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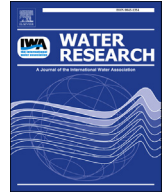
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A dynamic emulator for physically based flow simulators under varying rainfall and parametric conditions

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ABSTRACT

This work presents a method to emulate the flow dynamics of physically based hydrodynamic simulators under variations of time-dependent rainfall and parametric scenarios. Although surrogate modelling is often employed to deal with the computational burden of this type of simulators, common techniques used for model emulation as polynomial expansions or Gaussian processes cannot deal with large parameter space dimensionality. This restricts their applicability to a reduced number of static parameters under a fixed rainfall process. The technique presented combines the use of a modified Unit Hydrograph (UH) scheme and a polynomial chaos expansion (PCE) to emulate flow from physically based hydrodynamic models. The novel element of the proposed methodology is that the emulator compensates for the errors induced by the assumptions of proportionality and superposition of the UH theory when dealing with non-linear model structures, whereas it approximates properly the behaviour of a physically based simulator to new (spatially-uniform) rainfall time-series and parametric scenarios. The computational time is significantly reduced, which makes the practical use of the model feasible (e.g. real time control, flood warning schemes, hydraulic structures design, parametric inference etc.). The applicability of this methodology is demonstrated in three case studies, through the emulation of a simplified non-linear tank-in-series routing structure and of the 2D Shallow Water Equations (2D-SWE) solution (FLOW-R2D) in two computational domains. Results indicate that the proposed emulator can approximate with a high degree of accuracy the behaviour of the original models under a wide range of rainfall inputs and parametric values.

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1. Introduction

The simulation of surface water flow dynamics in urban and rural catchment scale is of great importance in water management. During the past four decades, several distributed or semi-distributed models, having a physical basis, have been developed, such as MIKE-SHE, SWAT or TOPKAPI software (Abbott et al., 1986; Mazzetti, 2015; Neitsch et al., 2002) among others. These conceptualisations simulate several processes (infiltration,

interception, snow melting, overland flow, groundwater flow, etc.) included in the water cycle using either differential or empirical equations. Usually, the overland flow propagation is approximated by simplified methods, such as the kinematic or dynamic wave equations and therefore cannot capture the non-linearities observed, especially in extreme events such as floods (Costabile et al., 2012a; Liang, 2010; Singh et al., 2014).

In the last few years, there is an increasing trend to simulate overland flow dynamics at catchment scale using the full form of the two-dimensional Shallow Water Equations (2D-SWE). Fiedler and Ramirez (2000) and Esteves et al. (2000) represent early attempts to use numerical solvers based on the full form of 2D-SWE

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to simulate the rainfall-runoff process in micro-scale catchments. The rapid increase in computational power led to several examples of application to real catchments (Costabile et al., 2012b, 2013; Liang et al., 2007; Nguyen et al., 2016; Singh et al., 2014).

Although the implementation of this kind of simulators is currently feasible in large-scale scenarios, the required computational time is a substantial limitation (in the order of hours-days). Therefore, the use of this type of physically based flow simulators in practice is still hampered (e.g. hydraulic design, real-time flood warning schemes, uncertainty analysis or parametric calibration).

Accelerating the sampling of hydrodynamic models is an area of high interest. Several approaches focus on exploiting the benefits of high performance computing (Kalyanapu et al., 2011; Vacondio et al., 2014) or efficient grid definitions (Stelling, 2012). These strategies reduce the time required for computing events of interest, however the computational burden is still prohibitive for intensive model evaluation.

The use of surrogate modelling is an alternative to approximate the behaviour of dynamic simulators at output variables of interest. Several authors have presented methods in which a large physically based model is substituted by a fast surrogate conceptual version (Bermúdez et al., 2018; Meert et al., 2018; van Daal-Rombouts et al., 2016). Other strategy focuses on learning directly the behaviour of the original simulator (building an interpolator between the parametric and output spaces). For instance, Wang et al. (2015) presented a data-driven emulator to facilitate uncertainty analysis in hydrologic modelling. A similar application for groundwater modelling can be found in Laloy et al. (2013). Carbajal et al. (2017) described a comparison of surrogate methods (mechanistic vs. data-driven) based on Gaussian processes to emulate the dynamics of urban drainage routing models. More applications can be found in urban hydrology (Machac et al., 2016a, 2016b). These methods have the advantage of representing a mapping between model parameters and the simulator output space, which allow for a direct use in calibration, inference or uncertainty analysis schemes. However, they are generally hard-bounded to the rainfall time-series in which they were trained. This means that the model emulator is only valid for changes in the parametric space under a particular rainfall event and boundary conditions (outside those conditions a new sampling and training would be necessary). This has posed a strong limitation on the application of data-driven emulators in hydrology.

A potential approach to incorporate the rainfall variability in the data-driven emulator is to encode the rainfall process as a set of discrete parameters (representing rainfall intensity at each time step), which is added to the model parametric space to be emulated (Mahmoodian et al., 2017). However, common techniques used for model emulation as polynomial chaos expansion (PCE) or Gaussian processes (GP) are sensitive to the dimensionality of the parameter space, allowing only for a reduced number of parameters to be accounted for. This technique is limited to only short rainfall events, or very coarsely discretised. Another surrogate approach could be the use of recurrent neural networks (RNN, e.g. long-short term memory configurations (Hochreiter and Schmidhuber, 1997)). These structures are designed to accommodate time-dependent processes. However, RNN implementations are expected to require a prohibitive number of simulator samples to guarantee that variations of time-dependent rainfall are sufficiently explored. Sajikumar and Thandaveswara (1999) provided an early example describing a rainfall-runoff process using a neural network by learning patterns from monitoring data. Although this could replicate the behaviour of a given status of the system, it did not allow for representing parameter variations or virtual changes in the system.

A way to cope with the approximation of physically-based flow

simulators responses to new rainfall series is the hybrid combination of the hydrological Unit Hydrograph (UH) theory with hydrodynamic modelling (Bellos and Tsakiris, 2016). With this technique, an UH is derived using a physically based 2D hydrodynamic simulator. Then, the rainfall event is simulated abstracting from the precipitation losses due to infiltration, sewer drainage, interception etc., and composing the total flow response using proportionality and superposition of the UH. With this scheme a flood event can be readily evaluated. Nevertheless, the derivation of the UH is parameter dependent, and thus practical model use is still severely hampered (e.g. quantification of uncertainty, sensitivity analysis, calibration, etc.). Bellos et al. (2017) addressed this issue by generalising the UH derivation with the use of a surrogate model for a uniform distribution of Manning coefficient values, thus including the parameter dependency. However, the solution of the 2D-SWE is often highly non-linear, which is strongly manifested when dealing with small catchments (characterised by fast response). This violates the assumption of linearity in the UH theory, thus rendering significant errors in the estimated hydrograph.

In this work, we present a new methodology to emulate physically based hydrodynamic simulators. This is based on encoding the rainfall process as unitary responses through a dedicated sampling scheme and the use of a polynomial chaos expansion surrogate model which compensates for the effect of non-linearities due to the superposition and proportionality composition of the UH. The mismatch observed in the results derived by the hybrid technique and the full implementation of the physically based model in previous attempts (Bellos and Tsakiris, 2016; Bellos et al., 2017) is significantly reduced. This new surrogate technique allows the modeller to capture the behaviour of the real model to variations of time-dependent rainfall (spatially uniform) and parameter scenarios at a significant computational time reduction (in the order of milliseconds-seconds).

In order to demonstrate the presented methodology, we compare the results derived by a simulator, the conventional use of UH linear theory and the new proposed surrogate model, in three case studies: a synthetic catchment which is represented by a simplified non-linear tank-in-series flow routing structure and two catchment geometries where the rainfall-runoff process is described by the full form of 2D-SWE.

2. Methods and materials

2.1. Model based unit hydrograph

The Unit Hydrograph (UH) theory (Dooge, 1959) is based on the assumption that there is a unique runoff response after a unitary rainfall depth, during a specific time interval, for every catchment. A commonly accepted unitary depth is 10 mm ($1 \cdot m^{-2}$) of rainfall, whereas the time interval varies and depends on the characteristics of the catchment, such as the size, time of concentration etc. With a given UH of a catchment, every runoff can be derived using as input data the rainfall event, based on the principles of the proportionality and superposition. The runoff response for rainfall depth in every time step is derived assuming that this rainfall depth is proportional to the corresponding unitary depth and therefore the responses should be proportional as well (principle of proportionality). The individual runoff responses are composed in time to represent the response for the given rainfall event (principle of the superposition).

The UH theory has been often used to approximate the behaviour of catchments where limited data is available (ungauged basins). This is done using synthetic UHs, which are derived based on the catchment's characteristics (e.g. Snyder's US or the Soil Conservation Service UH, etc.). Alternatively, UHs of several durations

can be derived from monitoring data when available. In this particular case, the objective is to represent the behaviour of a hydrodynamic simulator. Thus, a set of tailored simulations can be drawn from the model in order to capture its unitary reaction by using the principles of UH theory. From this set of samples, an emulator structure was applied to generate an interpolation map between new parameter and rainfall scenarios and the approximated response of the hydrodynamic simulator.

2.2. Polynomial chaos expansion (PCE)

A weighted sum of orthogonal polynomials can be used to link a vector of random variables to space-time model outputs (Xiu and Karniadakis, 2003; Xiu, 2010) if the mapping is smooth. In this case, we denote a deterministic flow model M as:

$$Q(t) = M[m_0, I(t), \theta], \quad (1)$$

which has a set of initial conditions m_0 , time dependent inputs $I(t) \in \mathbb{R}^m$ and a vector of model parameters $\theta \in \mathbb{R}^d$ and which solution renders the simulated flow dynamics at a certain location, $Q(t) \in \mathbb{R}^m$. Then, we aim to find a linear combination of polynomials (only dependent on the parametric space) which approximate a map between θ and $Q(t, \theta)$ as:

$$Q(t, \theta) \approx \mathbf{c}(t)^T \cdot \phi(\theta) \quad (2)$$

in which $\phi(\theta) \in \mathbb{R}^{N \times 1}$ is a series of N orthogonal polynomials constructed as basis of the joint probability density function of the parameter space θ and $\mathbf{c}(t) \in \mathbb{R}^{N \times 1}$ is a vector of coefficients $c_i(t) \in \mathbb{R}^m$ to be fitted to the particular model response.

The output space $Q(t, \theta)$ is interpolated through a weighted sum of polynomials. The fitting process is performed by deriving the model output at $i = 1 \dots K$ known parameter combinations ($\theta = q_i$) as $M[m_0, I(t)|\theta = q_i] = Q(t|q_i)$. The model samples and the polynomial approximation can be written as a system of equations:

$$\begin{bmatrix} Q(t|q_1) \\ \vdots \\ Q(t|q_K) \end{bmatrix} = \begin{bmatrix} \phi_1(q_1) & \cdots & \phi_N(q_1) \\ \vdots & \ddots & \vdots \\ \phi_1(q_K) & \cdots & \phi_N(q_K) \end{bmatrix} \cdot \begin{bmatrix} c_1(t) \\ \vdots \\ c_N(t) \end{bmatrix}, \quad (3)$$

in which the only unknown factors are the coefficients $c_i(t)$. This system can be expressed in matrix form as:

$$\mathbf{Q}(t|q) = \mathbf{P}(q) \cdot \mathbf{c}(t), \quad (4)$$

for which $\mathbf{P} \in \mathbb{R}^{K \times N}$ is the matrix of polynomials values corresponding to each parameter sample. By ensuring that the system is overdetermined ($K > N$), this system can be approximated by a least squares minimisation:

$$\mathbf{c}(t) = (\mathbf{P}(q)^T \cdot \mathbf{P}(q))^{-1} \cdot \mathbf{P}(q)^T \cdot \mathbf{Q}(t|q), \quad (5)$$

thus the values of $\mathbf{c}(t)$ are approximated so they map the selected polynomial basis $\phi(\theta)$ and the sampled output series $\mathbf{Q}(t|q)$. Then the expression of equation (2) can be used to interpolate the targeted output series to different values of the parameter set. This is known as a non-intrusive collocation method, other fitting methods and sampling strategies are discussed in Hadigol and Doostan (2018).

The orthogonal polynomials should be chosen as basis of the parameter probabilistic space. Xiu and Karniadakis (2002) provided a range of known polynomial basis and stochastic variable distributions. In this case, training parameter distributions were always considered independent and uniformly distributed. This has

associated the Legendre polynomials. The creation of orthogonal polynomial series was done using the implementation of Gautschi (1994), which uses a three-term recursion relation for univariate polynomials:

$$\begin{aligned} \phi_{n+1}(\theta_i) &= \phi_n(\theta_i)(\theta_i - A_n) - \phi_{n-1}(\theta_i)B_n \\ A_n &= \frac{E[\theta_i \phi_n^2]}{E[\phi_n^2]}, B_n = \frac{E[\phi_n^2]}{E[\phi_{n-1}^2]}, \phi_{-1} = 0, \phi_0 = 1 \end{aligned} \quad (6)$$

where $\phi_n(\theta_i)$ represents the n th polynomial of the i th parameter. As the parametric space is considered stochastically independent, the multivariate orthogonal expansion was obtained by multiplying the univariate ones:

$$\phi_n(\theta) = \phi_n(\theta_1) \cdots \phi_n(\theta_d). \quad (7)$$

In practice, the polynomial series is truncated at a certain order p , which is selected such that a desired level of accuracy is achieved. Then, the number of polynomials (and thus of associated $c_i(t)$ to be approximated) is:

$$N = \frac{(p+d)!}{p!d!} \quad (8)$$

which is related to the polynomial truncation order p and to the dimensionality of the parameter vector d .

2.3. Emulator structure

A polynomial chaos emulator can be used to represent an interpolation map between model parameters and the model unitary hydrograph response (Bellos et al., 2017). This is done by propagating a unitary rainfall event of 10 mm at combinations of model parameter $\theta = q_i$ and fitting a PCE (as described previously) to the output unitary response, $UH_{10mm}(t, \theta)$:

$$UH_{10mm}(t, \theta) \approx \mathbf{c}_{10mm}(t)^T \cdot \phi_{10mm}(\theta). \quad (9)$$

The total hydrograph shape is then reconstructed for any given rainfall event and combination of parameters. This relies on the proportionality and superposition assumptions of the UH theory, which has proven insufficient to capture the real model dynamics in previous attempts (Bellos et al., 2017). The observed error in the comparison between the hydrodynamic simulator and the composition of the UH was separated in two sources: a) error due to the proportionality assumption; b) error due to the superposition assumption.

According to the proportionality principle, the UH relates linearly to rainfall intensity. This assumption is not valid when dealing with a non-linear model structure. In order to correct for this error source, the behaviour of the unitary hydrograph to rainfall intensity was transferred to the PCE emulator. This was achieved by training the emulator through variations of the model parametric space and of the unitary rainfall intensity (R) (instead of using a fixed 10 mm event to derivate the UH):

$$UH_p(t, \theta, R) \approx \mathbf{c}_p(t)^T \cdot \phi_p(\theta, R). \quad (10)$$

With this approach, the emulator UH_p included the proportional non-linear effect. This corrected for the proportionality error of the classical UH theory, which was tested by reproducing the behaviour of a non-linear tank-in-series model to variations of unitary rainfall intensity.

On the other hand, the superposition error is linked to the model dynamic state. According to UH theory, the flow response is

unitary and independent in previous states and therefore fails to capture non-linear processes. In order to transfer the information of the system state to the emulator structure, we propose a new method to sample the real simulator and to build a unitary rainfall emulator (UH_{PS}). Fig. 1 depicts the emulator development process. This structure was based on two simplification phases. First, a PCE emulator scheme was built following these steps: 1) a series of samples were drawn from the model parametric space $\theta = q_i$ and from two extra parameters R and R_p (which represented two consecutive unitary rainfall steps with duration Dt , selected following the UH theory). 2) Two samples were drawn from the original simulator using the same parameter sample (q_i) but using a rainfall time-series input of $\mathbf{R}_T(t) = [R_p, R, 0, \dots]_{Dt}$ and

$\mathbf{R}_p(t) = [R_p, 0, 0, \dots]_{Dt}$ respectively (which are vectors of input rainfall intensity at a given Dt time step). The difference between the two output hydrographs was computed as $M(\theta = q_i, \mathbf{R}_T(t)) - M(\theta = q_i, \mathbf{R}_p(t))$, which provided an approximation of the state response of the model equations when a rainfall intensity R_p preceded a rainfall intensity R . This response contains the proportionality non-linear error information along with the superposition error (at one rainfall lag). The set of unitary responses was stored in a database.

3) The model unitary responses from the database were used to train a PCE emulator as:

$$UH_{PS}(t, \theta, R, R_p) \approx \mathbf{c}_{ps}(t)^T \cdot \phi_{ps}(\theta, R, R_p). \quad (11)$$

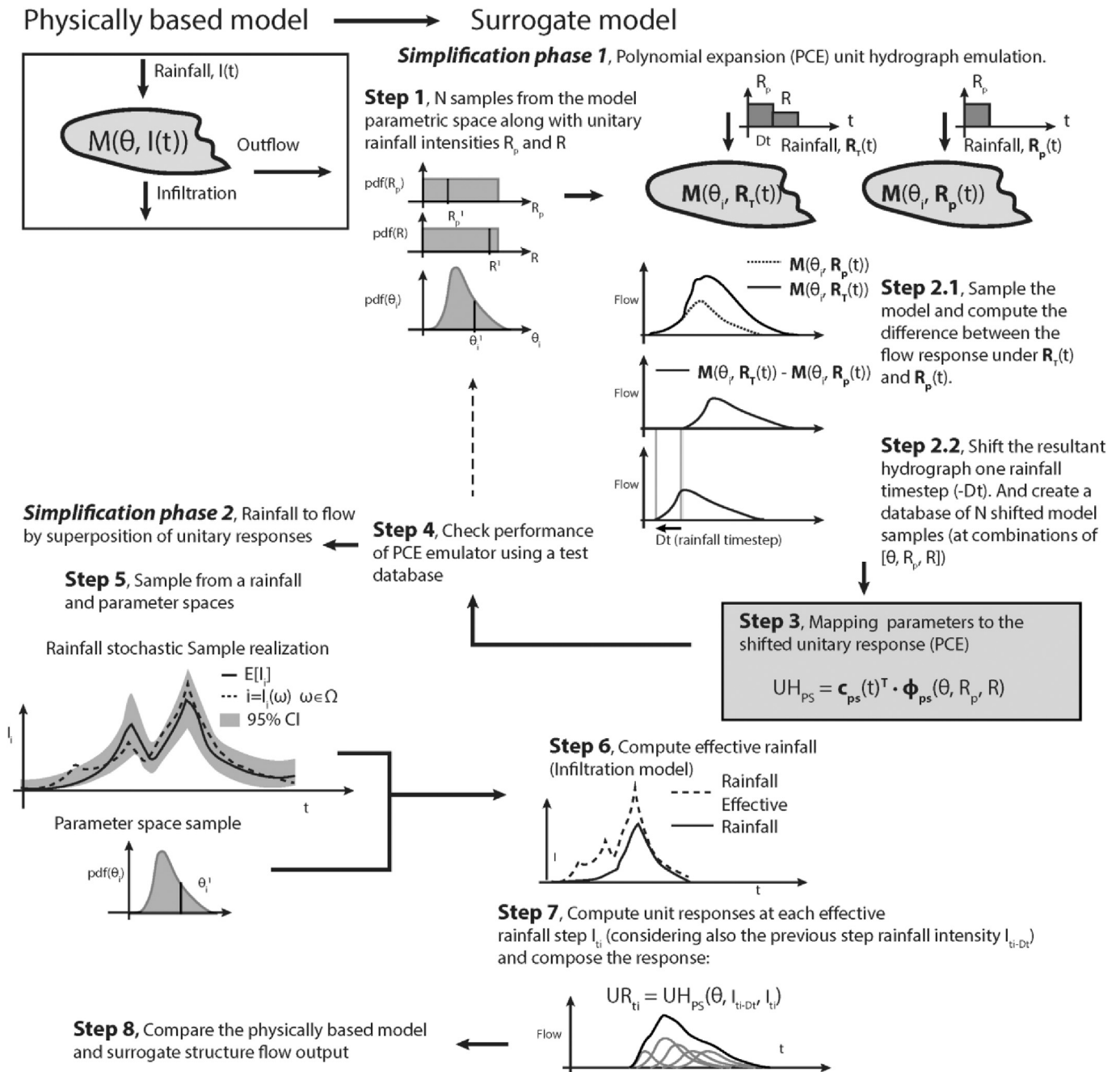


Fig. 1. Emulator conceptual scheme for the correction of superposition and proportional non-linear errors (UH_{PS}).

4) The performance of the unitary emulator was tested on several samples, which were not used to train the model. Once fitted the interpolator (PCE), a second simplification phase is performed; 5) the unitary responses from UH_{PS} are used to reconstruct new rainfall-parametric scenarios; 6) Effective rainfall is computed (if required) and 7) superposing all unitary model responses obtained from equation (11), which corresponds to the unitary response of the model under the parameter set θ and the given rainfall event. Additionally, initial boundary conditions can also be included in the emulation phase by conceptualising them as extra model parameters.

2.4. Case studies

2.4.1. Simplified flow model

In order to illustrate the impact of non-linearities in the basic assumptions of the unit hydrograph theory (superposition and proportionality) a basic synthetic model was used (Fig. 2). This simple rainfall-runoff model structure was conceptualised as a chain of non-linear tanks:

$$\frac{dV_i}{dt} = Q_{in} - Q_{out} \quad (12)$$

$$Q_{out} = a \cdot V_i^b$$

where V_i represents the volume stored at the i^{th} tank, Q_{in} the flow entering in the tank from the previous structure and Q_{out} represents the outflow, which follows a non-linear relationship with the current tank storage (Eq. (1)). The discharge is driven by a proportional coefficient a and an exponential parameter b . The runoff was calculated as $Q_{in\ tanks} = A \cdot R$ from a certain area (A), and was separated in two lines of five and three tanks, which converged at the outflow (Fig. 2).

Both tank lines shared the exponential parameter b but had different proportional coefficients, namely a and a_r . Infiltration was set to 0. Thus the model was composed by a set of Ordinary Differential Equations (ODEs):

$$Q_{outflow} = M_{simplified}(a, a_r, b, A, R(t)), \quad (13)$$

represented by $M_{simplified}$ which depends in the set of tank-parameters, the catchment's area A and in a rainfall input $R(t)$. The parameters were manually selected ($a = 1.4$, $a_r = 2.2$, $b = 1.2$ and $A = 5$) in order to force a non-linear dynamic behaviour. Rainfall time-series were supplied with a frequency of 10 min. The effect of non-linearities and its correction through the use of the proposed emulator were computed on the simplified model at the fixed set of parameters.

Additionally an example is provided in which the full parameter space was used as an input for the emulator. The surrogate structure was trained using 3000 samples drawn from a Latin hypercube sampling (LHS) scheme of the full parametric space (a , a_r , b , A , R_p), where the first four elements referred to model parameters,

and the last two encoded the rainfall process. Distribution and ranges used at the training dataset are described in Table 1.

An uncertainty analysis scheme was also implemented using the emulated structure from an elicited parameter probability distribution (Table 2). A total of 1000 samples were drawn from a Monte-Carlo sampling scheme assuming independency of parameters. This contained the four model parameters (a , a_r , b) and a rainfall multiplier ($K_{rainfall}$), which modified the rainfall input.

2.4.2. Physically based flow model

The applicability of the proposed emulation technique in physically based real scale models was tested by representing the dynamic response of the full solution of the 2D-SWE in two synthetic studies. A computational domain was created using a parabolic shape to represent a surface elevation model (Fig. 3). The surface elevation model $z(x, y)$ (in meters) adopted the following form:

$$z(x, y) = (\alpha - \alpha_0 \cdot x) \cdot (y - y_0)^2 - \beta \cdot x + c \quad (14)$$

where $\alpha = 10^{-4}$, $\alpha_0 = 1.5 \times 10^{-7}$, $y_0 = 250$, $\beta = 5 \times 10^{-3}$, and $c = 10$. The computational domain was discretised in square-shaped cells of 10×10 m, whereas a gate of 100 m width was located at the outlet of the catchment where runoff was measured. The system had a surface of 0.26 km^2 , which is representative of a small catchment characterised by fast response (Model SWE_parabola). Additionally, a set of five obstacles (square reflective boundaries) was located near the centre of the computational domain (Model SWE_urban).

The numerical solver used for the flow dynamics simulation was the FLOW-R2D model, which solves the full form of 2D-SWE. The implementation consisted on the Finite Difference Method and a modified version of McCormack numerical scheme (Bellos and Tsakiris, 2015). The time step was $\Delta t = 0.01$ s, whereas for the diffusion factor a typical value of $\omega = 0.999$ was selected. The Manning equation was used to represent friction. The threshold which distinguishes wet and dry cells was selected equal to $h_{dry} = 10^{-4}$ m. For numerical reasons, an initial thin film of water equal to 1.1×10^{-5} m was set up in the catchment. This film was infiltrated in the first 15 min through the sink term of the mass equation of the 2D-SWE in a constant rate, in order to preserve mass balance between rainfall and runoff volumes. The boundaries of the catchment were set as walls through the reflection boundary technique in order to preserve mass balance as well, whereas the outlet of the catchment was set as open boundaries (Tsakiris and Bellos, 2014). A rainfall input series with a time step of 15 min.

The emulator scheme was implemented using variations of the

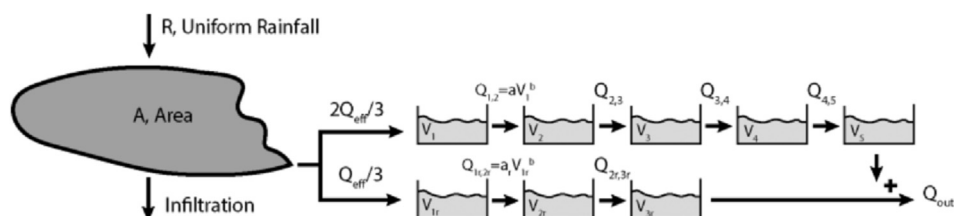


Fig. 2. Scheme for a simplified/lumped non-linear flow model.

Table 1

Parameter probability distributions used for training the simplified model emulator.

Parameter	a (–)	a_r (–)	b (–)	A (km^2)	R (mm)	R_p (mm)
Pdf	Uniform	Uniform	Uniform	Uniform	Uniform	Uniform
Range	[1, 1.6]	[1.8, 2.5]	[1.1, 1.2]	[4.5, 5.5]	[0.2, 20]	[0, 20]

Table 2
Parameter marginal distributions (simplified model uncertainty propagation).

Parameter	a (–)	a_r (–)	A (km ²)	b (–)	$K_{rainfall}$ (–)
Pdf	truncNorm	truncNorm	truncNorm	Uniform	Uniform
Parameters	$\mu = 1.4\sigma = 0.014$	$\mu = 2.2\sigma = 0.088$	$\mu = 5\sigma = 0.2$	–	–
Range	[1.2, 1.5]	[1.8, 2.5]	[4.5, 5.5]	[1.18, 1.95]	[0.95, 1.05]

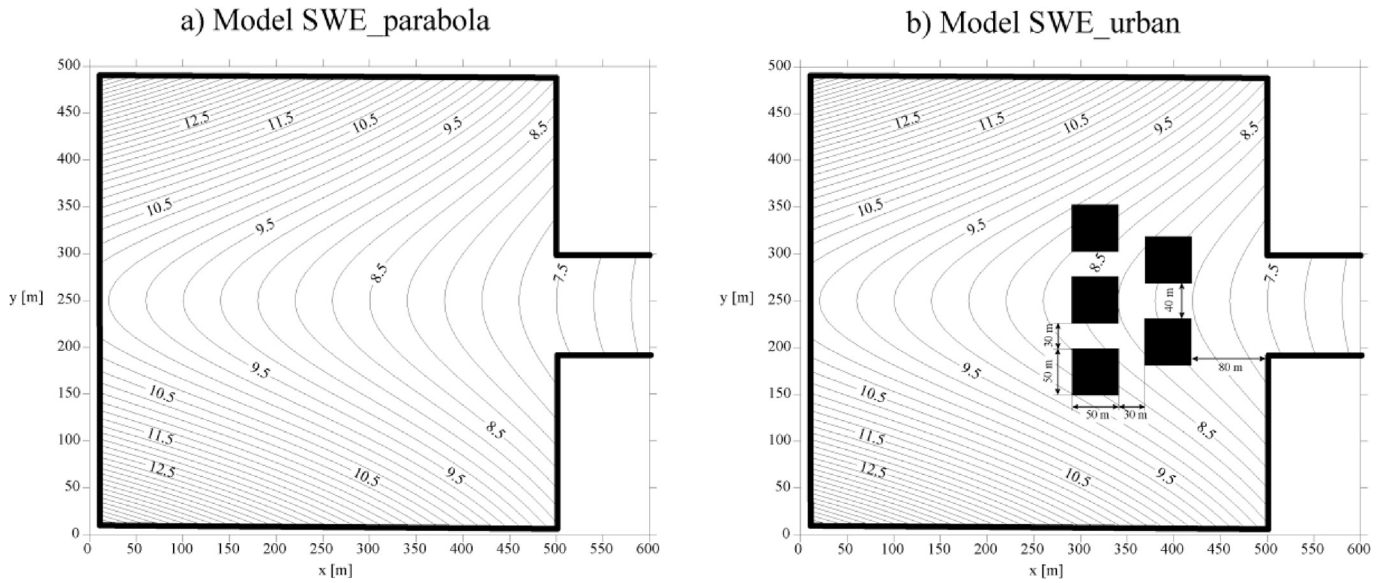


Fig. 3. Surface elevation and boundary conditions of the two 2D-SWE simulators.

surface manning roughness (n) as a model parameter (constant in the spatial domain). Table 3 presents the parametric distributions at training.

A total of 300 samples were performed on the two simulators (drawn from a LHS). The 2D-SWE simulator generated numerical instabilities at very low rainfall intensities. Thus the sampling scheme was reduced to $R_p > 0.2$ and $R > 0.2$. From the remaining dataset, 264 samples were used for training and 30 for validation of the PCE accuracy. A 5th order Legendre polynomial set was used in both cases. Additionally, a validation set of rainfall and parametric scenarios (Table B.1) was used to compare the fit between the original simulators and the proposed surrogate models.

2.5. Performance indicators

The fit between model and emulator derived flow time series was assessed by the Nash-Sutcliffe Efficiency (NSE, Nash and Sutcliffe (1970)):

$$NSE = 1 - \frac{\sum_{t=0}^T (E_t - S_t)^2}{\sum_{t=0}^T (S_t - \bar{S})^2}, \quad (15)$$

where E_t denoted the emulated and S_t the simulated values at time t , and $\bar{S}$ the mean value of the simulated series.

Table 3
Parameter probability distributions used for training the 2D-SWE model emulator.

Parameter	n ($s \cdot m^{-1/3}$)	R (mm)	R_p (mm)
Pdf	Uniform	Uniform	Uniform
Range	[0.03, 0.05]	[0.01, 20]	[0, 20]

Besides, a Peak relative error (PRE) index was used in order to assess the accuracy of the flow maximum peak emulation, which follows:

$$PRE = \frac{S_{peak} - E_{peak}}{S_{peak}}, \quad (16)$$

where S_{peak} and E_{peak} are the simulated and emulated values associated with the peak flow of the hydrograph.

3. Results and discussion

3.1. Correcting UH errors due to non-linearities

The simplified tank-in-series model was used to test the effect of superposition and proportionality assumptions in the reconstruction of hydrographs based in the UH linear theory. The model parameters were defined as described in the materials section to force a non-linear routing process ($b = 1.2$). Fig. 4 shows the mismatch between a UH linear derived hydrograph reconstruction (from a 10 mm/10 min rainfall) and the original simulator. In the x-axis, a set of unitary (10 min) rainfall events is supplied with a ramping intensity (between 1 and 50 mm). The color-map represents hydrograph response. The normalised residuals at each time-step are shown below, which were computed as:

$$\tilde{e}_t = \frac{S_t - E_t}{S_t}, \quad (17)$$

where S_t is the flow simulated at time t and E_t the corresponding emulated values. In the right (Fig. 4) the simulated, approximated (by the UH theory) and residual values are shown for a 30 mm unitary rainfall. The residual structure indicates that for rainfall

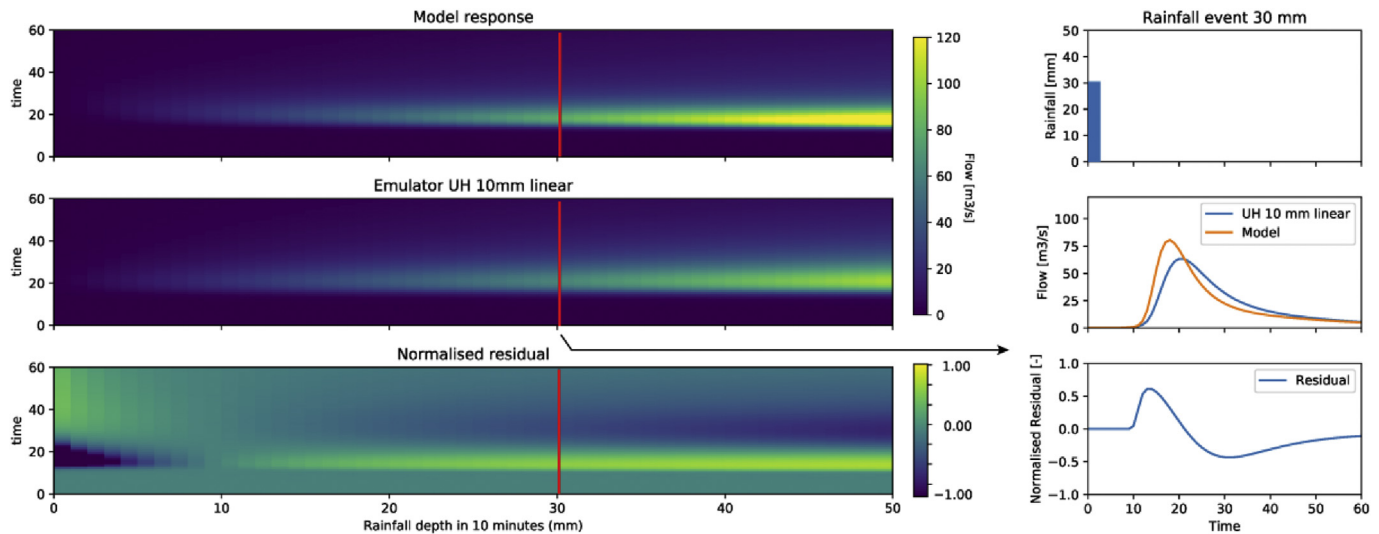


Fig. 4. Effect of non-linearities in the proportionality assumption of the unit hydrograph theory at the simplified model.

intensities above or below 10 mm the performance of the UH reconstruction rapidly decreases. This is due to the non-linear behaviour of the flow propagation, which explains why higher intensities are heavily underestimated and lower intensities overestimated through the linear representation of the UH.

Fig. 5 shows the effect of proportionality when using the UH_p emulator. In this case the rainfall intensity is included in the surrogate structure, and thus the unitary response derivation represents the effect of non-linearities due to proportionality. The residual structure indicates a high similarity between the emulator-simulator outputs, when using only unitary rainfall at varying intensities.

Fig. 6 depicts the errors due to the superposition of the unit hydrograph. In the x-axis a set of 100 rainfall events with varying duration and intensity were used as input for the simulator and for the UH_p emulator. The rainfall events had a random duration of between 10 and 50 min and a rainfall intensity ranging from 2 to 18 mm/10min. The x-axis was sorted by rainfall volume. In the right, the effect of a constant rainfall intensity of 12 mm/10min during 30 min is shown. The effect of non-linearities is still present in this case, although the proportional factor was corrected as shown in

Fig. 5. This indicates that the system state influences the response, and thus, should be accounted for in non-linear systems. Fig. 7 shows the correction done by the use of the proposed emulator structure (UH_{ps}). This structure partially compensates for the proportional and the superposition effects. The residual plot in Fig. 7 shows that these errors are significantly reduced in comparison with the previous scheme (UH_p).

The effect of the linear assumptions of the UH theory in hydrograph approximation have been reported in the literature for rural and urban catchments (Ding, 2011; Minshall, 1960; Musy, 1998). The example presented shows the separated effect of the superposition and proportionality simplifications of a unit hydrograph and a strategy to correct them in the emulator structure. With the use of the tank-in-series model it was possible to modify the level of non-linearity by changing the tank exponent (b). The reader is directed to the additional material (Figure A.1 and A.2) where the same effect was computed for the case $b = 1$, which shows the applicability of the UH theory in linear cases. Nevertheless, flow propagation processes are seldom linear, and thus this effect is expected to be relevant in most applications.

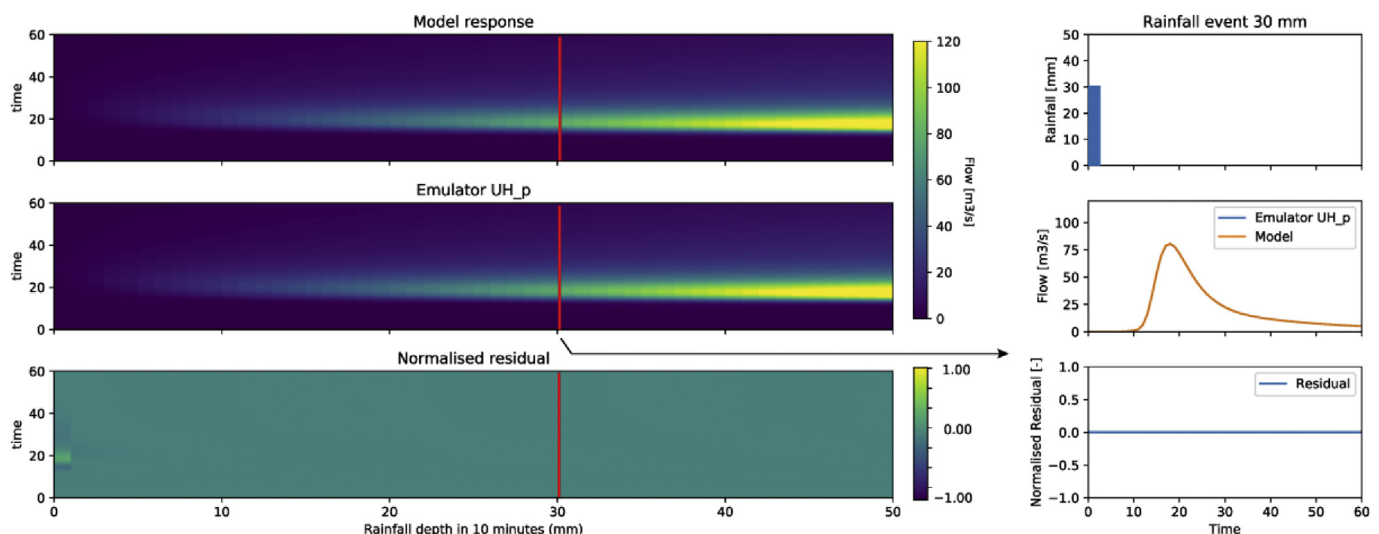


Fig. 5. Correction of the proportionality error at the simplified model (UH_p).

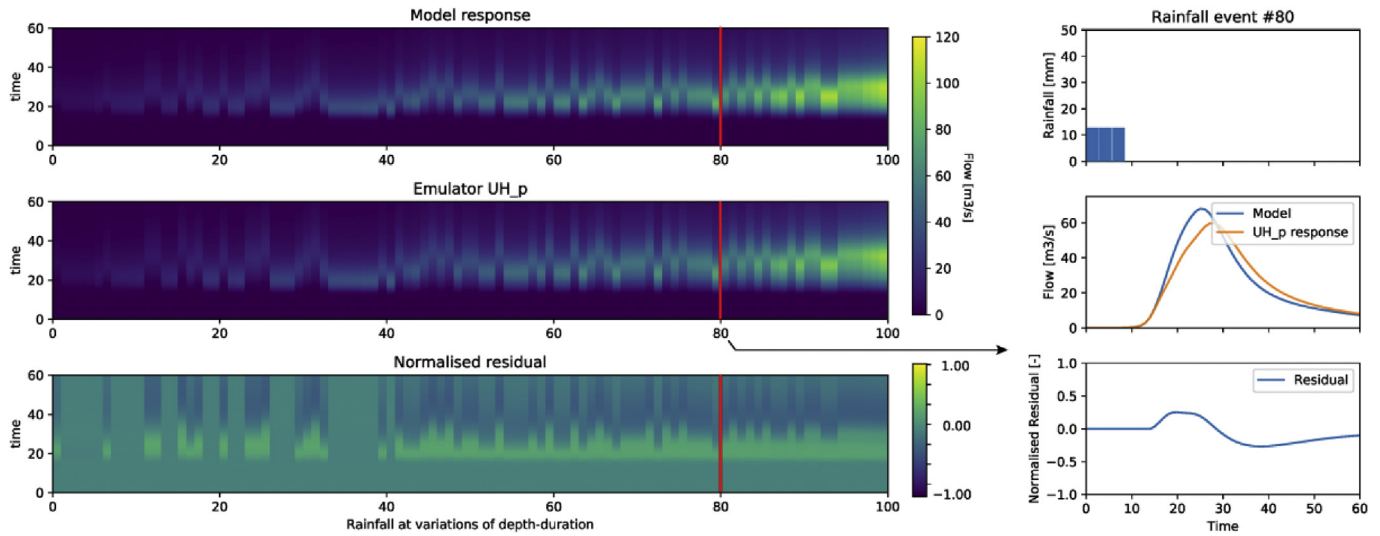


Fig. 6. Superposition error after correction of the proportional error (UH_p).

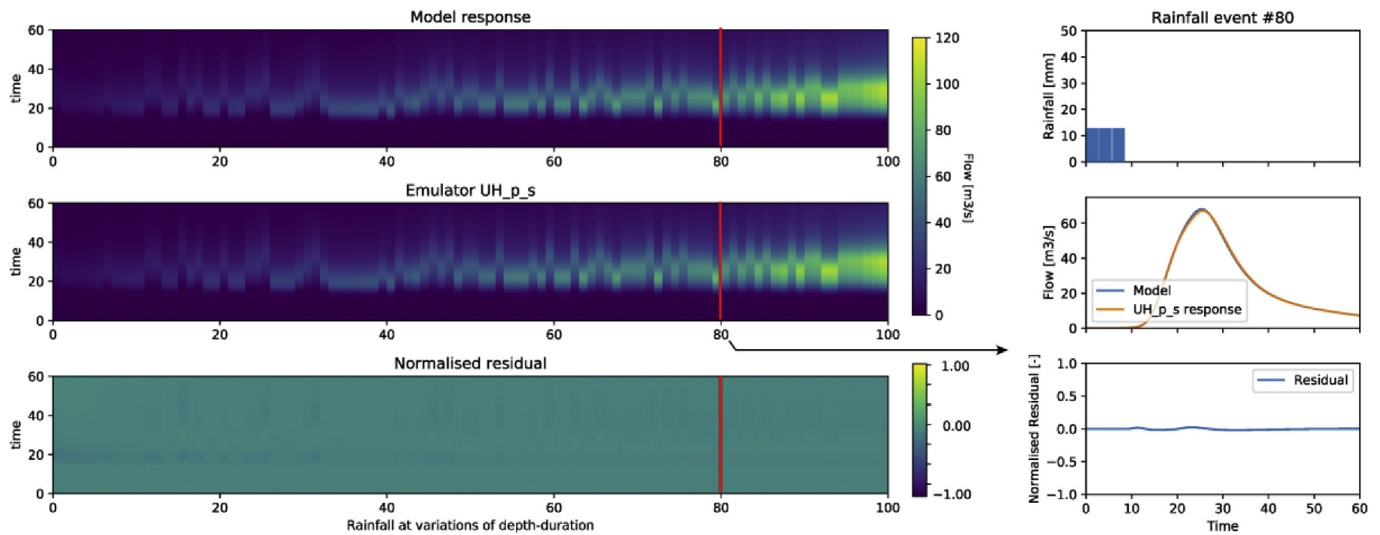


Fig. 7. Correction of superposition and proportionality (UH_{ps}).

3.2. Emulation of the simplified flow model

Once trained, the behaviour of the UH_{ps} emulator was compared with the simplified model response for combinations of rainfall and parametric scenarios. To that effect, 1000 samples were drawn from a Monte-Carlo sampling scheme of an elicited parameter distribution (Table 2). This contained the four model parameters (a , a_r , A , b) and a rainfall multiplier ($K_{rainfall}$). Fig. 8 displays the distribution of the performance indicators PRE and NSE between UH_{ps} and the original simulator. NSE is close to one indicating an accurate fit between simulated-emulated time-series. PRE reports the relative error in the peak reproduction, which is around 1.2% of the maximum flow.

Fig. 9 shows the graphical comparison of the UH_{ps} emulator and the simulator for the initial parameter sample at a particular rainfall series, along with the mean and 95% interval of the 1000 parameter samples performed on the emulator.

3.3. Emulation of the 2-D shallow water equations

The dynamics of the 2D-SWE were emulated following the same

process as in the simplified example. Fig. 10 shows the NSE values for the emulated-simulated unitary responses at 30 combinations of parameters contained in the testing dataset. This served to validate the emulator of the unitary responses.

We compared the emulator UH_{ps} (which takes into account the error due to proportionality and superposition), the emulator UH_p (only the proportionality error), the conventional composition of the UH linear (using 10 mm unitary rainfall) and the results derived from the 2D-SWE hydrodynamic simulators (SWE_parabola and SWE_urban) in a set of 8 validation scenarios (Appendix B, Table B.1), for varying rainfall time series and roughness coefficient values. Table 4 presents the NSE and PRE values for all cases comparing with the hydrodynamic simulator. There is a clear increase in performance by the use of the proposed emulator structure (UH_{ps}) when approximating the flow dynamics. This increase is denoted by the high NSE values and a PRE one order of magnitude lower than the other emulator structures. In general, the use of the proportional correction (UH_p) is not sufficient, and although it reproduces the hydrograph peak better than the simple use of the linear UH structure, denoted by the lower PRE values (specially in rainfall events where the maximum intensity differs from 10 mm as

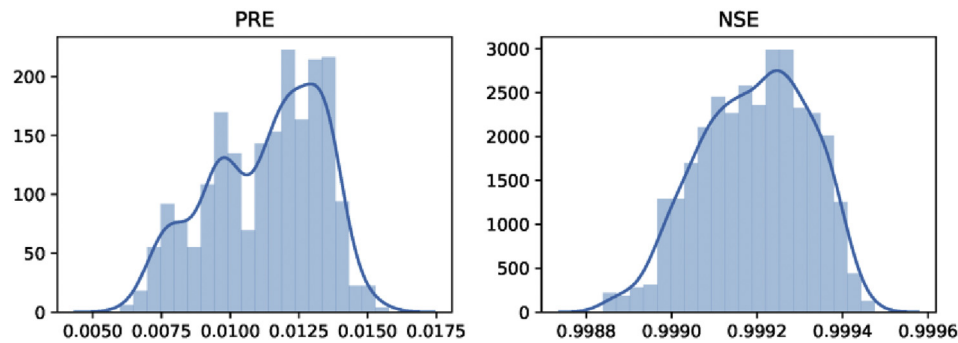


Fig. 8. Performance indicators for the comparison simulator-UH_{PS} (1000 samples). Peak relative error (PRE) and Nash-Sutcliffe Efficiency (NSE) histograms.

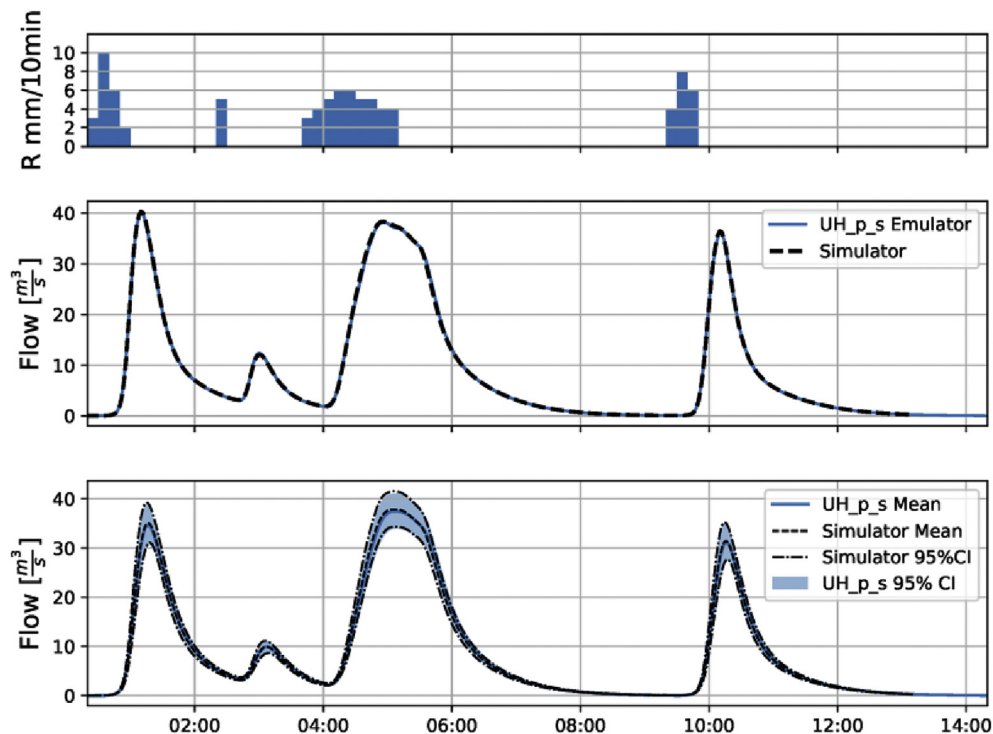


Fig. 9. Model vs. emulator comparison; Mean rainfall series (above), emulator and simulator response at parameter values ($a = 1.4$, $a_s = 2.2$, $b = 1.2$ and $A = 5$) (middle) and comparison of forward uncertainty propagation from 1000 samples from the emulator and simulator (below).

in Validation events 0 to 3), it is heavily affected by the superposition error as seen in the Validation events 4 to 7.

The use of UH_{PS} improves the reconstruction of the simulated hydrograph and it captures the timing of the flow peak in all tested cases for both geometrical scenarios. Fig. 11 shows a graphical comparison between the emulated and simulated values for the Validation_0 and Validation_1 scenarios for the simulator SWE_{urban}. UH_{PS} has a close fit to the simulator dynamics, with an error in the peak estimation of 1–5%. The comparison of SWE_{-parabola} and SWE_{urban} are also shown in Fig. 11 were the effect of geometrical obstacles of the second scheme generates a slightly delayed and attenuated flow response, which led to a decrease in performance of UH_{LINEAR} and UH_P. The reader is directed to the additional material for the graphical comparison at the 8 validation scenarios for the two simulators (Figure B.1 and B.2).

One of the advantages of the proposed methodology (UH_{PS} structure) is that the emulation errors can be decomposed directly in two sources: a) errors in the emulation of the unitary responses through a PCE and b) errors in the reconstruction of the hydrograph

by composition of the unitary responses. The errors in phase a) can be described by comparing the PCE emulator and the simulator in a set of test parameter scenarios. This source is dependent on the capability of the emulation technique used to represent the link between the unitary response and the parameter space, which can be reduced in two ways: 1) by carefully selecting the emulator structure, which should be capable of representing a dynamic output, such as a PCE (Xiu and Karniadakis, 2002), by using a Gaussian Process as in Carbajal et al. (2017), Bayesian networks (Conti and O'Hagan, 2010) or recurrent neural networks (Gers et al., 2002). 2) By increasing the training dataset size (sampling from the simulator). Phase b) involves reconstructing the hydrograph from the unitary responses. The effect of the proportionality simplification is well represented by including the rainfall intensity in the emulator structure. However, the superposition composition has a dependency on the system dynamics and the unitary rainfall length. For highly dynamic systems, high-frequency rainfall data could be necessary, and thus, accounting for only one temporal step in the superposition scheme might not be sufficient.

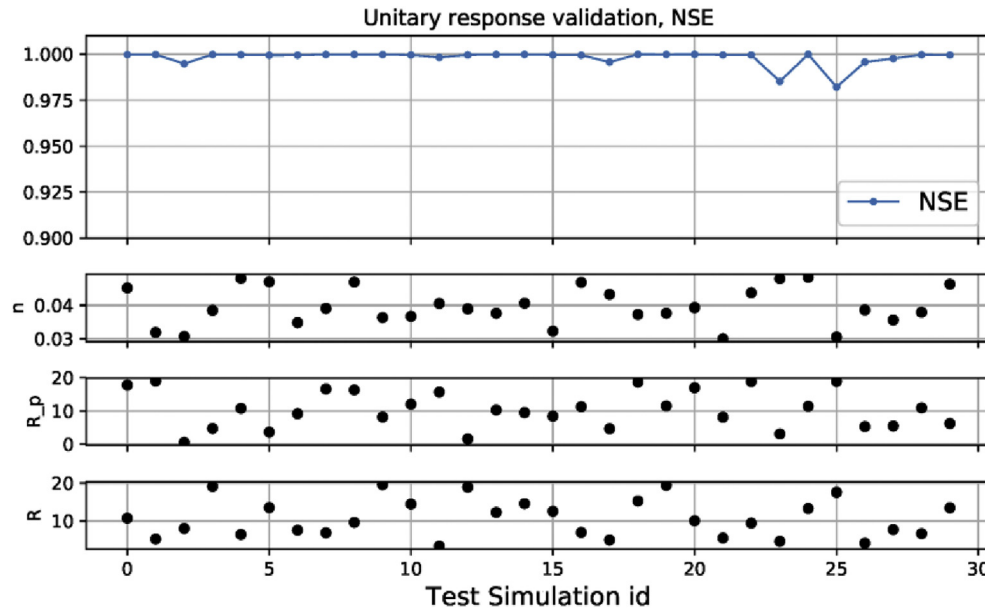


Fig. 10. NSE and parameter values for the UH_{ps} emulator unitary responses at the test database (SWE_parabola).

Table 4

Nash-Sutcliffe Efficiency and Peak relative error between simulated vs emulated (in the left, SWE_parabola, and in the right, shaded, SWE_urban).

	NSE						PRE					
	UH_{LINEAR}		UH_p		UH_{ps}		UH_{LINEAR}		UH_p		UH_{ps}	
Validation_0 (n=0.035)	0.64	0.53	0.74	0.65	0.988	0.987	0.46	0.51	0.18	0.23	-0.04	-0.03
Validation_1 (n=0.042)	0.53	0.36	0.65	0.54	0.989	0.983	0.48	0.53	0.24	0.27	-0.043	-0.01
Validation_2 (n=0.037)	0.46	0.48	0.59	0.61	0.985	0.988	0.51	0.52	0.28	0.24	0.055	-0.02
Validation_3 (n=0.043)	0.39	0.34	0.52	0.53	0.987	0.981	0.52	0.54	0.3	0.28	0.032	0.007
Validation_4 (n=0.036)	0.62	0.6	0.48	0.37	0.996	0.988	0.42	0.44	0.43	0.49	0.026	-0.049
Validation_5 (n=0.040)	0.6	0.55	0.41	0.25	0.996	0.986	0.42	0.45	0.45	0.51	0.012	-0.03
Validation_6 (n=0.038)	0.57	0.52	0.49	0.38	0.996	0.996	0.46	0.45	0.45	0.45	0.02	-0.04
Validation_7 (n=0.041)	0.53	0.45	0.43	0.28	0.997	0.996	0.48	0.47	0.47	0.48	0.016	-0.03

A limitation of the proposed methodology is that its applicability is restricted to rainfall spatial homogeneity. The generalisation to spatio-temporal rainfall variability poses a challenge since it will increase significantly the degrees of freedom of the unitary response, which should be captured by the emulator phase, thus requiring a much larger number of samples from the real simulator.

Also, in practice the number of accounted parameters is limited in this approach. When using the PCE emulator, the number of polynomials follows equation (8), which depends on the dimension of the parameter space (d) and the grade of the polynomial series (p). This relationship grows rapidly, forcing to increase the number of samples from the original model. Thus, for large dimensional spaces the number of required model samples could render the training impractical.

For instance, the training of the SWE_parabola and SWE_urban

emulators was done through 260 unitary responses requiring a total of 1040/2080 computation-hours (training was performed in the HPC platform of the Computational Centre of the National Technical University of Athens), details are provided in Table 5. The emulator sampling at the validation tests took ~40 ms per iteration (in a 2.2 GHz Intel Core i7) which represents a significant time reduction. The benefit of proposing an emulator is strongly case dependent and is linked to the number of required parameters and shape of the simulator response. Fig. 12 provides a measure for the increase in performance (measured by the decrease in L2 norm) with the training data set size for the three tested emulators. The stabilization of performance can be used to design a sequential sampling scheme, which can reduce the number of simulator samples.

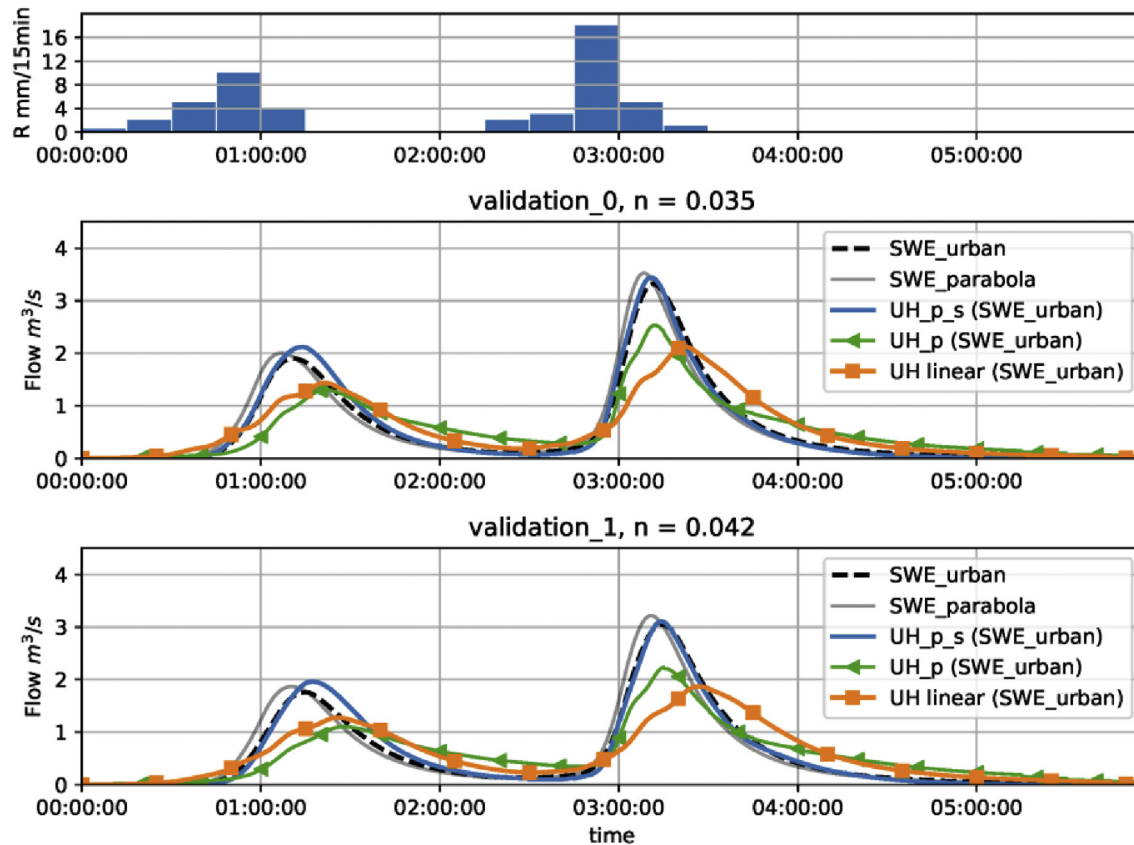


Fig. 11. Validation of the SWE_urban emulator. Graphical comparison of the response of the real model under a rainfall event and two manning values (0.035 and 0.042 respectively) against; use of the classical unit hydrograph theory from a 10 mm rainfall (UH linear), the correction of the proportionality error only (UH_p) and the proposed emulator structure (UH_{ps}).

4. Conclusion

In this work a novel methodology to perform emulation of flow derived from hydrodynamic simulators is presented. This method allows approximating hydrographs generated by physically based hydrodynamic modelling under variations of model parameter values and rainfall series. This method is based on the combined use of the unit hydrograph theory (UH) and a polynomial chaos expansion (PCE) emulator. The use of the unit hydrograph theory is based upon the assumption that the underlying process is linear. This assumption is seldom met in physically based hydrodynamic simulators since the driving equations are fundamentally non-linear. In this new approach, information of the non-linear reaction of the model is encoded in the PCE structure by means of a dedicated sampling scheme.

The performance of the emulator was tested in three case studies; a) a simplified flow routing model based on a non-linear tank cascade, b-c) two synthetic computational domains simulated through the full form of the 2D Shallow Water Equations. In the three simulators the proposed emulator structure could approximate an output hydrograph under various combinations of rainfall time-series and model parameters. A comparison between

the performance of the proposed emulator structure (UH_{ps}) and the use of the classical UH theory is also provided. This demonstrated that errors induced by the linear assumption of the UH theory can be significant when dealing with simulators based on the solution of the 2D-SWE.

The method still has several limitations. For instance, the emulator can only accept spatially uniform rainfall time series. This can pose a severe constrain when dealing with large-scale catchments. Also, rainfall series inputs should have a constant sampling frequency. Errors in the emulator-simulator structure are expected to increase if the selected rainfall step-duration is much smaller than the catchment's concentration time for highly non-linear models, since the unit hydrograph superposition error will become dominant. The number of independent parameters is also limited in practice. This is a limitation of the emulator structure used (PCE) since the number of required model samples increases rapidly with the dimensionality of the parametric space. Nonetheless other data-driven surrogate strategies can be easily implemented. Further research should be conducted in these areas.

The proposed methodology has the potential to significantly increase the range of applications of physically based flow propagation schemes, which is currently hampered by the computational burden.

Table 5

Computational time of training vs. operation.

	# training samples	Simulator (time)		Emulator (time)
		sample	Validation scenario	Validation scenario
SWE_parabola	260	~14,400 s	~22,000 s	~0.040 s
SWE_urban	260	~29,000 s	~40,000 s	~0.040 s

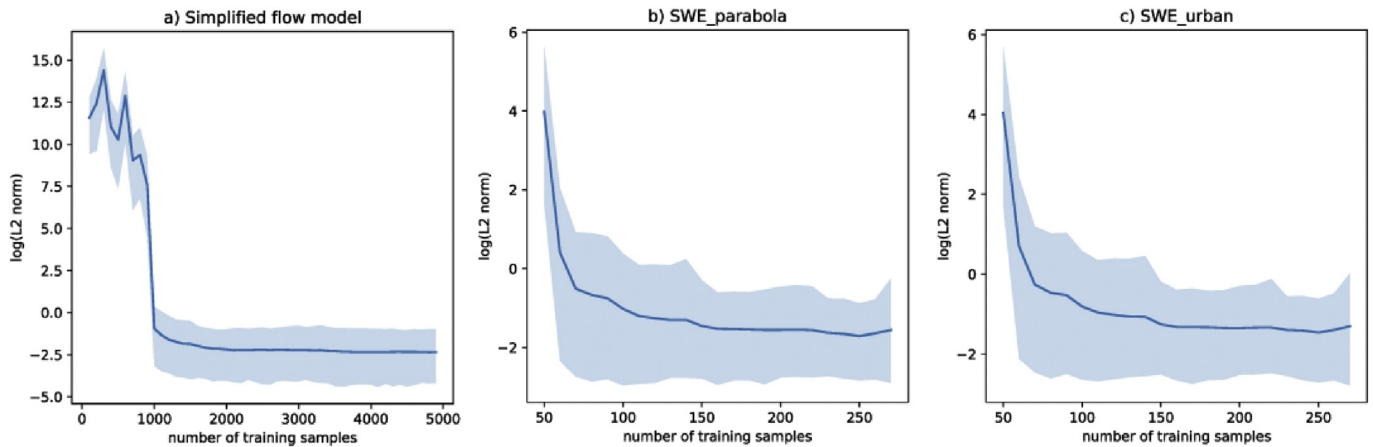


Fig. 12. Emulator performance (mean and 95% quantile for L2 norm in logarithmic scale) and number of training samples. Number of parameters and polynomial degree in each case: a) 6–6, b) 3–5 and c) 3–5.

Author contributions

AMR developed the required software and carried out the simulations and data analysis. **VB** produced the design and simulations from the physically based model (FLOW-R2D). **AMR** and **VB** wrote the manuscript. The work was performed under the supervision of **JL** and **FC**. All authors copy-edited the manuscript.

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access provided to the use of the computation facilities.

Appendix A. Uh simplification in linear models

When using a linear model the assumptions of proportionality and superposition of the unit hydrograph are congruent with the underlying dynamics. Figure A.1 shows the comparison between the simplified model described in the first case study (using $b = 1$, thus a set of linear tanks) and the use of a unit hydrograph derived from the response at 10 mm rainfall for an increasing unitary rainfall intensity from 1 to 50 mm/10min. Figure shows the same comparison for the joint proportionality and superposition assumptions for rainfall inputs of varying length (10–50 min) and intensity (1–20 mm/10min). In those cases the classical UH theory can describe the model behaviour correctly, which is denoted by the almost null residual map.

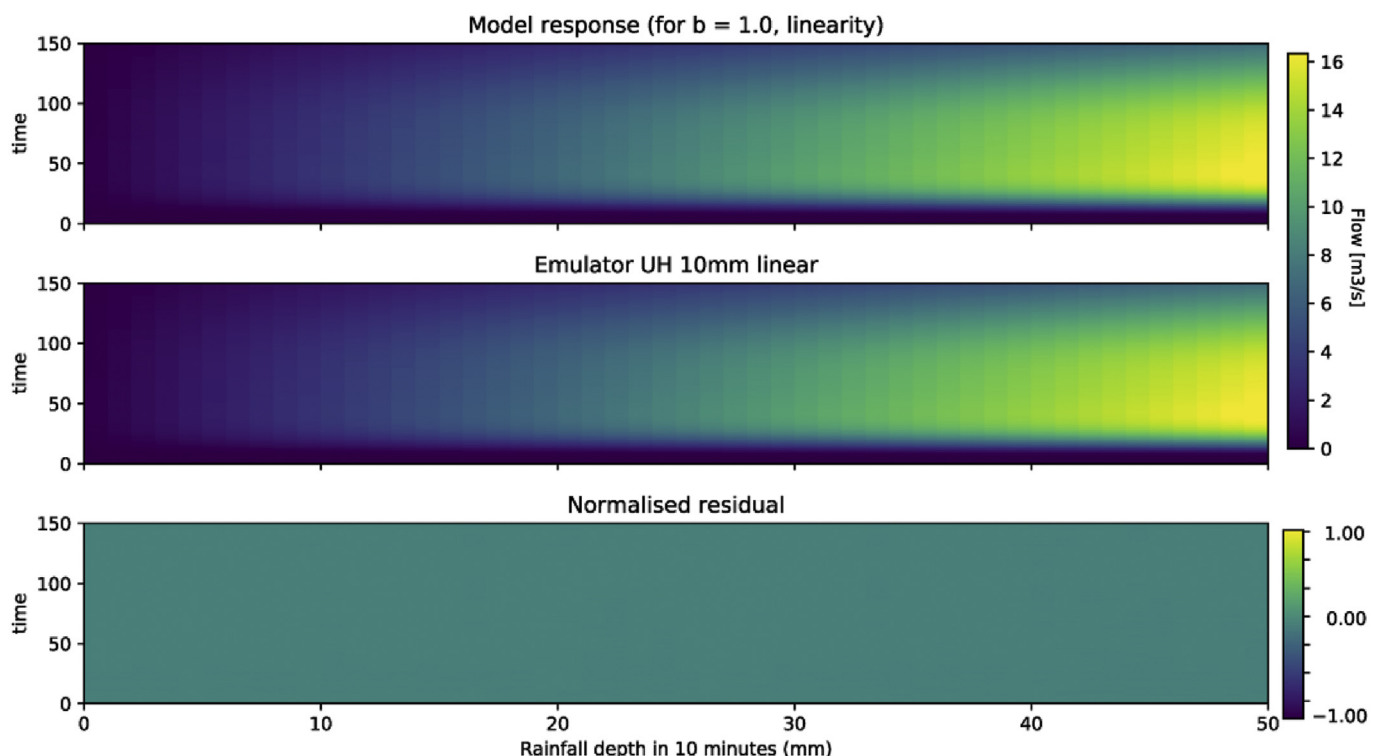


Fig. A.1. Comparison of model vs linear unit hydrograph proportionality composition for a simplified linear model ($b = 1$).

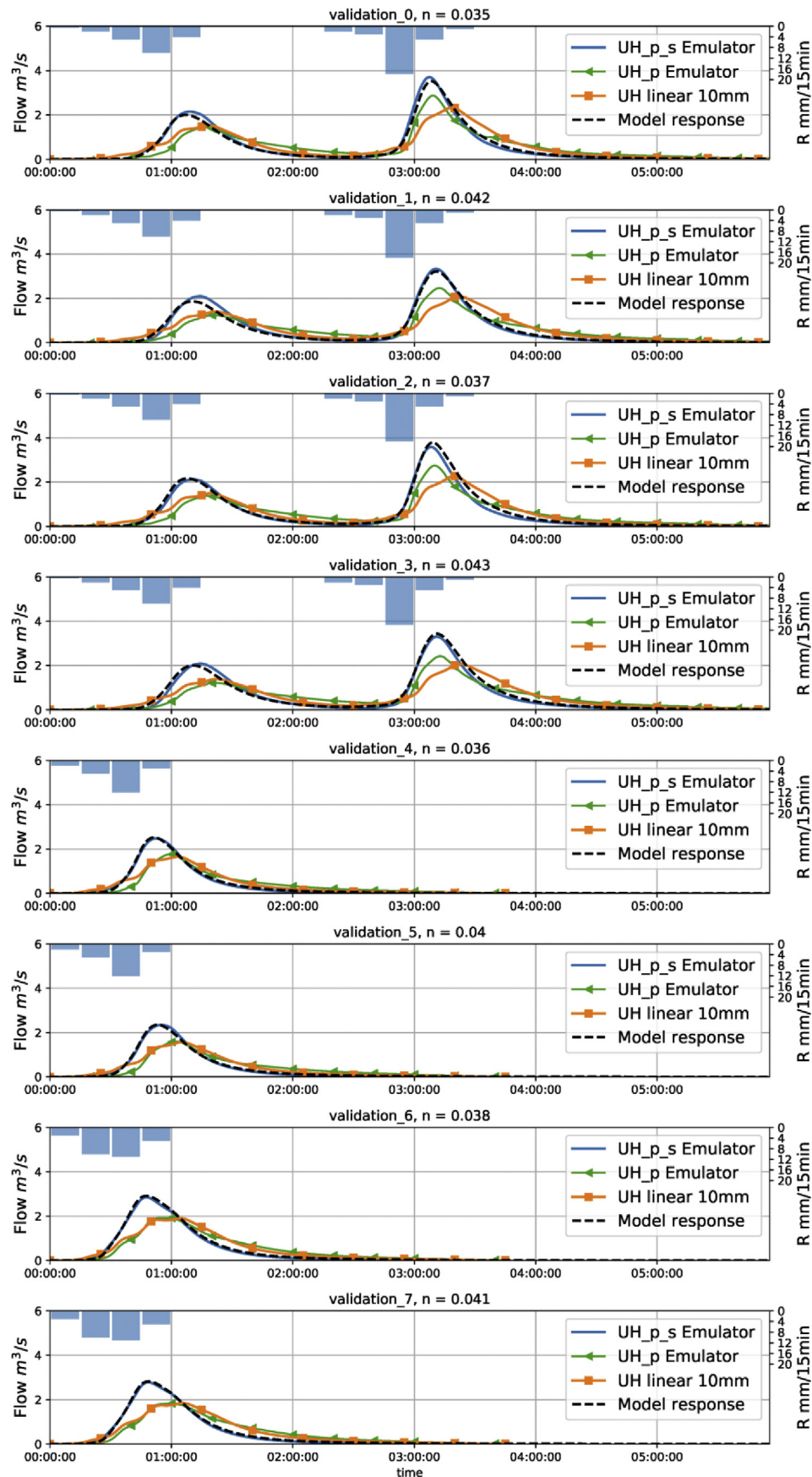


Fig. B.1. Validation comparisons emulator vs SWE_parabola simulator.

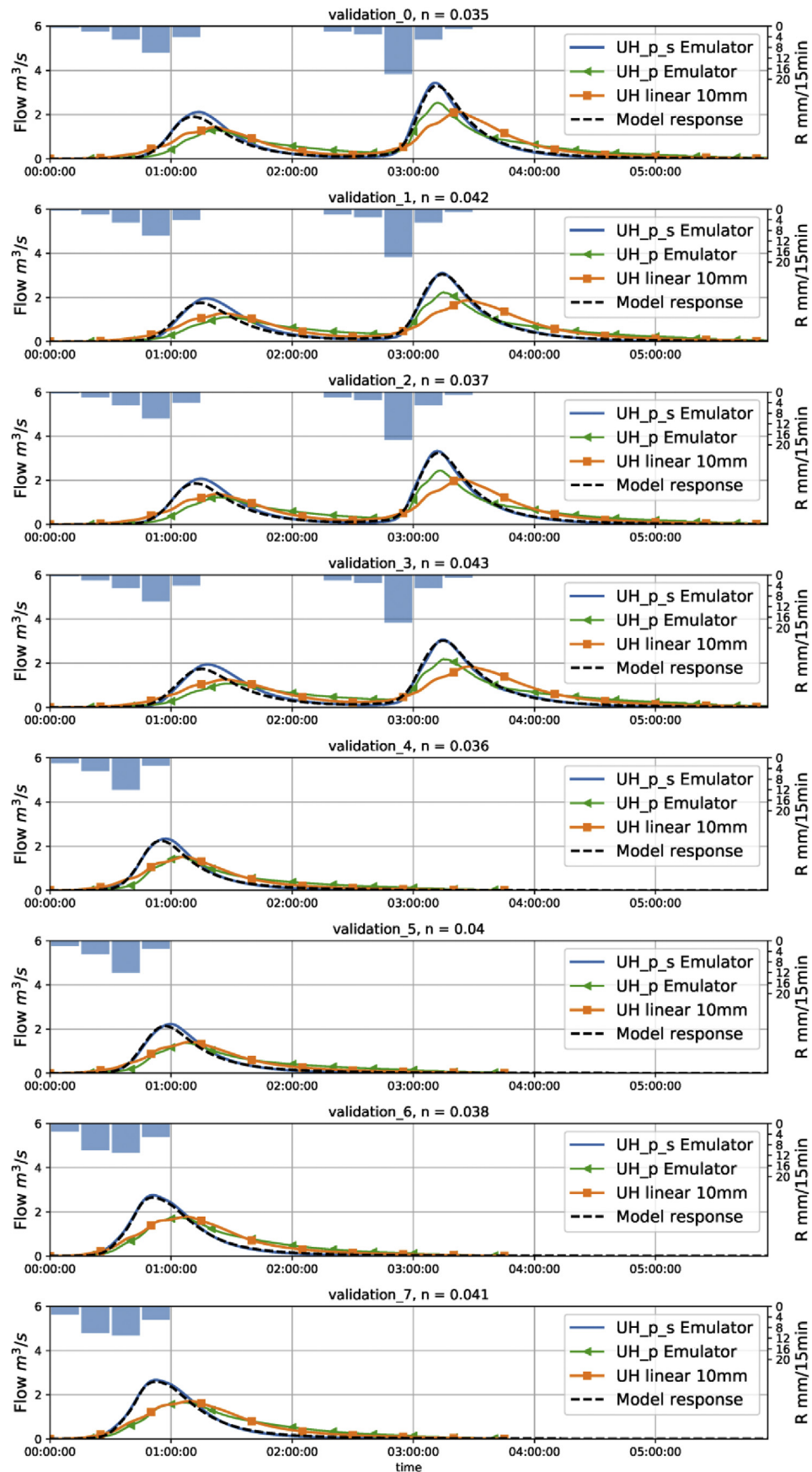


Fig. B.2. Validation comparisons emulator vs SWE_urban simulator.

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