HydroPol2D – Distributed Hydrodynamic and Water Quality Model: Challenges and Opportunities in Poorly-Gauged Catchments (Supplemental Material)

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I. Supplemental Material Organization

This supplemental material is organized as follows:

- Sec. II: Performance Indicators.
- Sec. III: HydroPol2D - Numerical Modeling Details.
  - Sec. III-A: Matrixwise Stormwater Runoff Mass Balance Equation.
  - Sec. III-B: Warm-up Process and Initial Values.
  - Sec. III-C: Conversion Factor from SWMM Wash-Off model to HydroPol2D.
  - Sec. III-D: Evapotranspiration Modeling.
  - Sec. III-E: Soil Recovery and Groundwater Replenishing.
- Sec. IV: Watershed Geometrical Indicators.
- Sec. V: Water Quality Calibration Module.
- Sec. VI: HydroPol2D - Detailed Results of Water Quality Modeling - Event 4.
- Sec. VII: HydroPol2D - Input data structure.

Since we here present matrixwise expressions that increase modeling speed by avoiding elementwise calculations, let us define some numerical operations and definitions, as follows:

Supplemental Materials' Notation: Italicized, boldface upper and lower case characters represent matrices and column vectors: a is a scalar, $\boldsymbol{a}$ is a vector and $\boldsymbol{A}$ is a matrix. Matrix $\boldsymbol{I}_n$ denotes an identity square matrix of dimension n-by-n, whereas $\boldsymbol{O}_{m\times n}$ and $\mathbf{1}_{m\times n}$ denotes a zero and one matrix with size m-by-n, respectively. The notations $\mathbb{R}$ and $\mathbb{R}_{++}$ denote the set of real and positive real numbers. The notations $\mathbb{R}^n$ and $\mathbb{R}^{m\times n}$ denote a column vector with n elements and an m-by-n matrix in $\mathbb{R}$. The element-wise product or Hadamard product is defined as $\boldsymbol{x} \circ \boldsymbol{y} := [x_1y_1, x_2y_2, \ldots, x_ny_n]^T$ multiplications. Similarly, the element-wise division or Hadamard is defined as $\boldsymbol{x} \oslash \boldsymbol{y} := [\frac{x_1}{y_1}, \frac{x_2}{y_n}, \ldots, \frac{x_n}{y_n}]^T$. The element-wise p power of a matrix $\boldsymbol{A}$, $(\boldsymbol{A}^{\circ p})$, with $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ and $p \in \mathbb{R}$ is given by $a_{i,j}^p$ for $i \in \mathbb{N}_{++}$, and $j \in \mathbb{N}_{++}$.

II. Performance Indicators

1) Nash-Sutcliffe-Efficiency

The Nash-Sutcliffe-Efficiency (NSE) metric is calculated in terms of the observed variable (e.g., generally flow discharge) and the modeled variable such that [1]:

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$$\mathrm{NSE} = 1 - \frac{\sum_{i=1}^{n}\left(y_{\mathrm{obs}}^{i} - y_{\mathrm{m}}^{i}\right)^2}{\sum_{i=1}^{n}\left(y_{\mathrm{obs}}^{i} - \overline{y_{\mathrm{obs}}^{i}}\right)^2} \tag{S1}$$

where y_{obs} is the observed or the assumed true variable, whereas y_{m} is the variable. The indexes herein expressed as i and n represent the time in which the observations were made and the number of observations, respectively. NSE ranges from $-\infty$ to 1 (inclusive), with negative values indicating that the observed mean has smaller squared error than the modeled results. Ideally, a NSE = 1 indicates a perfect match between modeled and observed values.

2) Coefficient of Determination

The coefficient of determination determines the correlation between the observations. It ranges from 0 to 1, with 1 corresponding to a perfect correlation between modeled and observed data, and can be calculated as:

$$r^2 = \left(\frac{\sum_{i=1}^{n}\left(y_{\mathrm{m}}^{i} - \overline{y_{\mathrm{m}}^{i}}\right)\left(y_{\mathrm{obs}}^{i} - \overline{y_{\mathrm{obs}}^{i}}\right)}{\sqrt{\sum_{i=1}^{n}\left(y_{\mathrm{m}}^{i} - \overline{y_{\mathrm{m}}^{i}}\right)^2 \sum_{i=1}^{i}\left(y_{\mathrm{obs}}^{i} - \overline{y_{\mathrm{obs}}}\right)^2}}\right)^2 \tag{S2}$$

3) Root-Mean-Square-Error

The Root-Mean-Square-Error (RMSE) index measures the average difference between predicted and observed variables and can be calculated as follows [2]:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_{m}^{i} - y_{\mathrm{obs}}^{i}\right)^2}{n}} \tag{S3}$$

4) PBIAS

The Percent bias (PBIAS) measures the average tendency of the modeled values to be larger or smaller than observations. PBIAS ranges from $-\infty$ to $+\infty$. Ideally, PBIAS should be zero, with positive values indicating overestimation bias, whereas negative values indicates model underestimation bias. PBIAS can be calculated as [3]:

$$\mathrm{PBIAS} \ = \frac{\sum_{i=1}^{n}\left(y_{\mathrm{obs}}^{i} - y_{\mathrm{m}}^{i}\right)}{\sum_{i=1}^{n} y_{\mathrm{obs}}^{i}} \tag{S4}$$

III. HydroPol2D - Numerical Modeling Extra Details

HydroPol2D is a numerical hydrodynamic and pollutant transport and fate model. A pseudo-code of the model is presented in Algorithm 1.

A. *Matrixwise Stormwater Runoff Mass Balance Equation*

The mass balance equation can be written as follows:

$$\frac{\mathrm{d}\boldsymbol{H}(t)}{\mathrm{d}t} = \boldsymbol{B}_i \circ \boldsymbol{I}(t) + \frac{1}{A}\boldsymbol{B}_Q \circ \boldsymbol{Q}(t) - \boldsymbol{F}(\boldsymbol{H}(t), \boldsymbol{F}_d(t)) - \boldsymbol{E}_{TR}(t) + \sum_{i=1}^{m}\left(\overbrace{\boldsymbol{B}_d(\boldsymbol{H}(t))\boldsymbol{Q}_{out}(\boldsymbol{H}(t))}^{\boldsymbol{Q}_{in}(\boldsymbol{H}(t))} - \boldsymbol{Q}_{out}(\boldsymbol{H}(t))\right) \tag{S5}$$

where $\boldsymbol{B}_i$ and $\boldsymbol{B}_Q \in \mathbb{R}^{n\times p}$ are boolean time invariant matrices representing cells that receive rainfall and inflow, respectively, $\boldsymbol{B}_d(\boldsymbol{H}(t)) \in \mathbb{R}^{n\times p}$ is the flow distribution time-variant matrix function derived from the celullar automata rules, $\boldsymbol{H}(t) \in \mathbb{R}^{n\times p}$ is the water surface depths, $\boldsymbol{I}(t) \in \mathbb{R}^{n\times p}$ is the rainfall intensity, $\boldsymbol{F}(\boldsymbol{H}(t), \boldsymbol{F}(t)) \in \mathbb{R}^{n\times p}$ is the infiltration rate, $\boldsymbol{F}_d \in \mathbb{R}^{n\times p}$ is the accumulated infiltration depth, $\boldsymbol{E}_{TR}(t) \in \mathbb{R}^{n\times p}$ is the evapotranspiration rate, $\boldsymbol{Q}_{in}(t)$ and $\boldsymbol{Q}_{out}(t) \in \mathbb{R}^{n\times p}$ are inflows and outflows from each cell, assuming a Von-Neumann squared grid, m is the the number of neighbour cells from a given cell, n and p represents the number of cells in Cartesian coordinates in the domain and t is a time index.

Expanding Eq. (S5) by a 1st order Taylor's approximation, we can derive an explicit numerical solution for the water surface due to overland flow problem neglecting high order, such that:

$$\boldsymbol{H}(t+\Delta t) = \overbrace{\boldsymbol{H}(t) + \Delta t\left(\boldsymbol{B}_i\boldsymbol{I}(t) + \frac{1}{A}\boldsymbol{B}_Q\boldsymbol{Q}(t) - \boldsymbol{F}(\boldsymbol{H}(t), \boldsymbol{F}_d(t), \boldsymbol{E}_{TR}) - \boldsymbol{E}_{TR}(t)\right)}^{\boldsymbol{H}_{ef}(t)} + \Delta t\sum_{i=1}^{m}\left(\boldsymbol{Q}_{in}^{i}(\boldsymbol{H}(t)) - \boldsymbol{Q}_{out}^{i}(\boldsymbol{H}(t))\right) \tag{S6}$$

where $\boldsymbol{H}_{ef}(t) \in \mathbb{R}^{n\times p}$ is the effective depth for overland flow routing. To solve Eq. (S6), we develop a weighted cellular automata approach using Manning's equation to estimate matrix $\boldsymbol{Q}_{out}$, and using topological relationships between cells, we

TABLE S1: Variable definitions, dimensions, and units, where n and p define the domain, and m represent the number of boundary cells per cell.

Class	Symbol	Description	Dimension	Units
Input Matrices and Data	$\boldsymbol{I}(t)$	Rainfall intensity	$\mathbb{R}^{n\times p}$	LT^{-1}
	$\boldsymbol{E}_{TR}(t)$	Evapotranspiration rate	$\mathbb{R}^{n\times p}$	LT^{-1}
	$\boldsymbol{Q}(t)$	Inflow hydrograph	$\mathbb{R}^{n\times p}$	L^{3}T^{-1}
	ω	Cell area	$\mathbb{R}$	L^2
	$\mathbb{C}$	Set of cells	N.A	N.A
	$\mathbb{O}$	Set of outlet cells	N.A	N.A
	$\mathbb{B}$	Set of domain borders	N.A	N.A
	Δx	Average cell width	$\mathbb{R}$	L
	Δt	Model time-step	$\mathbb{R}$	T
	α_1	Time-step coefficient for water quantity	$\mathbb{R}$	T
	α_2	Time-step coefficient for water quality	$\mathbb{R}$	T
	σ	Slope tolerance	$\mathbb{R}$	LL^{-1}
Infiltration model	$\boldsymbol{F}(t)$	Infiltration rate	$\mathbb{R}^{n\times p}$	LT^{-1}
	$\boldsymbol{F}_d(t)$	Infiltrated depth	$\mathbb{R}^{n\times p}$	L
Flood routing model	$\boldsymbol{H}(t)$	Water surface depth	a	L
	$\boldsymbol{B}_i$	Rainfall incidence matrix	a	N.A
	$\boldsymbol{B}_q$	Inflow hydrograph incidence matrix	a	N.A
	$\boldsymbol{B}_d(H(t))$	Flow distribution matrix	a	N.A
	$\boldsymbol{Q}_{in}(t)$	Inflows in each cell	$\mathbb{R}^{n\times p}$	L^{3}T^{-1}
	$\boldsymbol{Q}_{out}(t)$	Outflows in each cell	$\mathbb{R}^{n\times p}$	L^{3}T^{-1}
	$\boldsymbol{H}_{ef}(t)$	Effective depth for overland flow	$\mathbb{R}^{n\times p}$	L
Cellular Automata	**WSE**	Water surface elevation	$\mathbb{R}^{n\times p}$	L
	s_0^b	Outlet slope boundary condition	$\mathbb{R}$	L.L-1
	g	Gravity acceleration	$\mathbb{R}$	L^{3}T^{-2}
	$\boldsymbol{N}$	Manning's roughness coefficient	$\mathbb{R}^{n\times p}$	TL$^{-1/3}$
	Δh_{min}	Minimum assumed water level difference	$\mathbb{R}$	L
	$\Delta\boldsymbol{V}$	Available free volume within boundary cells	$\mathbb{R}^{n\times p\times(m+1)}$	L^3
	$\Delta\boldsymbol{H}_{ef}$	Available water depth within boundary cells	$\mathbb{R}^{n\times p\times(m+1)}$	L
	$\Delta\boldsymbol{V}_{min}$	Minimum intercell volume transfer	$\mathbb{R}^{n\times p}$	L^3
	$\Delta\boldsymbol{V}_{max}$	Maximum intercell volume transfer	$\mathbb{R}^{n\times p}$	L^3
	$\boldsymbol{\Omega}$	Weights for each direction	$\mathbb{R}^{n\times p\times m}$	N.A
	$\boldsymbol{V}_m$	Maximum outflow velocity per each cell	$\mathbb{R}^{n\times p}$	LT^{-1}
	$\boldsymbol{I}_{tot}^*$	Total intercell volume	$\mathbb{R}^{n\times p}$	L^3
	$\boldsymbol{V}_{min}$	Minimum intercell transferable volume	$\mathbb{R}^{n\times p}$	L^3
Build-up and wash-off	$\boldsymbol{\Phi}$	Wash-off rate	$\mathbb{R}^{n\times p}$	MT^{-1}
	$\boldsymbol{C}_1$	Build-up coefficient	$\mathbb{R}^{n\times p}$	ML^{-2}
	$\boldsymbol{C}_2$	Build-up exponent	$\mathbb{R}^{n\times p}$	T^{-1}
	$\boldsymbol{C}_3$	Wash-off coefficient	$\mathbb{R}^{n\times p}$	(LT^{-1})^{C_4}T^{-1}
	$\boldsymbol{C}_4$	Wash-off exponent	$\mathbb{R}^{n\times p}$	N.A
	$\boldsymbol{B}_{out}^i$	Mass of pollutant washed for direction i	$\mathbb{R}^{n\times p}$	M
	$\boldsymbol{W}_{out}^{tot}$	Sum of washed pollutant for all directions	$\mathbb{R}^{n\times p}$	M
	$\boldsymbol{B}$	Available mass of pollutant in each cell	$\mathbb{R}^{n\times p}$	M
	$\boldsymbol{C}(t)$	Instantaneous pollutant concentration	$\mathbb{R}^{n\times p}$	ML^{-3}'

derive $\boldsymbol{Q}_{in}(t)$ in terms of $\boldsymbol{Q}_{out}(t)$ by calculating $\boldsymbol{B}_d(\boldsymbol{H}(t))$. Details of how to solve the WCA2D model can be found in [4] and [5] and are described later in Algorithm 2.

B. Warm-Up Process and Initial Values for Modeling

Before starting the hydrodynamic simulations, a warm-up process was simulated to represent the initial conditions of water depths in the TPS and the initial mass of pollutants in the catchment. Initial tests indicated that simulating an event with a hydrograph in the channel inlet provides better warm-up depths in the channel than a rainfall simulation on the grid (i.e., water accumulates only in the channel). Thus, a constant hydrograph with a flow of 0.3 m^{3}s^{-1}for 24 hours was simulated at the beginning of the open stream (coordinates 202762.24; 7563794.99 UTM 23S shown in Fig. 5). This initial flow can represent an eventual base flow and clandestine sewage releases that are often released into the creek. The same inflow is also considered in rain-on-the-grid events. The downstream boundary condition of the domain was assumed to be the critical flow condition, and the outlet pixels were considered the two lowest elevation pixels on the domain boundary. The outlet represents a 25-m wide area with 2 pixels.

A different warm-up process was used to represent the initial conditions of the pollutant mass of the cells. Typically, build-up

Algorithm 1: Main Algorithm, where $\boldsymbol{\gamma}, \boldsymbol{\tau}, \boldsymbol{\theta}$, and $\boldsymbol{\beta}$ are time vectors and $\boldsymbol{F}_d$ is the accumulated infiltration depth. The details of all input data are described in Table S1 in the supplemental material section

input: Input maps and parameters from .TIFF and .xlsx files (i.e., Digital Elevation Model, Land Use and Land Cover Map) time, minimum and maximum time-step, stability method, outlet boundary cells, cells receiving rainfall, cells receiving inflow hydrograph, recording times for maps and for hydrograhps, outlet boundary condition type, outlet boundary condition slope, flag to correct water balance, flag to simulate water quality, antecedent dry days, flag do correct time-step
set: Hydrologic, Hydrodynamic, and Water Quality distributed parameters according to input maps
while $t <$ *Routing Time* **do**
  compute: Infiltration Capacity through Green-Ampt Model
  compute: Inflow Rate from rainfall, inflow hydrograph and neighbor cells outflow
  compute: Infiltration Rate = min(Infiltration Capacity, Inflow Rate)
  compute: Cellular Automata Weighted System from and Algorithm 2 and find $\boldsymbol{Q}_{out}, \boldsymbol{H}_{ef}, \boldsymbol{I}^*_{tot}$
  compute: Build-up and Wash-off problem and determine spatial washed mass of pollutant and concentration
  if $t \in \boldsymbol{\gamma}$ **then**
    Check stability criteria and refresh time-step
  end if
  compute: Disaggregation of inflow and rainfall to the time-step used
  if $t \in \boldsymbol{\tau}$ **then**
    Resize all state matrices to the new coordinate system
  end if
  compute: 2-D discretized solution of mass balance of stormwater runoff and pollutant mass
  compute: Water Balance Error
  if *Water Balance Error* $>$ *Tolerance* **then**
    Redistribute water balance error in the inflow cells
  end if
  if $t \in \boldsymbol{\theta}$ **then**
    Save maps of water surface depths and pollutant concentration
  end if
  if $t \in \boldsymbol{\beta}$ **then**
    Save hydrographs and pollutugraphs at the outlet
  end if
end while
output: Export Hydrographs, Pollutographs, .TIFF maps, and GIFs of water surface elevations and pollutant distributions over time

models assume that the accumulation of pollutants in the catchment is uniform for each type of land use [6]. Therefore, in a scenario in which the entire catchment had been washed previously (e.g., a relatively large storm), for an accumulated mass equivalent to an ADD, permeable and impermeable areas would deterministically have the same accumulated mass of pollutants in each cell. A previous simulation was performed with ADD $= 10$ days and rainfall of RP $= 1/12$ years to determine more realistic conditions for the accumulation of pollutants, which is equal to the rainfall event with a probability exceedance relative to the period of 1 month, assuming a duration of 60 min. The hypothesis is that this event theoretically represents an initial condition of the catchment not fully washed, where a pattern of accumulation is established on the streets, buildings, and channels.

C. Conversion Factor from SWMM to HydroPol2D

Converting wash-off parameters from concentrated modeling to distributed modeling requires a conversion factor f_c that can be estimated as:

$$f_c = \left(\frac{3600 \times 1000}{\Delta x^2}\right)^{C_3^*} \tag{S7}$$

where Δx is the pixel size (m) and f_c converts C_3^*, the wash-off coefficient for concentrated modeling, to C_3, the wash-off coefficient for distributed modeling.

The application of the aforementioned equation for different pixel resolutions and C3 and C4 values are shown in the following figure:

Algorithm 2: Cellular automata pseudocode

input: Cell elevations, initial surface water depths, $\boldsymbol{N}$, $\boldsymbol{H}_0$, Δt, Δx, s_0^b, c, Velocity to the steepest direction $\boldsymbol{V}_m$, Intercell Volume $\boldsymbol{I}_{tot}$ previous outflow volumes, Minimum water depth Δh_{min} Set of cells $\mathbb{C}$, Outlet cells $\mathcal{O}$, Domain borders $\mathbb{B}$
for *i = 1 to m* **do**
  compute: $\Delta \boldsymbol{H}_{ef,i} = \mathbf{WSE} - \mathbf{WSE}_i,\ \Delta \boldsymbol{H}_{ef} \in \mathbb{R}^{n \times p \times (m+1)}, \mathbf{WSE} \in \mathbb{R}^{n \times p}$
end for
if *Outlet Type = 1* **then**
  compute: $\Delta \boldsymbol{H}_{ef,m+1} = s_0^b \Delta x\ \forall\ \mathbb{C} \in \mathbb{O}$
else
  compute: $\Delta \boldsymbol{H}_{ef,m+1} = \boldsymbol{H}_{ef}^{\circ -1/6} g^{0.5} \circ \boldsymbol{N}\ \forall\ \mathbb{C} \in \mathbb{O}$
end if
$\boldsymbol{H}_{ef,m+1} \leftarrow 0\ \forall\ \mathbb{C} \in \mathbb{B}$
$\boldsymbol{\Delta H}_{ef} \leftarrow 0\ \forall\ \Delta \boldsymbol{H}_{ef} \leq \Delta h_{min}$
compute: $\Delta \boldsymbol{V} = A \Delta \boldsymbol{H}_{ef},\ \Delta \boldsymbol{V} \in \mathbb{R}^{n \times p \times (m+1)}$
$\Delta \boldsymbol{V} \leftarrow c,\ \forall\ \Delta \boldsymbol{V} = 0$
compute: $\Delta \boldsymbol{V}_{max} = \max(\Delta \boldsymbol{V}),\ \Delta \boldsymbol{V}_{max} \in \mathbb{R}^{n \times p}$
compute: $\Delta \boldsymbol{H}_{ef,max} = \max(\Delta \boldsymbol{H}_{ef}),\ \Delta \boldsymbol{H}_{ef,max} \in \mathbb{R}^{n \times p}$
compute: $\Delta \boldsymbol{V}_{min} = \min(\Delta \boldsymbol{V}),\ \Delta \boldsymbol{V}_{min} \in \mathbb{R}^{n \times p}$
compute: $\boldsymbol{\Omega} = (\Delta \boldsymbol{V}_{tot} + \Delta \boldsymbol{V}_{min}) \oslash \Delta \boldsymbol{V},\ \boldsymbol{\Omega} \in \mathbb{R}^{n \times p \times (m+1)}$
compute: $\boldsymbol{\Omega}_{max} = \max(\boldsymbol{\Omega}),\ \boldsymbol{\Omega}_{max} \in \mathbb{R}^{n \times p}$
compute: $\boldsymbol{V}_m = \min(\sqrt{g} \boldsymbol{H}_{ef}^{\circ 0.5}, \boldsymbol{N} \oslash \max(\boldsymbol{H}_{ef} - \boldsymbol{H}_0)^{\circ 2/3} \circ (\boldsymbol{H}_{ef,max}(1/\Delta x))^{\circ 0.5}),\ \boldsymbol{V}_m \in \mathbb{R}^{n \times p}$
compute: $\boldsymbol{I}_{tot}^* = \min(\omega \boldsymbol{H}_{ef}, (\Delta x/\Delta t) \boldsymbol{V}_m \circ \boldsymbol{H}_{ef}, \boldsymbol{I}_{tot}^p + \Delta \boldsymbol{V}_{min}),\ \boldsymbol{I}_{tot}^* \in \mathbb{R}^{n \times p}$
compute: $\boldsymbol{I}_{tot}^* \leftarrow \mathrm{sum}_3(\boldsymbol{\Omega} \circ \boldsymbol{I}_{tot}^*)$
compute: $\boldsymbol{Q}_{out} = 1/(\Delta t A) \boldsymbol{I}_{tot}^*,\ \boldsymbol{Q}_{out} \in \mathbb{R}^{n \times p \times m}$
compute: $\boldsymbol{H}_{ef} \leftarrow \boldsymbol{H}_{ef} - (1/\omega) \boldsymbol{I}_{tot}^*$
output: $\boldsymbol{Q}_{out},\ ,\boldsymbol{H}_{ef},\ \boldsymbol{I}_{tot}^*$

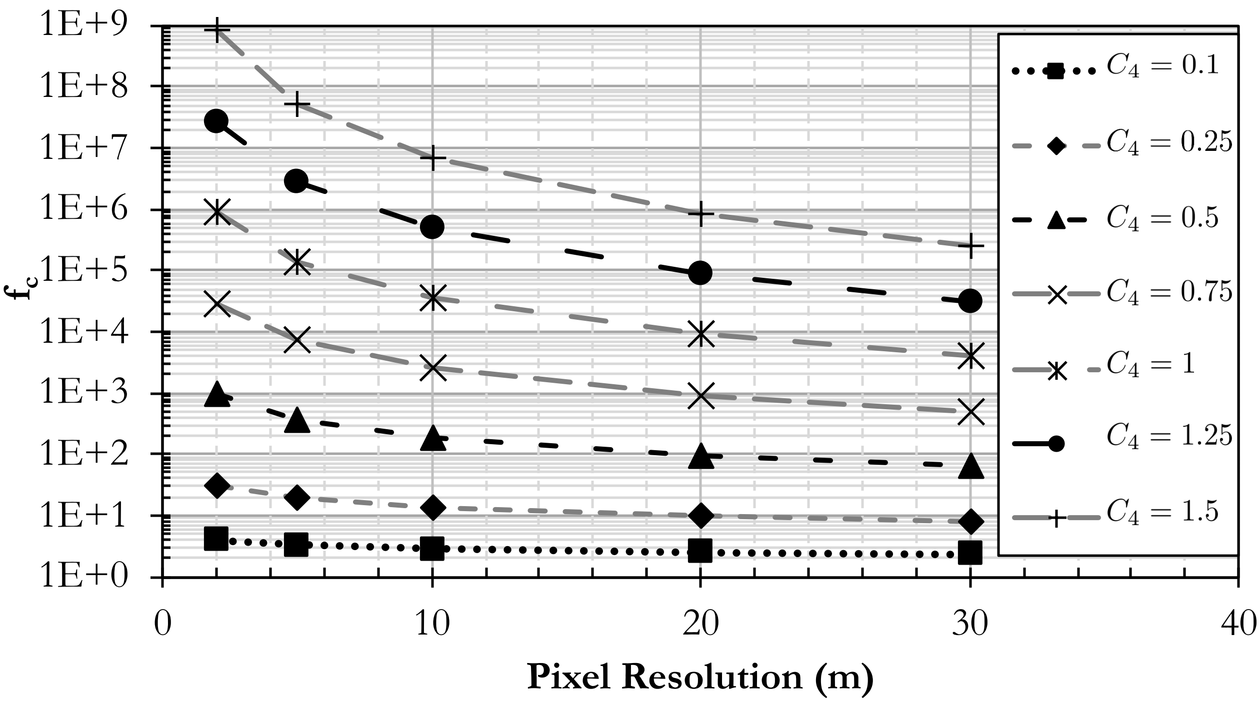

Fig. S1: Conversion factor from SWMM to HydroPol2D wash-off parameters.

D. Evapotranspiration Modeling

Although not often considered in rapid and intense flood modeling, evapotranspiration (ET) is important in continuous simulation models. ET is the process of evaporation in the soil-plant system transferring water to the atmosphere [7]. Several models are available to estimate the reference evapotranspiration (E_{to}) flux in monthly [8], daily [9], or even sub-daily scale [10]. The input data required to simulate it varies, and the proper selection of the model should be done according to data availability at the catchment. In this paper, we use the Penman-Monteith model, which requires spatialized data of wind speed at 2m from surface, relative humidity, temperature and radiation. The latter, however, can be indirectly estimated with the method presented as follows. Let (i, j) collect the central coordinate of a specific cell. The rate of evapotranspiration can be estimated as:

$$e_{to}^{i,j} = \frac{0.408 \times \Delta^{i,j}(r_n^{i,j} - g^{i,j}) + \gamma^{i,j} \times \frac{900}{t^{i,j}+273} \times u_2^{i,j} \times (e_s^{i,j} - e_a^{i,j})}{\Delta^{i,j} + \gamma^{i,j} \times (1 + 0.34 \times u_2^{i,j})} \tag{S8}$$

where $\Delta^{i,j}$ = slope vapor pressure curve ($\mathrm{kPa°C^{-1}}$), $\mathrm{r_n^{i,j}}$ = net radiation at the crop surface ($\mathrm{MJm^{-2}day^{-1}}$), $g^{i,j}$ = soil heat flux density ($\mathrm{MJm^{-2}day^{-1}}$), $\gamma^{i,j}$ = psychrometric constant constant ($\mathrm{kPa°C^{-1}}$), $t^{i,j}$ = mean daily air temperature at $2\ \mathrm{m}$ height in ($°\mathrm{C}$), $u_2^{i,j}$ = wind speed at 2 m height ($\mathrm{ms^{-1}}$), $e_s^{i,j}$ = saturation vapor pressure (kPa) and $e_a^{i,j}$ = actual vapor pressure (kPa).

This model is programmed to be implemented with all the inputs required in Penman Monteith ($\Delta^{\mathrm{i,j}}$, $\mathrm{r_n^{i,j}}$, $\mathrm{g^{i,j}}$, $\gamma^{\mathrm{i,j}}$, $\mathrm{u_2^{i,j}}$, $\mathrm{e_s^{i,j}}$, $\mathrm{e_a^{i,j}}$ and $\mathrm{t^{i,j}}$), but due to the lack of sub-day data in several regions, we applied methods to simplify the database and reduce the number of input data. To this end, parameters such as $\gamma^{\mathrm{i,j}}$, $\mathrm{r_n^{i,j}}$, $\mathrm{e_s^{i,j}}$ and $\mathrm{e_a^{i,j}}$ can be estimated with the input of spatially referenced areas, altitudes, temperatures for each watershed cell and, considering, some coefficients according to the location and the day of the year [11], [12]. The $\gamma^{\mathrm{i,j}}$ variable can be quantified by establishing a relationship with atmospheric pressure (S9), which will only require the altitude data that is extracted from the digital elevation model ($\mathrm{z^{i,j}}$) (S10).

$$\gamma^{i,j} = 0.665 \times 10^{-3} \times p_{atm}^{i,j} \tag{S9}$$

$$p_{atm}^{i,j} = 101.3 \times \left(\frac{293 - 0.0065 \times \mathrm{z^{i,j}}}{293}\right)^{5.26} \tag{S10}$$

where $\mathrm{p_{atm}^{i,j}}$ = atmospheric pressure (kPa) and $\mathrm{z^{i,j}}$ = altitude (meters).

The simplifications made for $\mathrm{e_s^{i,j}}$ (kPa) (S11), $\mathrm{e_a^{i,j}}$ (kPa) (S12), $\Delta^{\mathrm{i,j}}$ ($\mathrm{kPa}°C^{-1}$) (S13), and $\mathrm{r_n^{i,j}}$ ($\mathrm{MJm^{-2}day^{-1}}$) (S14) are presented below. The only input required for them are $\mathrm{g^{i,j}}$ ($\mathrm{MJm^{-2}day^{-1}}$), day of the year ($\mathrm{d}$) ($1$ to $366 \in \mathbb{N}_{++}$), latitude ($\phi^{\mathrm{i,j}}$) (rad) and maximum ($\mathrm{t_{max}^{i,j}}$) ($°C$), minimum ($\mathrm{t_{min}^{i,j}}$) ($°C$) and average temperatures ($\mathrm{t^{i,j}}$) ($°C$).

$$e_s^{i,j} = 0.6108 \times \exp\left[\frac{17.27 \times t^{i,j}}{t^{i,j} + 237.3}\right] \tag{S11}$$

$$e_a^{i,j} = 0.61 \times \left(\frac{17.27 \times t_{min}^{i,j}}{t_{\mathrm{min}}^{i,j} + 237.3}\right) \tag{S12}$$

$$\Delta^{i,j} = \frac{4098 \times \left[0.6108 \times \exp\left(\frac{17.2 \times t^{i,j}}{t^{i,j}+237.3}\right)\right]^2}{t^{i,j} + 237.3} \tag{S13}$$

$$r_n^{i,j} = r_{ns}^{i,j} - r_{nl}^{i,j} \tag{S14}$$

where $\mathrm{r_{ns}^{i,j}}$ = short-wave radiation ($\mathrm{MJm^{-2}day^{-1}}$), expressed in following equation (S15) and $\mathrm{r_{nl}^{i,j}}$ = long-wave radiation ($\mathrm{MJm^{-2}day^{-1}}$), later detailed in (S21).

$$r_{ns}^{i,j} = (1 - \alpha) \times r_s^{i,j} \tag{S15}$$

where $\mathrm{r_s^{i,j}}$ = incident solar radiation ($\mathrm{MJm^{-2}day^{-1}}$) (S16) and α = 0.23, coefficient of the albedo for culture referee (grass). Note that α can change according to the land cover in the watershed. Therefore, r_s can be calculated as:

$$r_s^{i,j} = k_{rs} \times r_a^{i,j} \times \sqrt{(t_{max}^{i,j} - t_{min}^{i,j})} \tag{S16}$$

where $\mathrm{r_a^{i,j}}$ = solar radiation at the top of the atmosphere ($\mathrm{MJm^{-2}day^{-1}}$) (S17) and $\mathrm{k_{rs}}$ = coefficient of 0.16 to continental areas and 0.19 to coastal areas. The solar radiation, however, is a periodic function of ϕ and is related to the relative distance between the sun and the surface, such that:

$$r_a^{i,j} = \frac{118.08}{\pi} \times d_r^{i,j} \times \left[w_s^{i,j} \times \sin(\phi^{i,j}) \times \sin(\delta^{i,j}) + \cos(\phi^{i,j}) \times \cos(\delta^{i,j}) \times \sin(w_s^{i,j}) \right] \tag{S17}$$

where $\mathrm{d}_\mathrm{r}^{\mathrm{i,j}}$ = inverse relative distance between Earth and Sun (rad) (S18), $\mathrm{w}_\mathrm{s}^{\mathrm{i,j}}$ = sunrise angle (rad) (S19) and $\delta^{\mathrm{i,j}}$ = solar declination (rad) (S20). We can estimate d_r as a periodic function of d, such that:

$$d_r^{i,j} = 1 + 0.33 \times \cos\left(\frac{2 \times \pi}{365} \times \mathrm{d}\right) \tag{S18}$$

Moreover, w_s from (S17) is a function of the latitude and δ, such that:

$$w_s^{i,j} = \frac{\pi}{2} - \mathrm{arctg} \times \left[\frac{-\tan(\phi^{i,j}) \times \tan(\delta^{i,j})}{(1 - [\tan(\phi^{i,j})]^2 \times [\tan(\delta^{i,j})]^2)^{0.5}} \right] \tag{S19}$$

if $(1 - [\tan(\phi^{\mathrm{i,j}})]^2 \times [\tan(\delta^{\mathrm{i,j}})]^2) \leq 0$, we use $1\mathrm{e}-5$. Variable δ can be estimated as:

$$\delta^{i,j} = 0.409 \times \sin\left(\frac{2}{\pi} \times \mathrm{d} - 1.39\right) \tag{S20}$$

$$r_{nl}^{i,j} = \sigma \times \left[\frac{(t_{max}^{i,j} + 273.16)^4 + (t_{min}^{i,j} + 273.16)^4}{2} \right] \times (0.34 - 0.14 \times \sqrt{(e_a^{i,j})}) \times \left(1.35 \times \frac{r_s^{i,j}}{r_{so}^{i,j}} - 0.35\right) \tag{S21}$$

where σ = 4.903×10^{-9} ($\mathrm{MJm^{-2}day^{-1}}$) and $\mathrm{r}_{\mathrm{so}}^{\mathrm{i,j}}$ = incident solar radiation without clouds ($\mathrm{MJm^{-2}day^{-1}}$), resulting in:

$$r_{so}^{i,j} = (0.75 + 2 \times 10^{-5} \times \mathrm{z}^{\mathrm{i,j}}) \times r_a^{i,j} \tag{S22}$$

More background and rationale of these methods can be found in [12].

E. Soil Recover and Groundwater Replenishing

Three hydrological processes are assumed to occur in the soil media. The evapotranspiration and sub-surface drainage reduce the water content in the media, whereas infiltration from upper zone increases it. We focus here on the methods to estimate sub-surface exfiltration rate (f_g), which depends on the replenishing rate k_r and on the uppermost layer depth l_u, written as [13]:

$$k_r = \frac{\sqrt{k_{sat}/25.4}}{75} \tag{S23}$$

$$t_r = \frac{4.5}{\sqrt{k_{sat}/25.4}} \tag{S24}$$

$$l_u = 4\sqrt{k_{sat}/25.4} \tag{S25}$$

where k_r = replenishing rate (1/h), t_r = recovery time (h), and l_u = uppermost layer depth (m).

From previous equations, we can infer that the sub-surface exfiltration rate is given by:

$$f_g = (\theta_{sat} - \theta_i) k_r l_u 1000 \tag{S26}$$

where f_g = sub-surface exfiltration rate (mm/h), θ_{sat} = saturated soil content $(-)$, and θ_i = initial soil content $(-)$. Therefore, f_g is a constant sub-surface exfiltration rate applied in the water balance equation.

F. Interpolation of Rainfall ETP and Climatological Forcing

HydroPol2D allows interpolating spatially distributed input data using the Inverse-Distance-Weightning method [14], which is calculated as follows. Given a n_s number of stations with recorded values, we store the station values for a given time t in $\boldsymbol{z_s}(t) = [z_s^1(t),\ z_s^2(t), \dots z_s^{n_s}(t)]^T$. The stations are located at known projected coordinates x and y described by vectors $\boldsymbol{x_s}$ and $\boldsymbol{y_s}$, respectively. We apply the IDW method [14] by calculating the p-norm (i.e., projected distance for a euclidean norm) between each point of the meshgrid and the stations.

$$\hat{z}(\mathbf{x_s}, \mathbf{y_s}) = \frac{\sum_i^{n_c} w_i z_s^i}{\sum_i^n w_i},\ w_i = ||(\mathbf{x_s}, \mathbf{y_s}) - (\mathbf{x_i}, \mathbf{y_i})||_2^{-\beta} \tag{S27}$$

where n_c is the number of cells in the catchment, β is the weighting factor and is typically asssumed equals 2 to represent the Euclidean distance.

IV. Watershed Geometrical Indicators

A. Compactness Coefficient

The compactness coefficient relates the perimeter of the catchment and a perimeter of a circle with the same area such that:

$$k_c = \frac{0,28P}{\sqrt{A}} \tag{S28}$$

where P is the perimeter of the catchment and A is its area.

B. Form Factor

It is the relationship between the average width of the catchment (W) and the length of the catchment axis (L) (from the mouth to the farthest point in the area). The average width of the basin is typically determined by geoprocessing software. However, in the developed model, this width is estimated as follows:

$$\bar{L} = \sqrt{W^2 + H^2} \tag{S29}$$

where W and H are the largest $x - x$ length, and $y - y$ length in the 2-D spatial domain, respectively.

Therefore, the factor form is given by:

$$K_f = \frac{A}{\bar{L}} \tag{S30}$$

C. Circularity Index

The circularity index is the ratio between the catchment area and the correspondent perimeter of a circle with the same perimeter such that:

$$IC = 12,57\frac{A}{P^2} \tag{S31}$$

V. Water Quality Calibration Module

The decision variables for the optimization problem are the wash-off coefficients C_3 and C_4 and the problem is solved with the genetic algorithm for a 40 generation and population size of 100. The build-up coefficients C_1 and C_2 were not used in the calibration since the initial mass of salt is known. Let x be the decision vector collecting the optimized water quality parameters, such that $x = [C_3^{\mathrm{opt}}, C_4^{\mathrm{opt}}]^T$. Let $\boldsymbol{x}_l$ collect the lower boundary conditions of C_3 and C_4, such that $\boldsymbol{x}_l = [C_3^l, C_4^l]^T$. Similarly, let $\boldsymbol{x}_m$ collect upper bounds of the water quality parameters, such that $\boldsymbol{x}_m = [C_3^m, C_4^m]^T$. We want to formulate a calibration optimization problem such that the root mean square error (RMSE) between the observed solute concentration and modeled solute concentration is minimized. Therefore, we can write the objective function as follows:

$$\mathrm{OF} = \mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(C_{mod}^i - C_{obs}^i\right)^2}{n}} \tag{S32}$$

where C_{mod} and C_{obs} are the modeled and observed solute concentrations and n is the number of concentration observations.

The inputs for the optimization problem are:

- Hyetograph
- Watershed Parameters
- Observed Pollutograph (i.e., pollutant concentration)

The algorithm developed can also work with equality and inequality constraints. These are defined by matrices $\boldsymbol{A}_{\mathrm{eq}}$, $\boldsymbol{B}_{\mathrm{eq}}$, and $\boldsymbol{A}$, $\boldsymbol{B}$. Therefore, we can formally describe the optimization problem as follows:

$$\begin{aligned} &\min_{C_3, C_4} \text{Eq. (S32)} \\ \\ \text{s.t.}\quad &\text{HydroPol2D Dynamics} \\ &\boldsymbol{A}_{\mathrm{eq}}\boldsymbol{x} = \boldsymbol{B}_{\mathrm{eq}} \\ &\boldsymbol{A}\boldsymbol{x} \le \boldsymbol{B} \\ &\boldsymbol{x}_l \le \boldsymbol{x} \le \boldsymbol{x}_m \end{aligned} \tag{S33}$$

In Matlab, several solvers can be used to solve the previous equation (e.g., global search, pattern search. In this paper, we used the genetic algorithm solver. Since the problem is non-linear and non-convex, we aimed to provide relatively enough number of population and generation in the simulation to try catching global solutions. We assumed a 100-population and 40-generations in the modeling for both calibration, that is, for events with 0.5° and 2° slopes.

The optimized results for events with 0.5° are shown in Fig. S2. The resulting water quality parameters from the optimization simulation are $C_3^{\mathrm{opt}} = 9036.83813876743$ and $C_4^{\mathrm{opt}} = 0.243545935909623$.

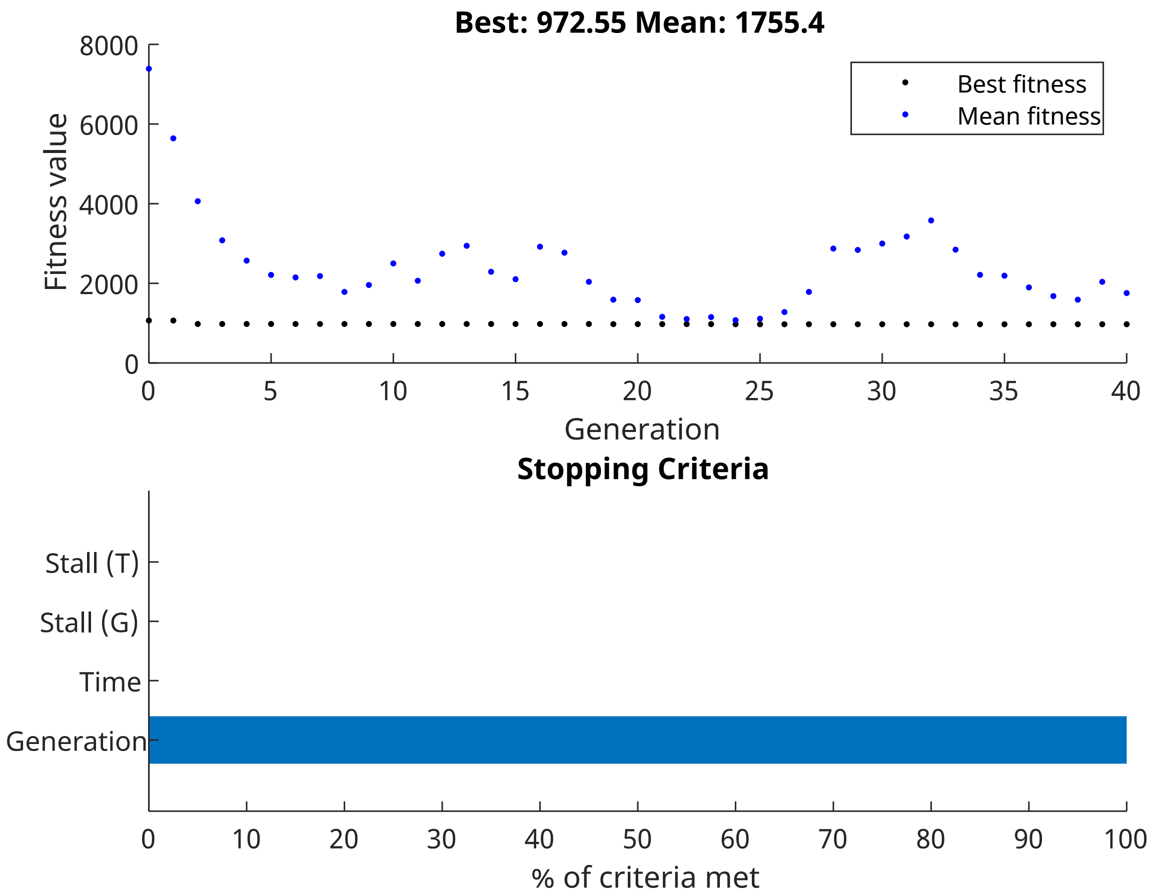

Fig. S2: Optimization Summary for Events with 0.5° slope. Results obtained using the genetic Algorithm to minimize the RMSE (mg/L) between the modeling and the observed solute concentrations

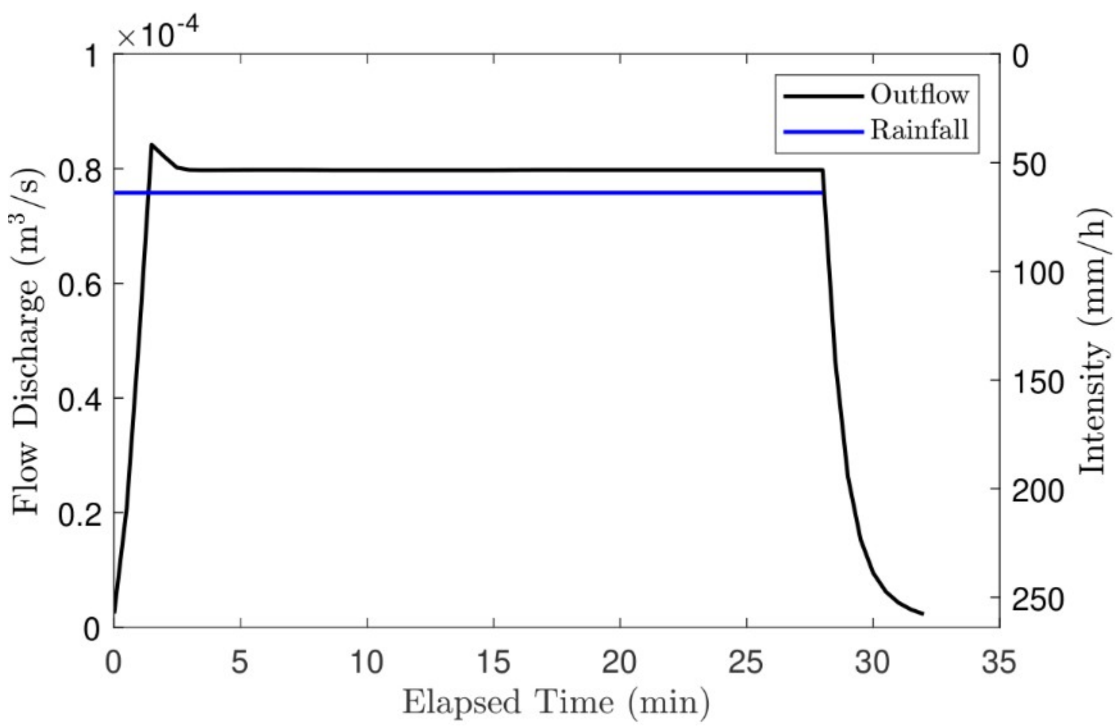

Fig. S3: Outlet hydrograph and Rainfall Intensity

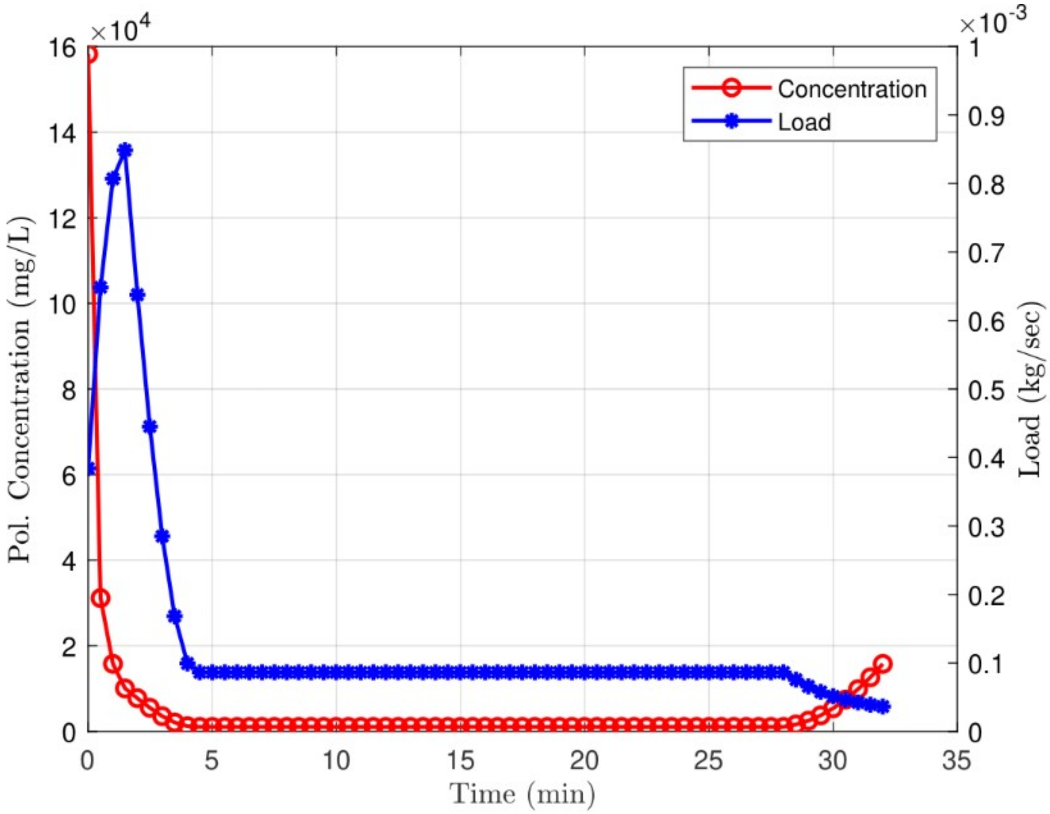

Fig. S4: Pollutograph and Load of diluted salt.

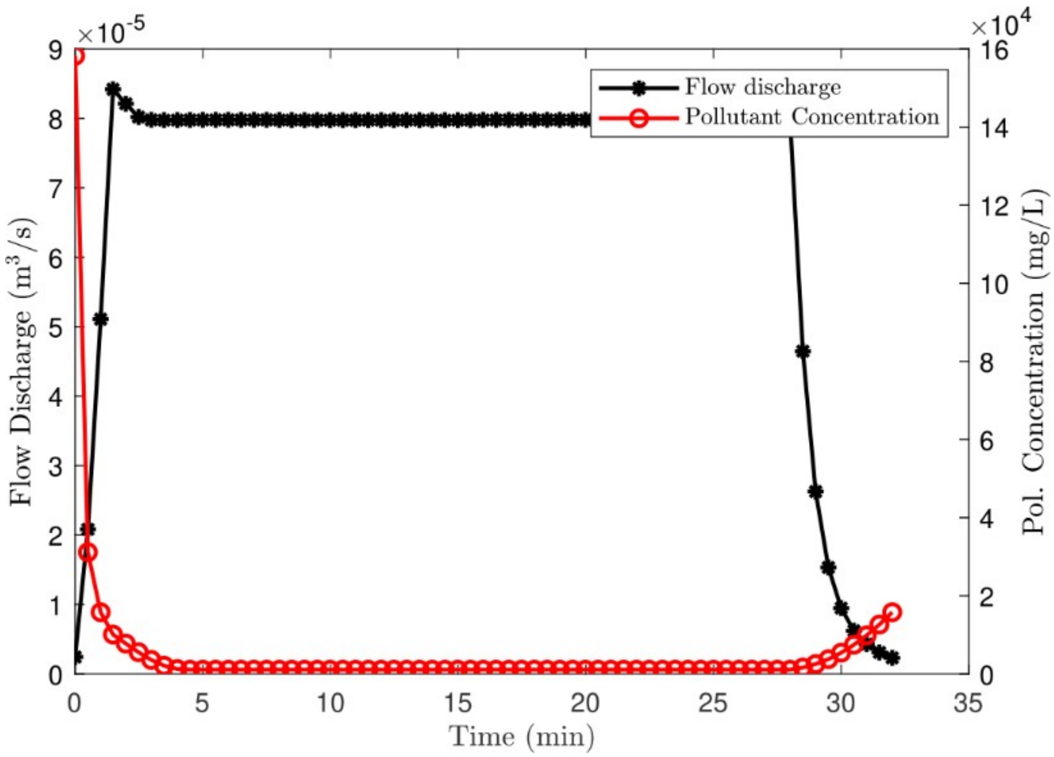

Fig. S5: Hysteresis effect where the peak of the concentration occurs before the flow discharge peak.

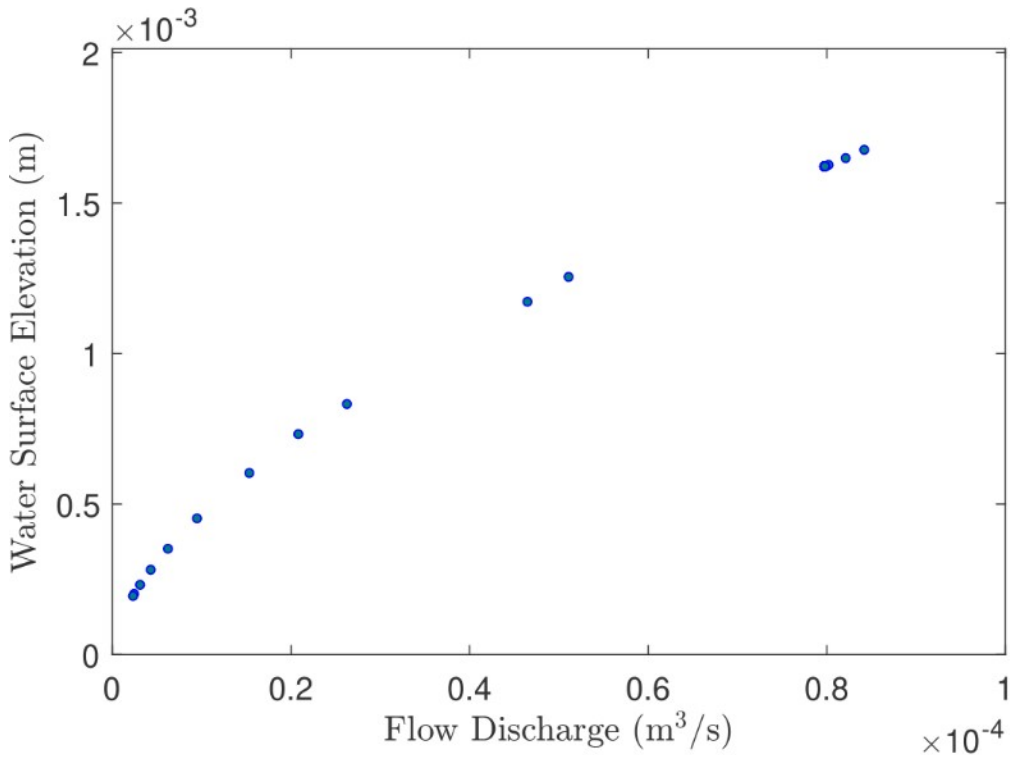

Fig. S6: Rating Curve at the outlet where the flow discharge is known for each stage.

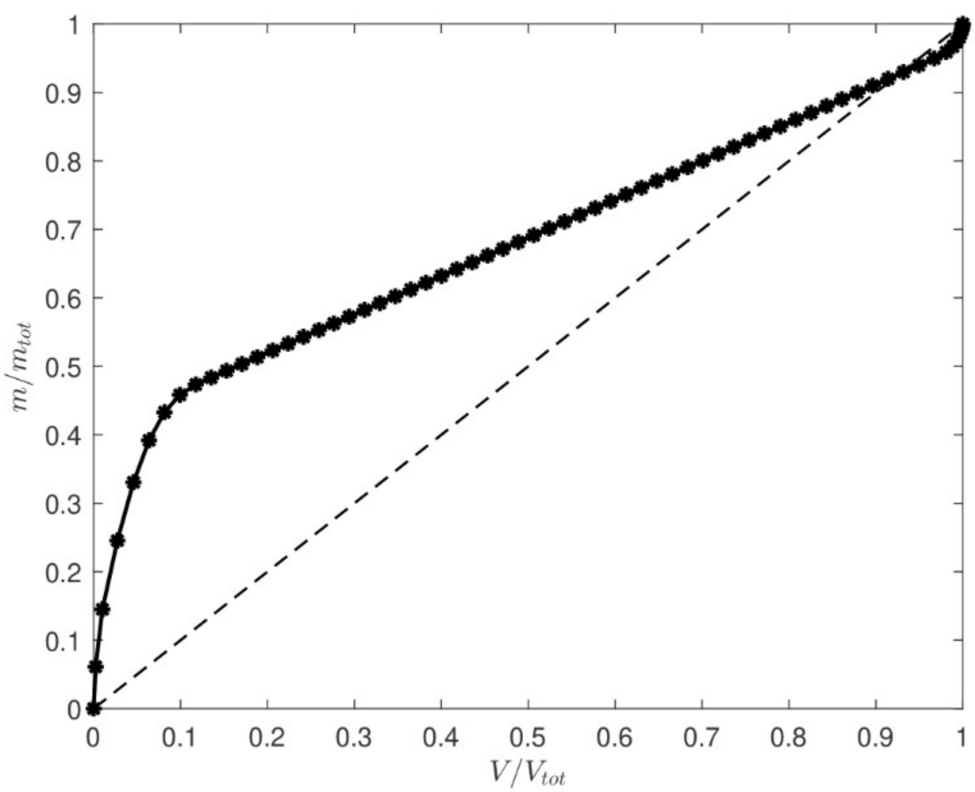

Fig. S7: M(V) Curve relating normalized runoff volume and normalized pollutant mass.

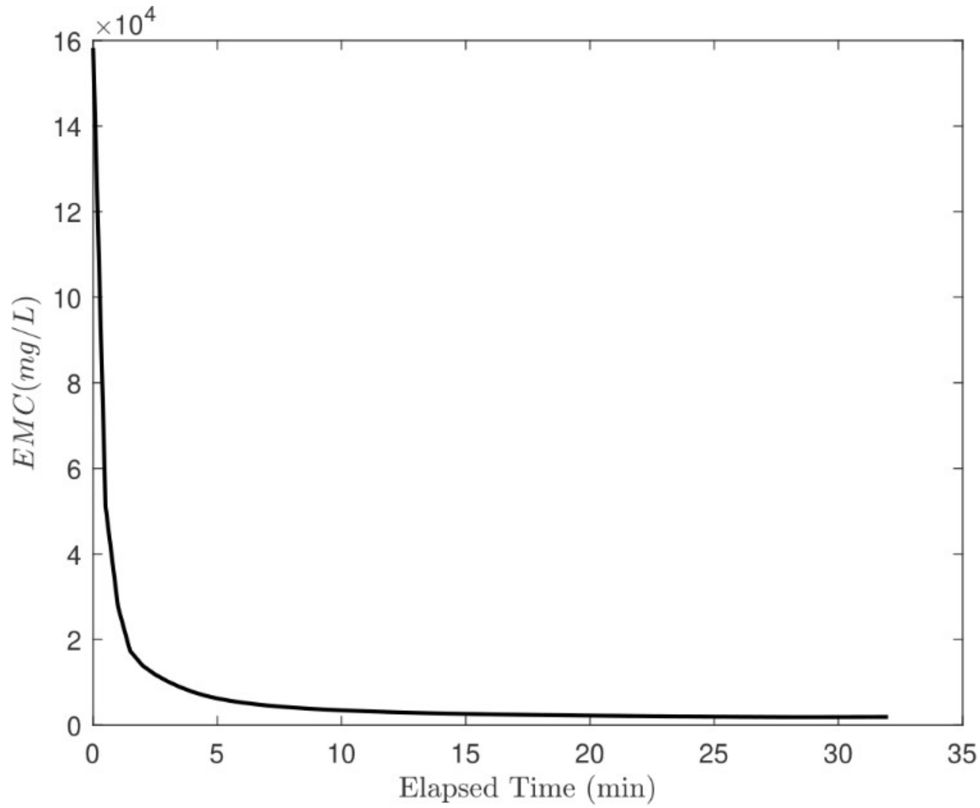

Fig. S8: EMC Curve relating the EMC variation with time.

VI. Detailed Results of Water Quality Modeling - Event 4

In the HydroPol2D model, users can access detailed reports, summary figures, and GIF files with spatial states shown in time. In this section, we show the HydroPol2D automatic results generated from the post-processing codes. The following graphs show (i) hydrographs and Rainfall, (ii) Concentrations and loads, (iii) Discharges and Concentrations, (iv) rating curve, (v) M(V) Curve, (vi) EMC variation with time. In addition to graphs, as mentioned above, all data are also saved and exported in .csv files. Finally, GIFs and .tifs from spatial data are generated and shown automatically on the screen.

VII. HydroPol2D - Input data structure

For the HydroPol2D input data structure, we use .xlsx sheets to facilitate the procedure of feeding the model with input data. In Fig. S9 is shown a general view of the general input data structure. Here, we briefly explain each input data section:

1) Running Control:this section defines the time-steps for each sub-component of the model. In addition, it defines the running control, that is, the beginning and end of the simulation. This section also includes the parameters of the CFL stability criteria.
2) General Flags: This section defines the model options allowed in HydroPol2D. Each value equals 1 indicates that a condition is implied in the model (e.g., $flag\_rainfall = 1$ means that rainfall is being model, whereas $flag\_rainfall = 0$ indicates that no infiltration is modeled). The user defines the modeling conditions, e.g., rainfall (lumped or distributed), model hydrodynamic structure (kinematic or diffusive), consideration of ETP calculation, among others.
3) Matricial Variables: This is used if and only if an inflow hydrograph is used and allows the model to use a different one to avoid calculation in large matrices. Therefore, the model change the size of the matrices according to the wet cells that were derived from the inflow hydrograph propagation.
4) Watershed Inputs and Cuts: Definition of the outlet conditions. The outlet type defines which outlet boundary condition is used, that is, normal flow or critical flow. Also, if the user wants to define more outlets than the ones already defined by finding the cells with the smallest elevation, she can define it by choosing the n_outlets_data. This variable adds more outlets near to the ones already defined by the topology.
5) Maps and Plots Control: In this section, we define the time that the spatial and source variables are recorded. Users must be aware of memory and processing capabilities of their machines such that the recording of the spatial variables is sufficiently accurate, but yet suitable for their computer memory. It also defines the threshold to map the variables.
6) CA Parameters: Definition of some thresholds for cellular automata.
7) Abstractions: coordinates definition to establish an initial area of interest to improve modeling performance (applicable

for warm-up procedure and CPU execution). The model allows the user to delineate a region of interest, defined by a squared region, using the local x and y coordinates (units or pixels) taken from the center of the left upper corner

8) Water Quality Inputs: here are defined the water quality model parameters.
9) DEM Smoothing, Imposemin, Resample, Bathymetry: Optional procedures to treat the used digital elevation model.
10) Directories: Here are defined the directories for the DEM, land use and land cover, soil type, warm-up depths (if apply), among others. Please note that Matlab must have access to these folders.
11) Human Instability: Here are the set variables to calculate humans stability against drag forces.
12) Observation Points: In this section are defined the coordinates for all the relevant point within the study area to analyze the modeling results and derive hydrographs, stages, and other charts related to the coordinates.
13) Synthetic Design Storms: The user can define synthetic storms with varied return periods, durations, and time intervals. Two options are allowed: Alternated Blocks and Huff rainfall distributions. However, in both cases users need to have a Sherman-type IDF curve.
14) Satellite Or Radar Rainfall: The HydroPol2D is capable to read rainfall data in .TIFF format, .bin binary data from compressed data, e.g., satellite data, or HDF5 data from radar.

In Fig. S10 is shown the HydroPol2D input structure related to rainfall (distributed or lumped) and evapotranspiration processes. For spatial rainfall data, it is necessary to inform the index code, the coordinates of the gauges, and their respective rainfall intensity records. The time is discretized with constant time-steps. Please, note that the coordinates must be in a projected coordinate system and must be the same reference from the DEM, LULC, and Soil maps. However, for lumped rainfall data, it is only necessary to inform the rainfall intensity records. Similarly, from the distributed rainfall case, for the ETP data, coordinates and gauge code stations are required, and the record data are such as: maximum, median and minimum air temperature, air speed above two meters from the surface (U_2), relative air humidity (UR), and solar radiation (G).

In Fig. S11 is shown the structure for inflow data, soil type and land use and land cover. For the inflow data, it is necessary to specify the hydrograph and coordinates from where the stream flow is entered as a boundary condition. Related to soil type, name of the soil, relative index, and hydraulic properties such as saturated conductivity (k_{sat}), suction head (ψ), initial water content (I_0), and water deficit (θ_{sat} - θ_i). In relation to land use and land cover, it is necessary to specify the name and index for each class. Please note that the indexes used in these folders must match with information stored in the input rasters .tif used when reading the general data. Furthermore, parameters for the hydraulic and water quality behavior are necessary, such as: manning roughness coefficient (n), initial abstraction (h_0), initial water depth condition (d_0), pollutant build-up and wash-off coefficients (C_1, C_2, C_3, C_4).

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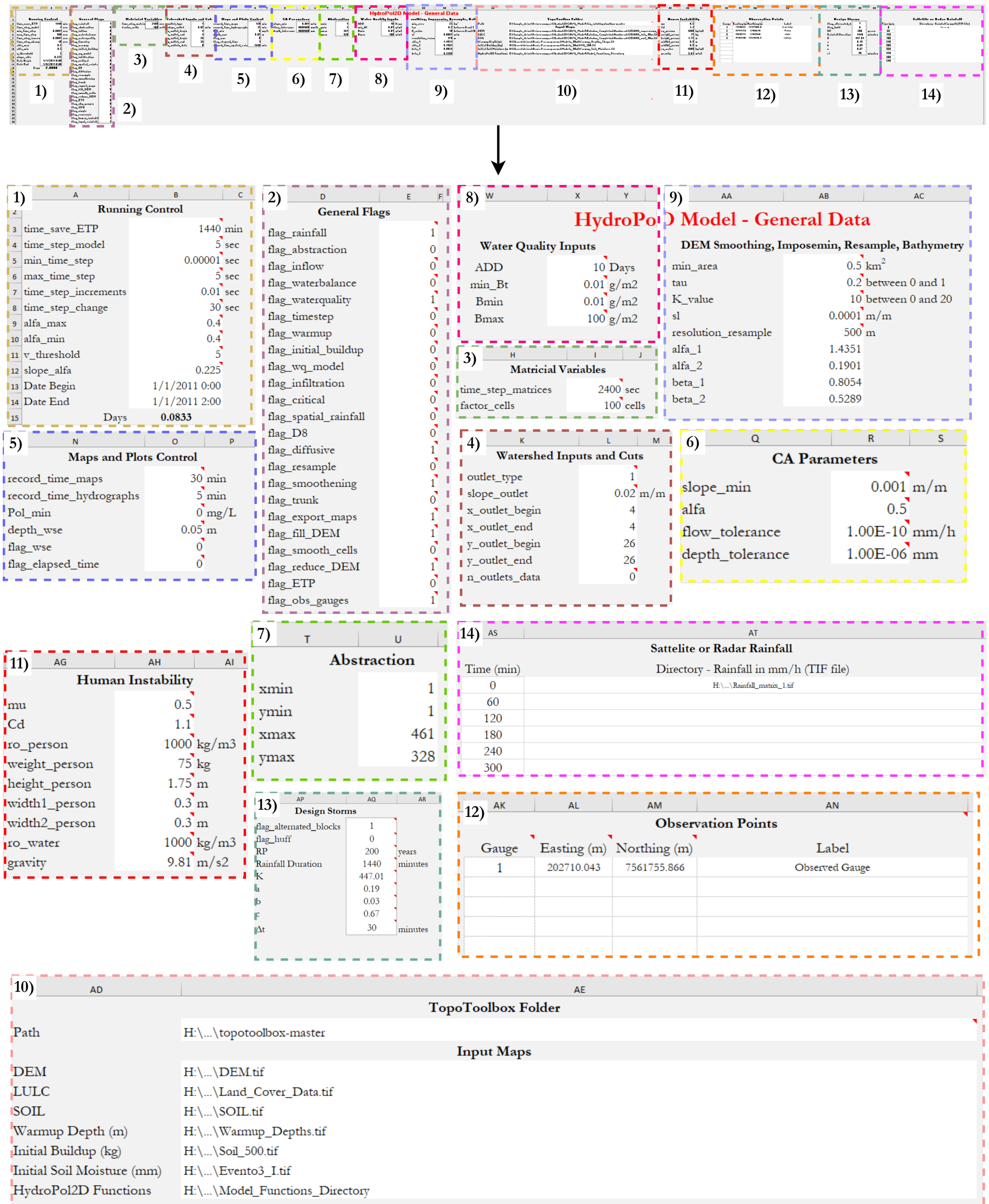


Fig. S9: HydroPol2D - General data input data structure. Sections 1, 2, 3, 4, 5, 6, 10, 12 are always required to be entered while the remainder sections are optional and might be only act

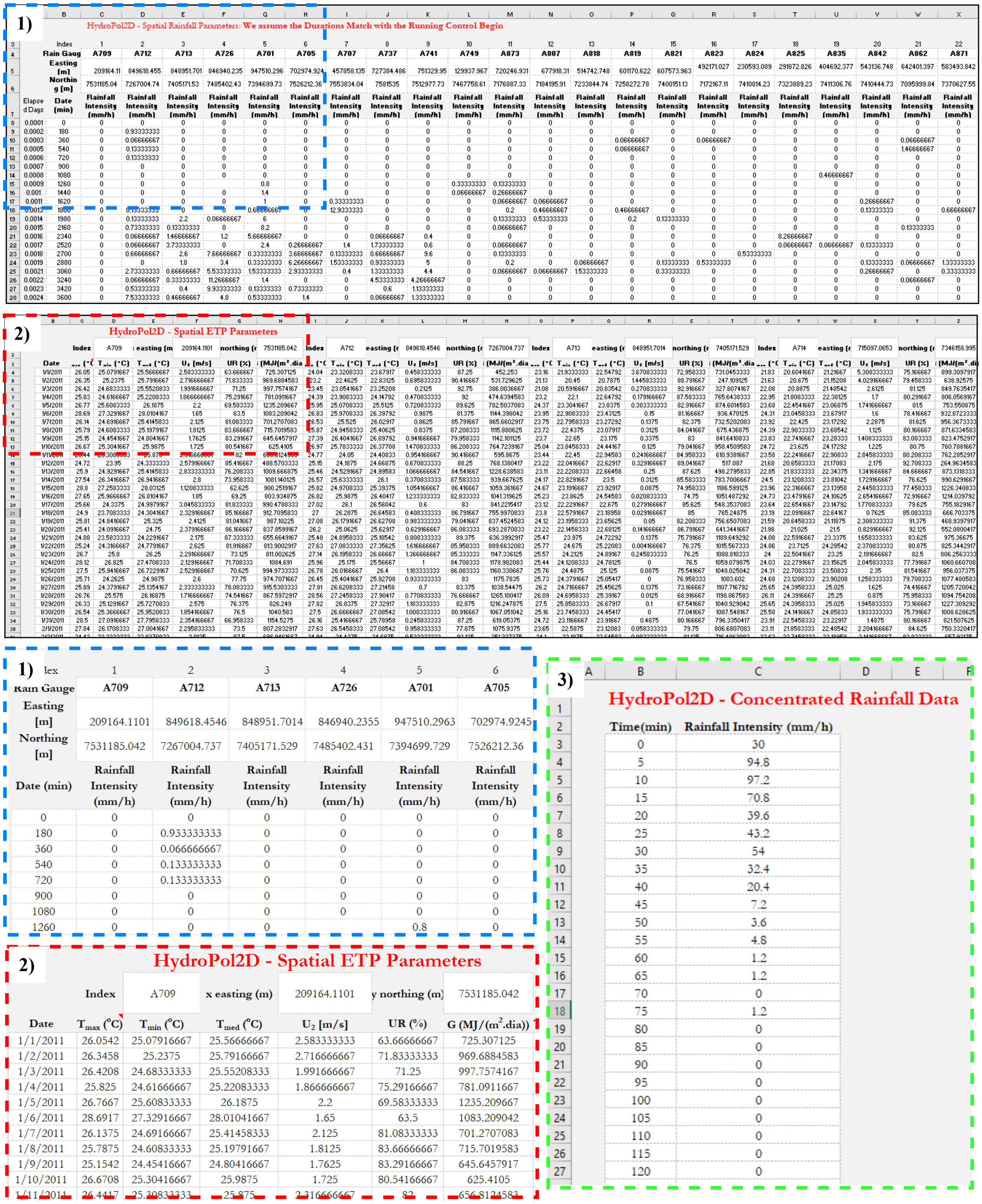
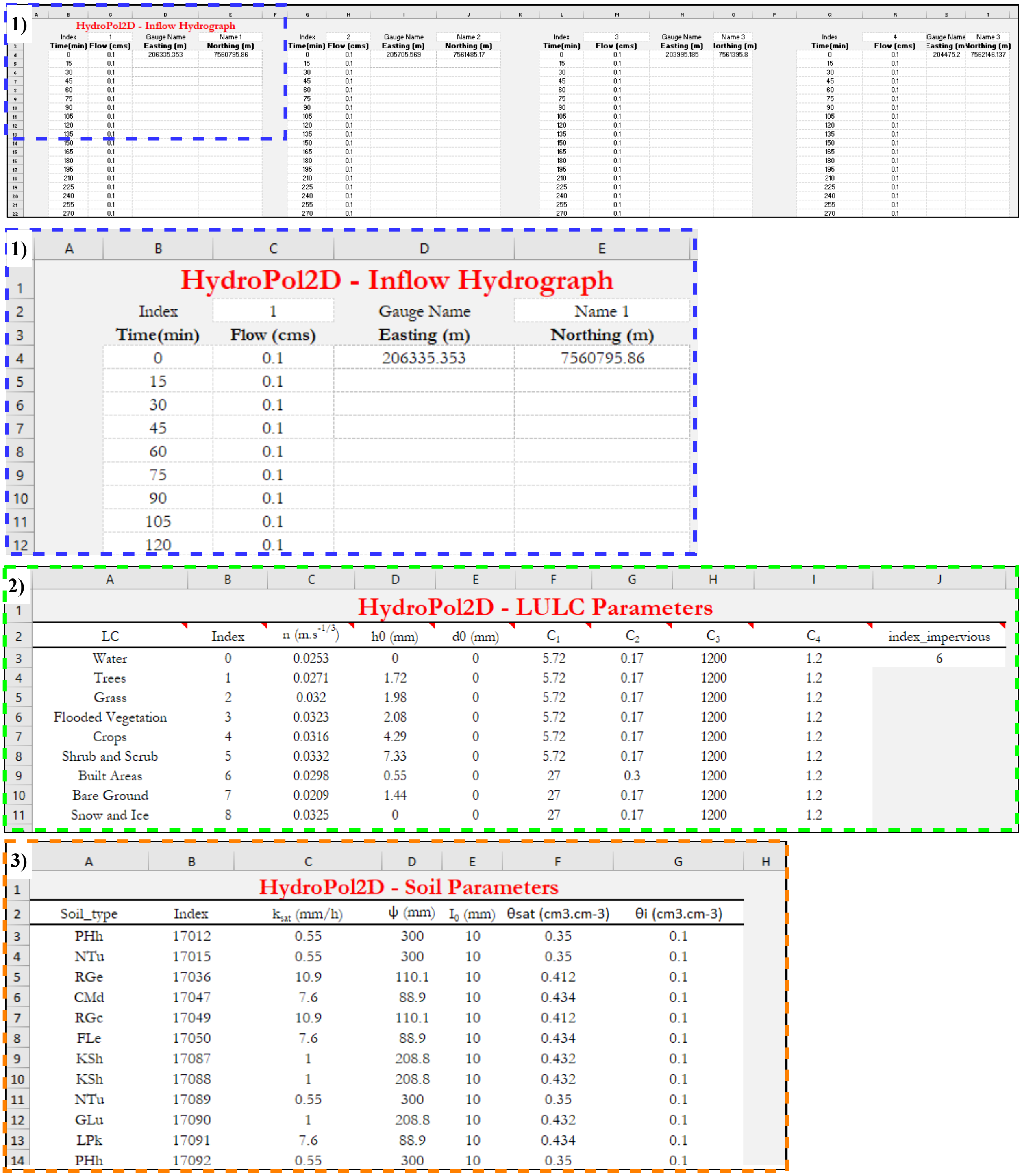


Fig. S10: HydroPol2D - ETP and rainfall input data structure.



1)

HydroPol2D - Inflow Hydrograph

Index	1	Gauge Name	Name 1	Index	2	Gauge Name	Name 2	Index	3	Gauge Name	Name 3	Index	4	Gauge Name	Name 3
Time(min)	**Flow (cms)**	**Easting (m)**	**Northing (m)**	**Time(min)**	**Flow (cms)**	**Easting (m)**	**Northing (m)**	**Time(min)**	**Flow (cms)**	**Easting (m)**	**lorthing (m)**	**Time(min)**	**Flow (cms)**	**Easting (m**	**Northing (m)**
0	0.1	206335.353	7560795.86	0	0.1	205705.569	7561485.17	0	0.1	203995.185	7561395.8	0	0.1	204475.2	7562146.137
15	0.1			15	0.1			15	0.1			15	0.1		
30	0.1			30	0.1			30	0.1			30	0.1		
45	0.1			45	0.1			45	0.1			45	0.1		
60	0.1			60	0.1			60	0.1			60	0.1		
75	0.1			75	0.1			75	0.1			75	0.1		
90	0.1			90	0.1			90	0.1			90	0.1		
105	0.1			105	0.1			105	0.1			105	0.1		
120	0.1			120	0.1			120	0.1			120	0.1		
135	0.1			135	0.1			135	0.1			135	0.1		
150	0.1			150	0.1			150	0.1			150	0.1		
165	0.1			165	0.1			165	0.1			165	0.1		
180	0.1			180	0.1			180	0.1			180	0.1		
195	0.1			195	0.1			195	0.1			195	0.1		
210	0.1			210	0.1			210	0.1			210	0.1		
225	0.1			225	0.1			225	0.1			225	0.1		
240	0.1			240	0.1			240	0.1			240	0.1		
255	0.1			255	0.1			255	0.1			255	0.1		
270	0.1			270	0.1			270	0.1			270	0.1		

1)

HydroPol2D - Inflow Hydrograph

Index	1	Gauge Name	Name 1
Time(min)	**Flow (cms)**	**Easting (m)**	**Northing (m)**
0	0.1	206335.353	7560795.86
15	0.1		
30	0.1		
45	0.1		
60	0.1		
75	0.1		
90	0.1		
105	0.1		
120	0.1		

2)

HydroPol2D - LULC Parameters

LC	Index	n ($m.s^{-1/3}$)	h0 (mm)	d0 (mm)	C_1	C_2	C_3	C_4	index_impervious
Water	0	0.0253	0	0	5.72	0.17	1200	1.2	6
Trees	1	0.0271	1.72	0	5.72	0.17	1200	1.2	
Grass	2	0.032	1.98	0	5.72	0.17	1200	1.2	
Flooded Vegetation	3	0.0323	2.08	0	5.72	0.17	1200	1.2	
Crops	4	0.0316	4.29	0	5.72	0.17	1200	1.2	
Shrub and Scrub	5	0.0332	7.33	0	5.72	0.17	1200	1.2	
Built Areas	6	0.0298	0.55	0	27	0.3	1200	1.2	
Bare Ground	7	0.0209	1.44	0	27	0.17	1200	1.2	
Snow and Ice	8	0.0325	0	0	27	0.17	1200	1.2	

3)

HydroPol2D - Soil Parameters

Soil_type	Index	k_{sat} (mm/h)	ψ (mm)	I_0 (mm)	θsat (cm3.cm-3)	θi (cm3.cm-3)
PHh	17012	0.55	300	10	0.35	0.1
NTu	17015	0.55	300	10	0.35	0.1
RGe	17036	10.9	110.1	10	0.412	0.1
CMd	17047	7.6	88.9	10	0.434	0.1
RGc	17049	10.9	110.1	10	0.412	0.1
FLe	17050	7.6	88.9	10	0.434	0.1
KSh	17087	1	208.8	10	0.432	0.1
KSh	17088	1	208.8	10	0.432	0.1
NTu	17089	0.55	300	10	0.35	0.1
GLu	17090	1	208.8	10	0.432	0.1
LPk	17091	7.6	88.9	10	0.434	0.1
PHh	17092	0.55	300	10	0.35	0.1

Fig. S11: HydroPol2D - Inflow, Land use and Land cover, and soil type input data structure.