation calculated using a

737   literature value of albedo, which could result in an overestimation of the storage capacity of the

738   pavement at the beginning of the precipitation event, which had a total volume of 6 mm. As a result,

739   the model predicted that the pavement retained all the precipitation volume. A better

740   characterization of evaporation could help in increasing the accuracy of the model, which is already

741   high.

742   Figure 10 directly compares the measured outflows with those calculated by the two

743   modeling scenarios. The red bisector line represents conditions when modeled and measured

744   outflows are perfectly matched. Linear regression lines are reported for both scenarios. Since the

745   Scenario I tends to overestimate the outflow fluxes, the difference between the bisector and the

29

746   linear regression line (gray) for scenario I is substantial. On the other hand, Scenario II tends to only

747   slightly underestimate the outflow fluxes, and thus the slopes of the bisector and the linear

748   regression line (black) for Scenario II are similar. The simulated hydrographs for both scenarios

749   tend to introduce some bias in the estimation of peak flows. This aspect is related to the choice of

750   the *NSE* as the objective function for the optimization. The *NSE* is focused on the general behavior

751   of the hydrograph rather than on particular components such as peak flows. A multi-objective

752   optimization that would include an objective function targeted to peak flow estimates could

753   represent a more appropriate approach if estimates of peak flows were the main goal of calibration.

754   However, even of great interest, the multi-objective optimization is out of the scope of this paper.

755   Overall, the validation process demonstrated the reliability of the calibrated models for both

756   scenarios.

757

758   **CONCLUSIONS**

759   In this paper, we investigated the suitability of the mechanistic model, HYDRUS-1D, to

760   correctly describe the hydraulic behavior of a permeable pavement installed at the University of

761   Calabria. We considered two different scenarios in describing the system. In Scenario I, we

762   assumed that flow on all layers can be described using a single-porosity model, while in Scenario II,

763   we assumed that a dual-porosity mobile-immobile model is needed to describe flow in the base and

764   subbase layers. The widely used Nash-Sutcliffe efficiency index was used to assess the models. A

765   Global Sensitivity Analysis, coupled with a Monte Carlo filtering procedure, was carried out before

766   the model calibration. Sensitivity analysis results suggested that the model is non-additive and

767   mainly driven by parameter interactions in both scenarios. The first-order effects only accounted for

768   56% of output variance for Scenario I and 53% for Scenario II. Sensitivity analysis also revealed

769   that the wear layer mainly influenced the hydraulic behavior of the pavement. A subsequent Monte

770   Carlo filtering procedure was applied to the runs performed during the sensitivity analysis in order

771   to identify the *behavioral* regions and to reduce parameter uncertainty. Both univariate and bivariate

30

772   Kernel Density Estimation plots were used to inspect the response surfaces and identify the

773   *behavioral* regions. This analysis revealed the high multimodality of the response surfaces, which

774   suggested the use of a global optimization algorithm for parameter estimation. Correlation

775   coefficients of the filtered sample were also computed, indicating a general low correlation between

776   parameters. Based on the results of the Monte Carlo filtering, a heuristic global optimization

777   method based on the Particle Swarm algorithm was used for parameter estimation. The calibrated

778   model for Scenario I exhibited an optimum $NSE = 0.43$, while for Scenario II, it reached $NSE=0.81$.

779   The optimized parameters were then validated against an independent set of experimental data,

780   resulting in $NSE = 0.43$ for Scenario I and $NSE = 0.86$ for Scenario II. The results of optimization

781   and validation clearly indicated that the implementation of the dual-porosity model for the base and

782   subbase layers produced more accurate results than the single-porosity model and described much

783   better the hydraulic behavior of pervious pavement. Results also confirmed the validity of the

784   assumption that the hydraulic behavior of the base and subbase layers was similar to the behavior of

785   a fractured rock, which is characterized by the highly permeable interconnected fractures and the

786   highly storative rock matrix. The main advantage in using a simple, dual-porosity, mobile-immobile

787   model with a saturation-based mass transfer is that this model requires only two additional

788   parameters compared to the single-porosity model. Further significant improvements could be

789   obtained by characterizing the hydraulic properties of the wear layer in the laboratory, as suggested

790   by the sensitivity analysis.

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1021   Figure 1. A schematic of the permeable pavement.

1022   Figure 2. Precipitation and subsurface flow during the optimization (top) and validation

1023   (bottom) time periods.

1024   Figure 3. Scatter plots for pair relations a_1-*NSE* (left) and n_1-*NSE* (right) for Scenario I. The

1025   red line is a regression line.

1026   Figure 4. Bivariate KDE plots (below diagonal), univariate KDE plots (diagonal), and

1027   correlation plots (above diagonal) for Scenario I.

1028   Figure 5. The average total index, S_T, for different layers for both scenarios.

1029   Figure 6. Scatter plots for pair relations a_1-*NSE* (left) and n_1-*NSE* (right) for Scenario II. The

1030   red line is a regression line.

1031   Figure 7. Bivariate KDE plots (below diagonal), univariate KDE plots (diagonal), and

1032   correlation plots (above diagonal) for Scenario II.

1033   Figure 8. Comparison between the modeled and measured hydrographs for Scenarios I (top)

1034   and II (bottom) for the optimization process.

1035   Figure 9. Comparison between the modeled and measured hydrograph for the two scenarios

1036   for the validation period.

1037   Figure 10. Comparison between the modeled and measured outflows for the two scenarios

1038   for the validation period.

1039

Soil Layer	Scenario I	Scenario II
Wear	Single Porosity	Single Porosity
Bedding	Single Porosity	Single Porosity
Base	Single Porosity	Dual Porosity – MIM
Sub-base	Single Porosity	Dual Porosity – MIM
Protection	Single Porosity	Single Porosity

1040   Table 1. Conceptual models representing water flow in the permeable pavement.

1041

Scenario	Number of parameters	Model runs
I	16	90000
II	20	110000

1042   Table 2. Number of parameters and HYDRUS-1D runs for both scenarios.

1043

	Scenario I	Scenario II
Parameter	Initial range	
θ_{s1} [-]	0.2-0.5	0.2-0.5
a_1 [1/cm]	0.001-0.3	0.001-0.3
n_1 [-]	1.1-4.5	1.1-4.5
K_{s1} [cm/min]	1.0-20.0	1.0-20.0
θ_{s2} [-]	0.2-0.5	0.2-0.5
a_2 [1/cm]	0.001-0.3	0.001-0.3
n_2 [-]	1.1-4.5	1.1-4.5
K_{s2} [cm/min]	1.0-20.0	1.0-20.0
θ_{s3} [-]	0.01-0.40	0.001-0.1
a_3 [1/cm]	0.001-0.3	0.001-0.3
n_3 [-]	1.1-4.5	1.1-4.5
K_{s3} [cm/min]	1.0-100.0	1.0-100.0
$\theta_{s,im3}$ [-]	-	0.15-0.4
ω_3 [1/min]	-	0.00001-0.009
θ_{s4} [-]	0.01-0.4	0.001-0.1
a_4 [1/cm]	0.001-0.3	0.001-0.3
n_4 [-]	1.1-4.5	1.1-4.5
K_{s4} [cm/min]	1.0-100.0	1.0-100.0
$\theta_{s,im4}$ [-]	-	0.15-0.4
ω_4 [1/min]	-	0.00001-0.009

1044   Table 3. Ranges of parameters used in the GSA for both scenarios.

1045

N	c_1	c_2	w
69	-0.267	3.395	-0.444

1046   Table 4. Parameters used in the PSO optimization.

1047

Parameter	S_1	S_1 (BCI)	Parameter	S_T	S_T (BCI)

38

Parameter			Parameter		
n_1 [-]	0.298	0.054	n_1 [-]	0.745	0.042
a_1 [1/cm]	0.102	0.040	a_1 [1/cm]	0.508	0.032
K_{s1} [cm/min]	0.051	0.040	K_{s1} [cm/min]	0.421	0.032
θ_{s3} [-]	0.023	0.024	θ_{s1} [-]	0.247	0.025
a_4 [1/cm]	0.020	0.023	n_4 [-]	0.224	0.146
a_2 [1/cm]	0.017	0.022	K_{s3} [cm/min]	0.210	0.127
n_3 [-]	0.014	0.029	n_3 [-]	0.194	0.035
K_{s4} [cm/min]	0.009	0.025	a_3 [1/cm]	0.181	0.024
n_4 [-]	0.009	0.035	a_2 [1/cm]	0.176	0.024
θ_{s1} [-]	0.009	0.028	n_2 [-]	0.176	0.028
n_2 [-]	0.007	0.023	a_4 [1/cm]	0.170	0.033
K_{s3} [cm/min]	0.004	0.022	θ_{s3} [-]	0.167	0.031
θ_{s4} [-]	0.001	0.022	θ_{s2} [-]	0.151	0.030
a_3 [1/cm]	-0.001	0.024	K_{s2} [cm/min]	0.138	0.023
θ_{s2} [-]	-0.004	0.019	K_{s4} [cm/min]	0.138	0.038
K_{s2} [cm/min]	-0.005	0.016	θ_{s4} [-]	0.136	0.022
Sum	0.563			> 1.0	

1048

1049 Table 5. First-order (S_1) and total (S_T) effect indices (in decreasing order) with their bootstrap
1050 confidence intervals (BCI) for parameters of Scenario I.

1051

Parameter	S_1	S_1 (BCI)	Parameter	S_T	S_T (BCI)
n_1 [-]	0.302	0.026	n_1 [-]	0.640	0.023
a_1 [1/cm]	0.054	0.029	a_1 [1/cm]	0.387	0.027
θ_{s3} [-]	0.030	0.045	n_3 [-]	0.383	0.020
n_3 [-]	0.026	0.024	θ_{s3} [-]	0.294	0.027
K_{s3} [cm/min]	0.018	0.022	a_3 [1/cm]	0.291	0.022
a_4 [1/cm]	0.018	0.020	θ_{s1} [-]	0.271	0.019
θ_{s2} [-]	0.017	0.018	a_4 [1/cm]	0.269	0.019
θ_{s4} [-]	0.014	0.022	K_{s1} [cm/min]	0.259	0.018
a_3 [1/cm]	0.013	0.025	n_4 [-]	0.256	0.013
K_{s2} [cm/min]	0.012	0.026	a_2 [1/cm]	0.229	0.017
K_{s4} [cm/min]	0.011	0.031	K_{s3} [cm/min]	0.222	0.017
θ_{s1} [-]	0.007	0.023	n_2 [-]	0.217	0.022
$\theta_{s,im3}$ [-]	0.006	0.017	θ_{s4} [-]	0.201	0.017
a_2 [1/cm]	0.005	0.016	K_{s2} [cm/min]	0.195	0.023
K_{s1} [cm/min]	0.001	0.022	K_{s4} [cm/min]	0.186	0.021
ω_4 [1/min]	-0.001	0.027	θ_{s2} [-]	0.185	0.018
n_2 [-]	-0.001	0.026	$\theta_{s,im3}$ [-]	0.149	0.016
ω_3 [1/min]	-0.003	0.021	ω_3 [1/min]	0.143	0.016
$\theta_{s,im4}$ [-]	-0.004	0.020	$\theta_{s,im4}$ [-]	0.138	0.013
n_4 [-]	-0.006	0.017	ω_4 [1/min]	0.125	0.020
Sum	0.534			> 1.0	

1052 Table 6. First-order (S_1) and total (S_T) effect indices (in decreasing order) with their
1053 bootstrap confidence intervals (BCI) for parameter of Scenario II.

1054

39

	Scenario I	Scenario II
Parameter	Reduced range	
θ_{s1} [-]	0.2-0.5	0.2-0.4
a_1 [1/cm]	0.001-0.1	0.001-0.15
n_1 [-]	3.0-4.5	1.1-2.8
K_{s1} [cm/min]	10.0-20.0	1.5-20.0
θ_{s2} [-]	0.25-0.5	0.2-0.4
a_2 [1/cm]	0.2-0.3	0.1-0.2
n_2 [-]	1.1-4.5	1.1-4.5
K_{s2} [cm/min]	1.0-20.0	3.0-20.0
θ_{s3} [-]	0.20-0.40	0.001-0.05
a_3 [1/cm]	0.001-0.05	0.001-0.05
n_3 [-]	1.1-4.5	1.5-4.5
K_{s3} [cm/min]	1.0-100.0	20.-100.0
$\theta_{s,im3}$ [-]	-	0.2-0.4
ω_3 [1/min]	-	0.00001-0.009
θ_{s4} [-]	0.01-0.2	0.001-0.05
a_4 [1/cm]	0.15-0.3	0.15-0.3
n_4 [-]	2.0-4.0	1.5-3.5
K_{s4} [cm/min]	1.0-100.0	1.0-100.0
$\theta_{s,im4}$ [-]	-	0.15-0.3
ω_4 [1/min]	-	0.00001-0.009

1055   Table 7. Reduced ranges of optimized parameters for the optimization process.

1056

				Scenario I					
Layer	θ_r	θ_s	a	N	K_s	L	$\theta_{r,im}$	$\theta_{s,im}$	ω
Wear	0.045	0.2	0.002	3.0	10	0.5	-	-	-
Bedding	0.03	0.3	0.3	4.47	20	0.5	-	-	-
Base	0	0.2	0.023	2.85	68.7	0.5	-	-	-
Sub-base	0	0.01	0.27	2.41	96.7	0.5	-	-	-
Protection	0.03	0.3	0.3	4.47	20	0.5	-	-	-
				Scenario II					
Wear	0.045	0.287	0.03	2.67	7.33	0.5	-	-	-
Bedding	0.03	0.298	0.113	3.04	3.87	0.5	-	-	-
Base	0	0.044	0.021	4.33	93.2	0.5	0	0.35	0.00017
Sub-base	0	0.001	0.247	2.17	56.3	0.5	0	0.29	0.0013
Protection	0.03	0.298	0.113	3.04	3.87	0.5	-	-	-

1057   Table 8. Optimized soil hydraulic parameters for both scenarios.

1058

	Scenario I		Scenario II	
Parameter	**Value**	**CI**	**Value**	**CI**
θ_{s1} [-]	0.2	0.057	0.287	0.007
a_1 [1/cm]	0.002	0.0006	0.029	0.0008
n_1 [-]	3	0.783	2.67	0.058
K_{s1} [cm/min]	10	4.4	7.33	0.272
θ_{s2} [-]	0.3	0.072	0.29	0.009

40

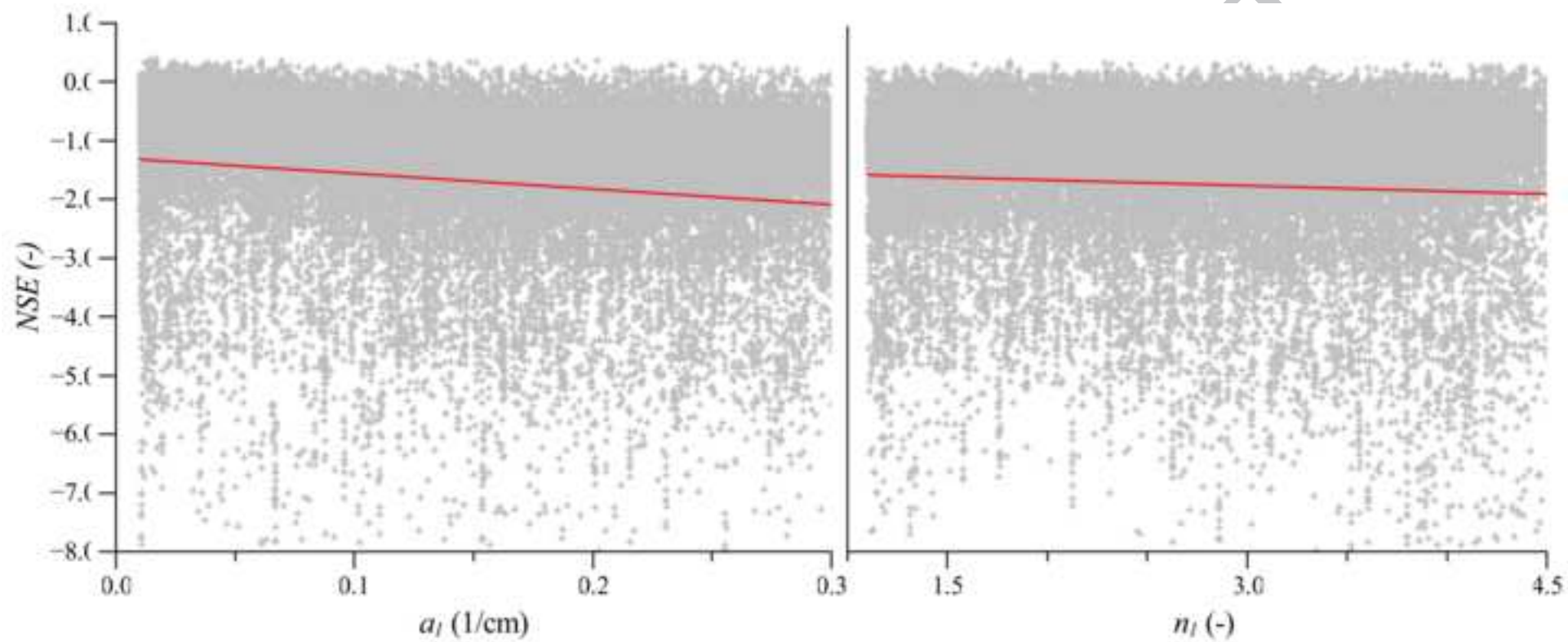|				
a_2 [1/cm]	0.3	0.062	0.11	0.002
n_2 [-]	4.47	1.08	3.04	0.052
K_{s2} [cm/min]	20	6.5	3.87	0.084
θ_{s3} [-]	0.2	0.048	0.044	0.001
a_3 [1/cm]	0.023	0.003	0.021	0.0005
n_3 [-]	2.85	0.537	4.33	0.139
K_{s3} [cm/min]	68.73	19.7	93.2	3.172
$\theta_{s,im3}$ [-]	-	-	0.35	0
ω_3 [1/min]	-	-	0.00017	0.000003
θ_{s4} [-]	0.01	0.002	0.001	0.00003
a_4 [1/cm]	0.27	0.018	0.247	0.004
n_4 [-]	2.41	0.121	2.17	0.039
K_{s4} [cm/min]	96.7	9.2	56.3	1.051
$\theta_{s,im4}$ [-]	-	-	0.288	0
ω_4 [1/min]	-	-	0.0013	0.00002

1059   Table 9. Confidence intervals (CI) for optimized parameters for both scenarios.

1060

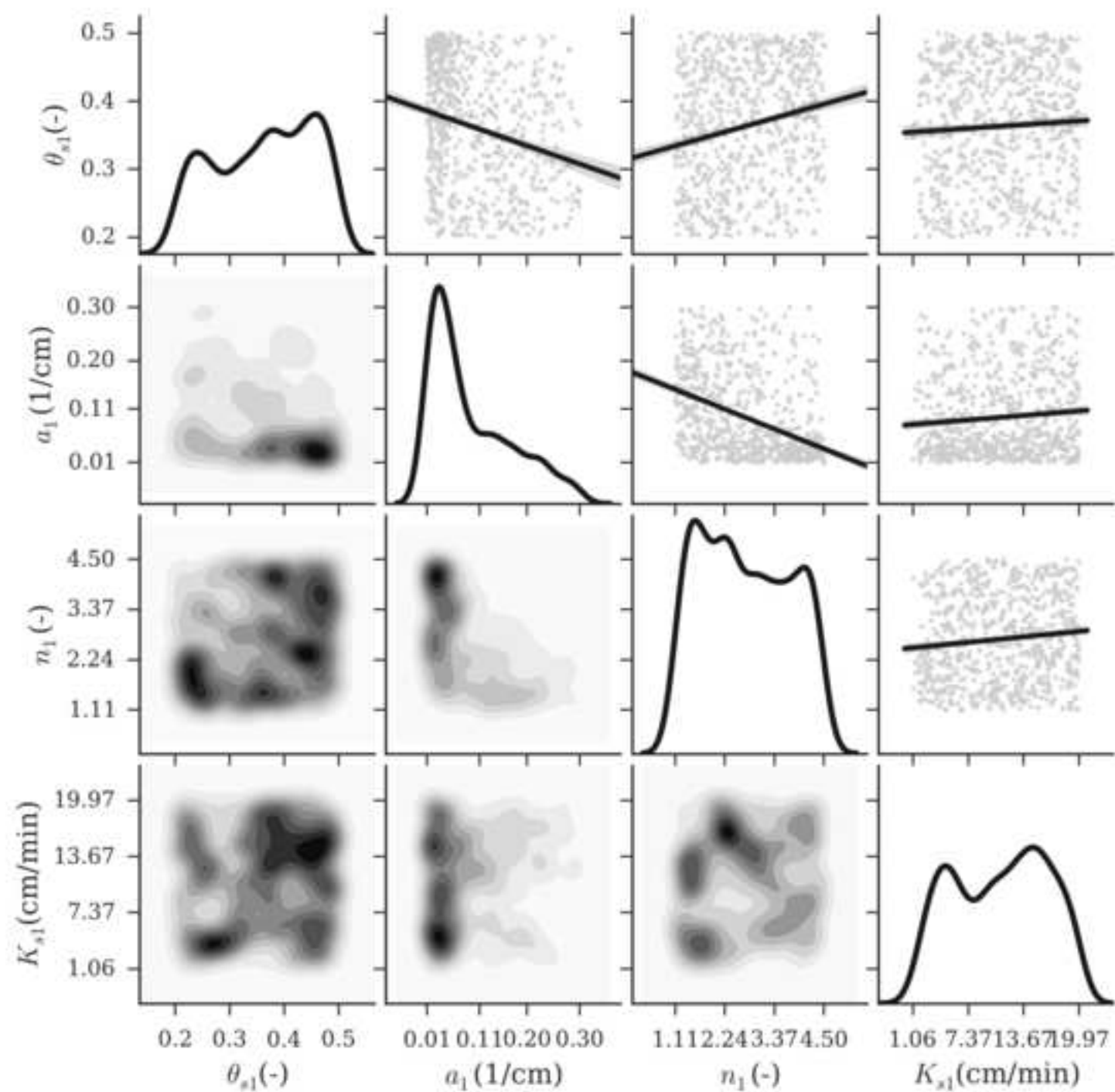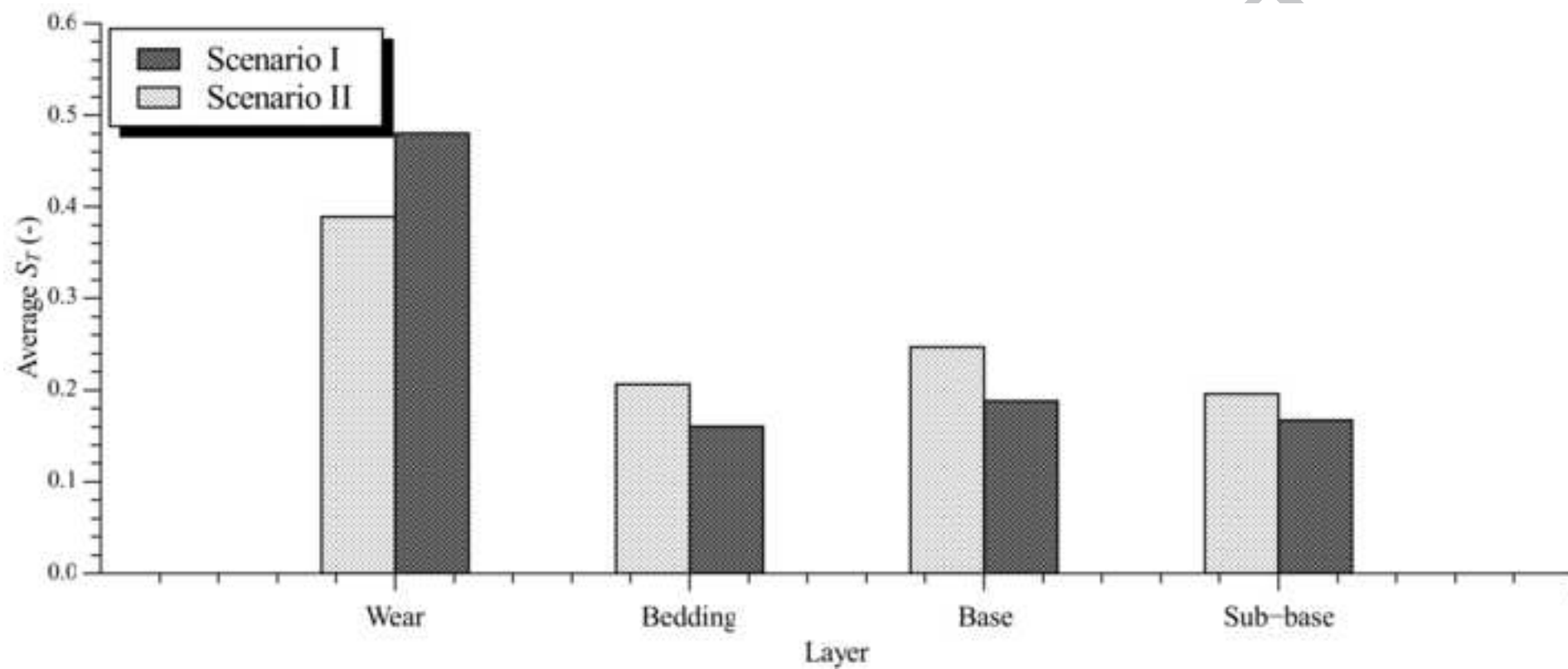1061   **Highlights**

1062   • Among Low Impact Development techniques permeable pavement are those that most lacks
1063   reliable and accurate modeling tools.
1064   • A mechanistic model is used for the analysis of the hydraulic behavior of a permeable
1065   pavement.
1066   • A Global Sensitivity Analysis is used to identify the main effect and interactions of soil
1067   hydraulic parameters.
1068   • The model is calibrated by using the metaheuristic Particle Swarm Optimization algorithm.
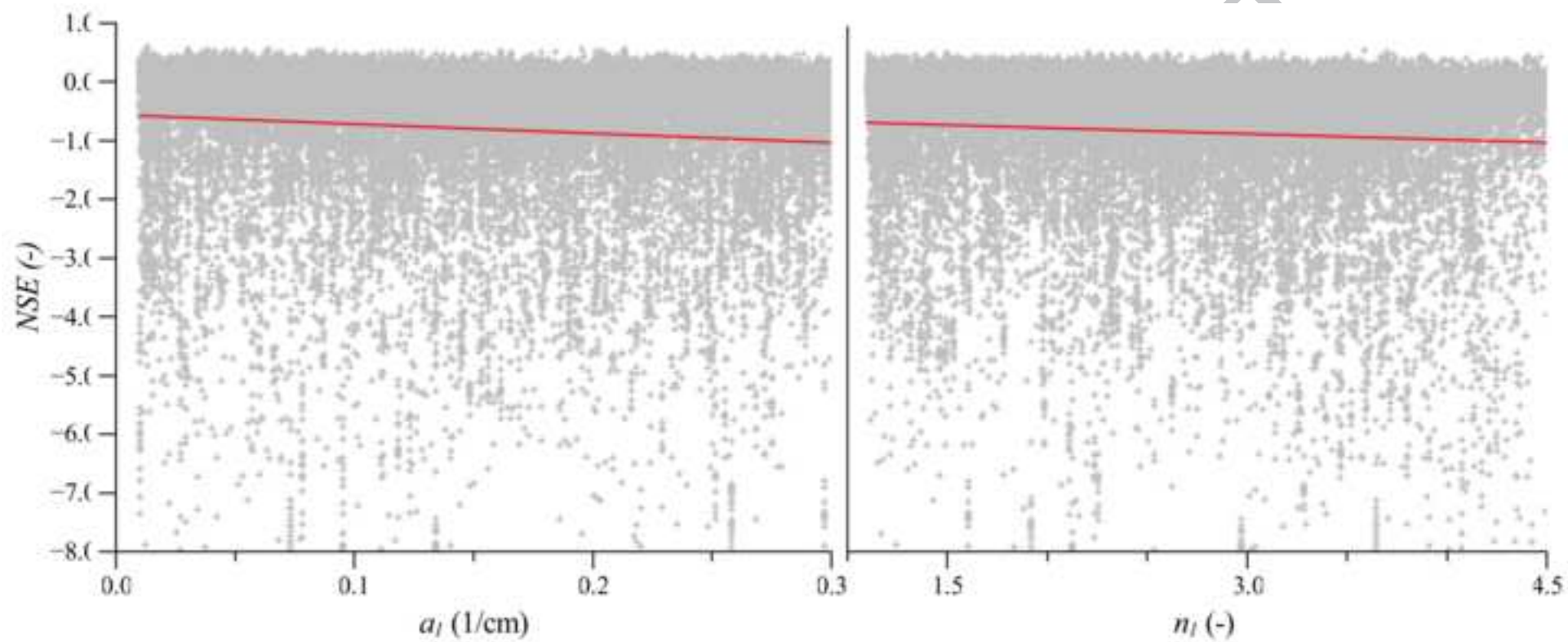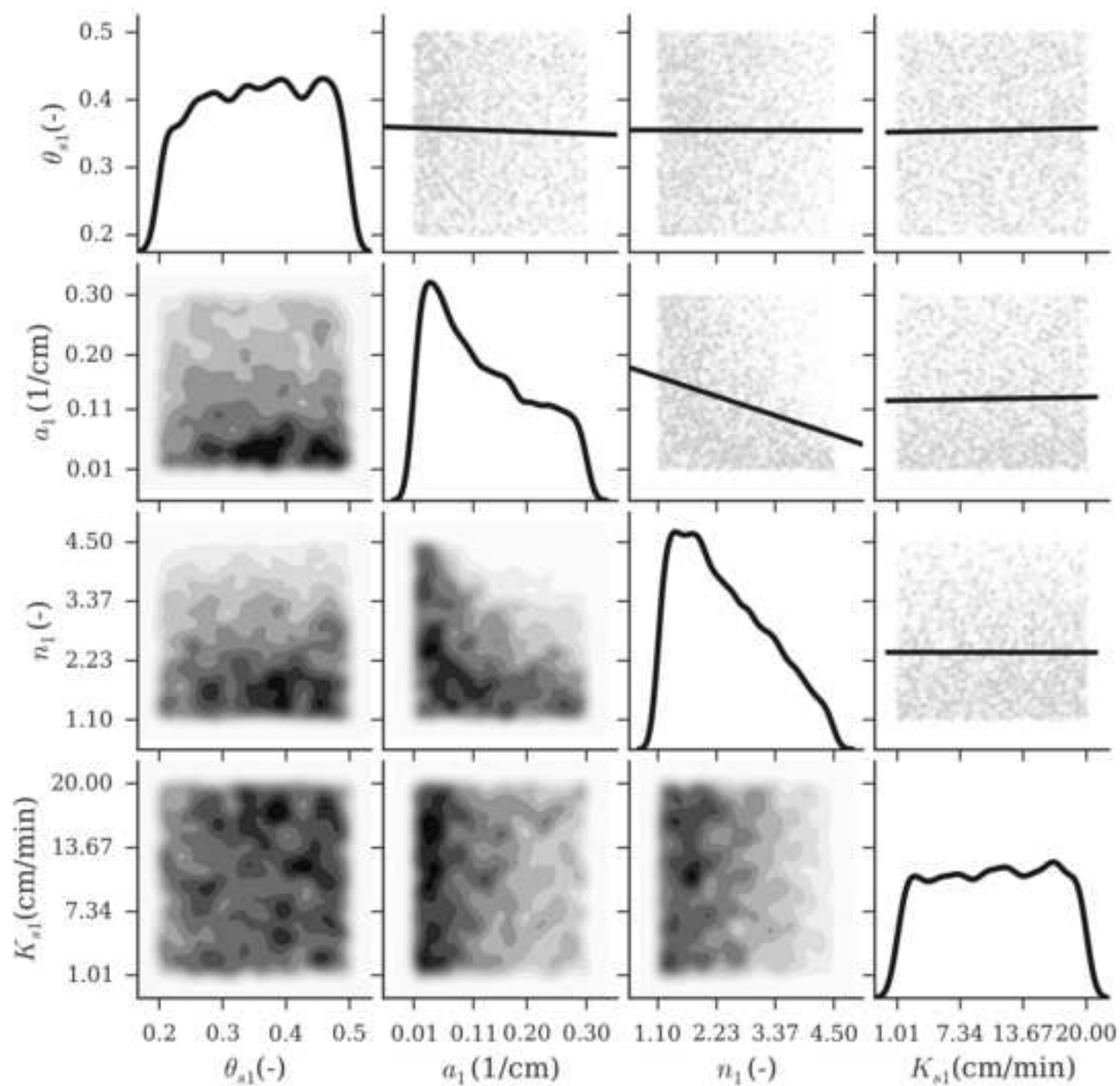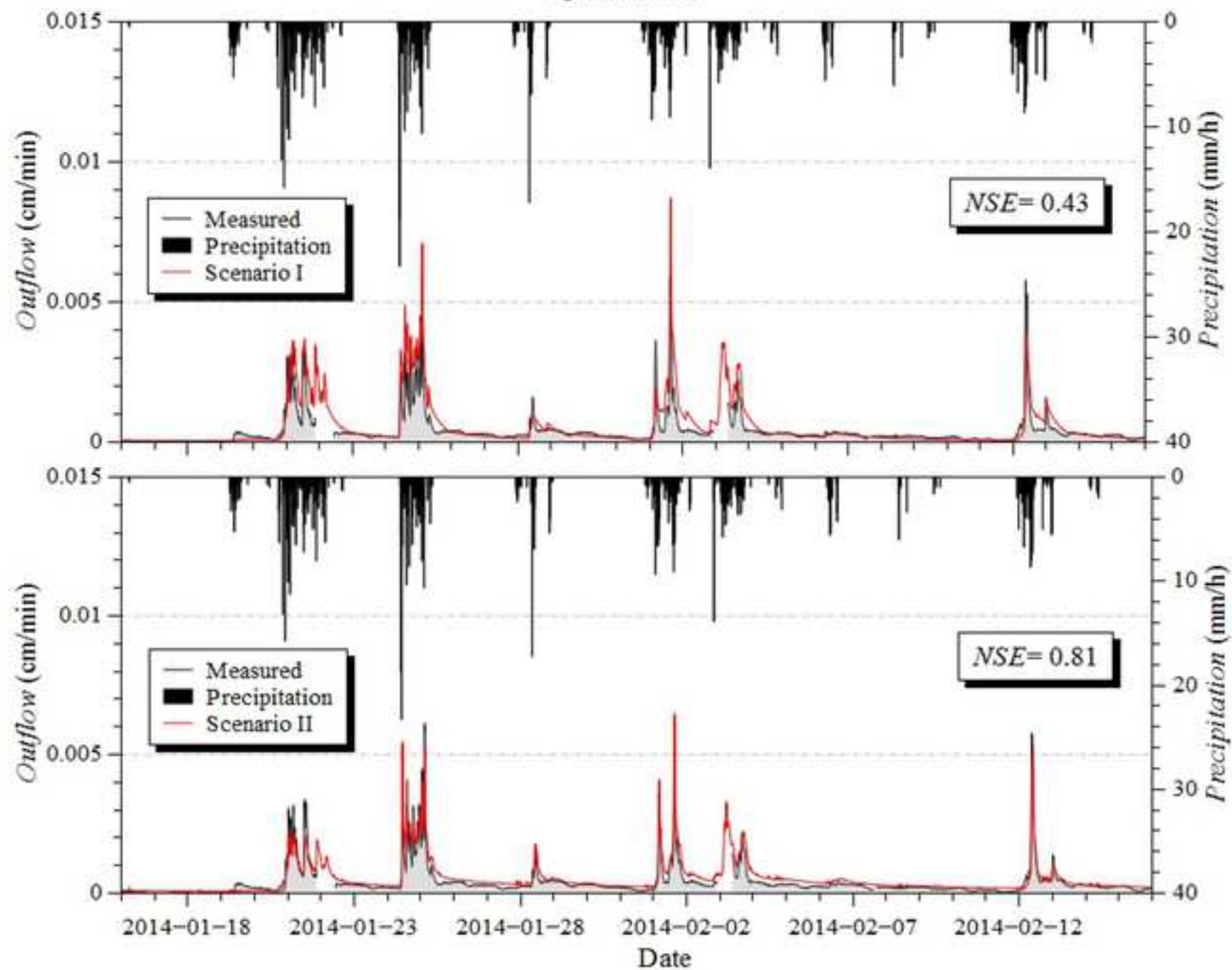1069   • The calibrated model is validated on an independent set of measurements with optimal
1070   results.

1071

Wear layer

Bedding layer

Geotextile

Base layer

Sub-base layer

Protection layer

Impervious geotextile

8 cm

5 cm

35 cm

98,5 cm

45 cm

5 cm

Optimization period

Validation period

Optimization

Legend:
+ Scenario I
+ Scenario II

$Q_{mod} = 1.37 Q_{meas}$
$Q_{mod} = 0.89 Q_{meas}$

Modeled outflow

Measured outflow