ERAHUMED DSS

Valerio Gherardi   Pablo Amador Crespo   Andreu Rico

Table of contents

Preface

The purpose of this book is to provide a comprehensive reference for the ERAHUMED Decision Support System. Here you can find the technical descriptions of the algorithms employed by the system, as well as the user manual for the accompanying software.

The Support System and, hence, this book are currently under development on Github. In particular, the {erahumed} R package is hosted here.

For general information on the ERAHUMED project, please refer to the official website. If you want to get in touch, you can contact any of us via e-mail:

- Andreu Rico (Coordinator)
- Pablo Amador (PhD Researcher)
- Valerio Gherardi (Software Developer)

1 Introduction

This is a book created from markdown and executable code.

See Martínez-Megías et al. (2024) for additional info.

Part I

Technical description

2 The ERAHUMED model: a bird's eye view

The ERAHUMED model for assessing the ecological status of the Albufera Natural Park consists of three key components:

- **Hydrology**: Water dynamics within the park
- **Exposure**: Estimating the exposure to toxic chemicals
- **Risk Assessment**: Evaluating the impact of exposure

From a spatial perspective, the natural park is divided into three types of water bodies: the Albufera lake, rice field clusters[1], and irrigation ditches, which hydrologically connect the lake to the fields. Each of the model's computational layers incorporates specific quantitative models to simulate the relevant processes across all water bodies. This is summarized in Figure 2.1, where arrows indicate downstream dependencies and define the logical computation order.

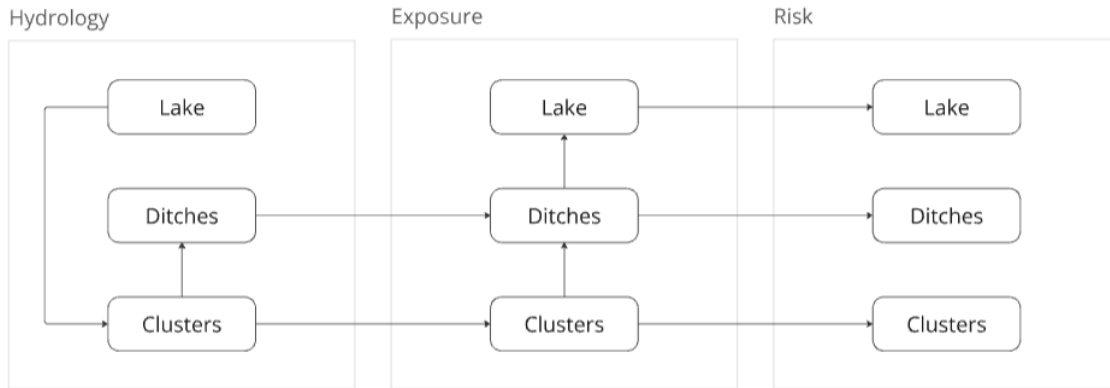Figure 2.1: Scheme of ERAHUMED model components. Directional arrows indicate the downstream dependencies of the various simulation layers.

To clarify this structure, we can summarize the role of each simulation layer in Figure 2.1 as follows:

---

[1]The exact definition of "clusters" is discussed in Section 4.4. For the purposes of this high-level description, we can think of them simply as groups of rice fields.

1. The system's hydrology, including water volumes and flows for all hydrological elements, is derived from minimal input data: daily water levels and sea outlet outflows for the Albufera lake. This is achieved through a set of simplifying assumptions about the hydrology of rice fields and irrigation ditches. Details on this model are provided in Chapter 4.

2. Exposure to chemicals is calculated by first simulating their application to rice fields based on typical cultivation patterns. The dispersion of chemicals is then modeled using a simplified set of differential equations designed to capture the key physical processes driving their spread. These calculations are described in detail Chapter 5.

3. The impact of chemicals is evaluated across all water bodies using a simplified approach based on Species Sensitivity Distributions, utilizing publicly available toxicity data for their estimation. This is described in detail in Chapter 6.

3 Model inputs

This chapter serves as a central reference for all input parameters used in ERAHUMED simulations.

3.1 Landscape parameters

Landscape parameters are collected in Table 3.1. In this table, a `numeric(n)` type indicates a numeric vector of `n` components, while `data.frame` inputs have more complex formats, detailed below.

3.2 Chemical-specific parameters

In addition to landscape parameters, ERAHUMED includes a set of parameters for each supported chemical, defining their physico-chemical and toxicological properties. At this stage, these parameters are internal and not reported here. However, our roadmap includes future support for customizing these parameters and defining new chemicals.

3.3 Data frame inputs

We detail in the following sections the format of data frame inputs.

3.3.1 Lake outflows and levels data frame

Time-series dataset that provides the observational hydrological data on the Albufera lake, along the template of `albufera_outflows` (the default value).

Table 3.2: Lake outflows and levels data frame [one row per day in the desired study frame.]

Column	Description
date	Date of measurement
level	Lake level (in meters above sea level)

Column	Description
outflow_pujol	Outflow at Pujol (meters cube per second)
outflow_perellonet	Outflow at Perellonet (meters cube per second)
outflow_perello	Outflow at Perello (meters cube per second)
is_imputed_level	Whether the `level` value was imputed.
is_imputed_outflow	Whether (any of) the outflows were imputed.

3.3.2 Weather data frame

A dataset that provides the relevant metereological time series, along the template of `albufera_weather` (the default value).

Table 3.3: Weather data frame [one row per day in the desired study frame.]

Column	Description
date	Date of measurement
temperature_ave	Average temperature.
temperature_min	Minimum temperature.
temperature_max	Maximum temperature.
precipitation_mm	Daily precipitation in millimiters.
evapotranspiration_mm	Daily evapotranspiration in millimiters.

3.3.3 Rice paddy management data frame

Dataset that provides the yearly schedule for irrigation and draining, along the template of `albufera_management` (the default value).

Table 3.4: Rice paddy management data frame [one row per day of year (29th of Feb. included) and per combination of the categorical variables `tancat` and `variety`.]

Column	Description
mm	numeric. Month of year (1 = January, 2 = February, *etc.*).
dd	numeric. Day of month.
tancat	logical. Whether the paddy is a tancat or not.
variety	character. Rice variety of the paddy under consideration.
sowing	logical. Whether `mm` and `dd` correspond to the sowing day.
ideal_irrigation	logical. Whether the paddy is scheduled to be irrigated on this day.
ideal_draining	logical. Whether the paddy is scheduled to be drained on this day.

Column	Description
ideal_height_eod	numeric. Scheduled water level of the paddy *at the end of the day* (that is, after irrigation and draining).

3.3.4 Chemical application schedules data frame

A dataset that provides the list of scheduled chemical applications, along the template of `albufera_ca_schedules`.

Table 3.5: Chemical application schedules data frame [one row per scheduled application.]

Column	Description
day	numeric. Scheduled day, counted starting from the sowing day, for the application under consideration.
rice_variety	character. Rice variety for this specific application.
chemical	character. Name of applied chemical.
kg_per_ha	numeric. Amount of chemical applied, in kilograms per hectare.
application_type	either `"ground"` or `"aerial"`. Application mode of the chemical to rice paddies.

Table 3.1: ERAHUMED input parameters

Parameter	Name	Unit	Group
\texttt{outflows_df}	Lake outflows and levels data frame	N/A	Hydrolo
\texttt{weather_df}	Weather data frame	N/A	Meteoro
\texttt{variety_prop}	Rice variety proportion	N/A	Environ
\texttt{seed}	\texttt{seed}	N/A	Hyperpa
\texttt{storage_curve_slope_m2}	Storage curve slope	m^2	Hydrolo
\texttt{storage_curve_intercept_m3}	Storage curve intercept	m^3	Hydrolo
\texttt{petp_surface_m2}	PET surface	m^2	Hydrolo
\texttt{management_df}	Rice paddy management data frame	N/A	Environ
\texttt{ideal_flow_rate_cm}	Ideal flow rate	cm	Hydrolo
\texttt{height_thresh_cm}	Cluster Height Threshold	cm	Hydrolo
\texttt{ditch_level_m}	Ditch water level	m	Hydrolo
\texttt{ca_schedules_df}	Chemical application schedules data frame	N/A	Environ
\texttt{drift}	Drift	1	Environ
\texttt{covmax}	Max interception potential	1	Environ
\texttt{jgrow}	Maturation cycle length	day	Environ
\texttt{SNK}	SNK	1	Environ
\texttt{dact_m}	Depth of active sediment	m	Environ
\texttt{css_ppm}	Suspended sediment concentration	ppm	Environ
\texttt{foc}	Fraction of organic content	1	Environ
\texttt{bd_g_cm3}	Bulk density of sediment	g $\cdot$ cm ^{2}	Environ
\texttt{qseep_m_day}	Seepage rate	m $\cdot$ day ^{1}	Environ
\texttt{wilting}	Wilting point	1	Environ
\texttt{fc}	Field capacity	1	Environ

4 Hydrological model of the Albufera Natural Park

4.1 Overview

4.2 Definition of hydrological elements

Our hydrological modeling represents the Albufera Natural Park in terms of three main hydrological elements (or "water bodies"): rice field clusters, irrigation ditches, and Albufera Lake.

The definition of rice field clusters and irrigation ditches used in our modeling is discussed in detail in Ref. [TODO: insert Pablo's paper reference]. For our purposes, we note that:

- The park's cultivation area is divided into rice field clusters, each comprising several rice fields that share the same hydrological management system (*tancat* or regular) and rice variety (*J.Sendra*, *Bomba* or *Clearfield*).

- Each cluster is assumed to drain into a single irrigation ditch, selected based on the shortest distance (see Ref. TODO for details).

4.3 Random assignation of rice variety

Since the actual rice variety cultivated in individual fields is unknown, a random variety is assigned to each cluster based on the following criteria:

- The proportion of cultivated surface allocated to each variety is determined by the `variety_prop` parameter (cf. Table 3.1).
- The *Bomba* variety is cultivated exclusively in *tancats*.
- The *Clearfield* variety is restricted to the northern part of the natural park, in clusters draining into ditches 1 to 19.

4.4 Scheme of the hydrological model

This schematic diagram represents the simplified hydrological model of the Albufera Natural Park employed by ERAHUMED. It highlights water flows across the three primary landscape elements defined in the previous Section. Key simplifying assumptions embedded in the model and visually summarized in the diagram are as follows:

- **Rice Clusters** Clusters are irrigated by external water sources and drain exclusively a single ditch. There is no direct hydrological interaction or exchange between individual clusters.

- **Ditches** Ditches collect water from the clusters and, potentially, from additional external sources, channeling all inflows directly into the Albufera lake.

- **The Albufera Lake** The lake receives water exclusively from the ditches. While two types of outflow are considered, namely direct discharge to the sea and water recirculation to the rice fields, the latter is typically negligible[1].
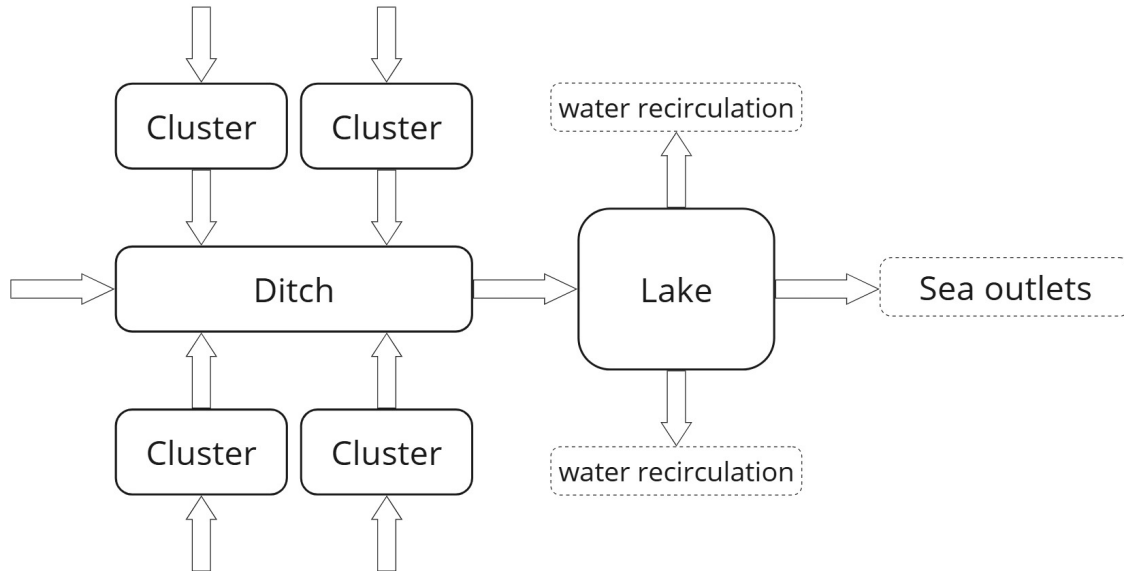
Figure 4.1: Scheme of ERAHUMED hydrological model of the Albufera Natural Park

---

[1]Further details on this are discussed in Section 4.5.1.

4.5 Water balance calculations

This section provides the details of the water balance calculations for (in the order of computation) the Albufera Lake, rice field clusters, and irrigation ditches of the park.

4.5.1 Albufera Lake

Water balance calculations for the Albufera Lake are relatively simple. The relevant equation expressing hydrological balance is:

$$\text{Volume Change} = \text{Inflow} - \text{Outflow} + \text{Precipitation} - \text{Evapotranspiration}. \tag{4.1}$$

The variables collected into the following table, that enter the balance equation 4.1, have direct correspondence with model input parameters listed in Chapter 3 (we use the notation `df$col` to indicate column `col` of data frame `df`).

Variable	Source	Units	Description
h_t	`outflows_df$level`	m	Lake water level daily time series
O_t^{Pujol}	`outflows_df$outflow_pujol`	m^3	*Pujol* outflow daily time series
$O_t^{\text{Perelló}}$	`outflows_df$outflow_perello`	m^3	*Perelló* outflow daily time series
$O_t^{\text{Perellonet}}$	`outflows_df$outflow_perellonet`	m^3	*Perellonet* outflow daily time series
P_t	`outflows_df$precipitation_mm`	mm	Precipitation (per unit area) daily time series
ET_t	`outflows_df$evapotranspiration_mm`	mm	Evapotranspiration (per unit area) daily time series
α	`storage_curve_intercept_m3`	m^3	Storage curve intercept
β	`storage_curve_slope_m2`	m^2	Storage curve slope
σ_{PET}	`petp_surface_m2`	m^2	PET surface

Calculated quantities are listed in the following table.

Variable	Units	Description
V_t	m^3	Lake water volume daily time series

15

Variable	Units	Description
$\Delta V_t \equiv V_{t+1} - V_t$	m^3	Lake water volume change daily time series
ΔV_t^{PET}	m^3	Lake water volume change due to precipitation and evapotranspiration daily time series
I_t	m^3	Lake total inflow daily time series
O_t	m^3	Lake total outflow daily time series

The volume time-series is computed as:

$$V_t = \alpha + \beta \cdot h_t, \tag{4.2}$$

while the volume changes due to precipitation and evapotranspiration are given by:

$$\Delta V_t^{\text{PET}} = \sigma_{\text{PET}}(\text{P}_t - \text{ET}_t), \tag{4.3}$$

Total inflow and outflow must satisfy Equation 4.1, which we may rewrite explicitly as:

$$\Delta V_t - \Delta V_t^{\text{PET}} = I_t - O_t, \tag{4.4}$$

Strictly speaking, O_t is not merely the sum of O_t^{Pujol}, $O_t^{\text{Perelló}}$ and $O_t^{\text{Perellonet}}$, but is rather calculated as follows:

$$O_t = \max\left[O_t^{\text{Pujol}} + O_t^{\text{Perelló}} + O_t^{\text{Perellonet}}, \Delta V_t^{\text{PET}} - \Delta V_t\right]. \tag{4.5}$$

The rationale is that the simple sum of estuaries outflows omits potentially important contributions from *water recirculation*, that is to say, water being pumped out from the lake for rice-field irrigation, by the so-called *tancats*. Such amount of recirculated water is hard to estimate and, in the lack of a better model, we simply assume this to be negligible, *except* when a positive amount is required by Equation 4.4 itself, due the physical constraint that $I_t \geq 0$.

Once O_t is calculated through Equation 4.5, I_t can be immediately obtained from Equation 4.4. Notice that whenever the aforementioned compensating outflow term due to water recirculation is included (which happens when the maximum in Eq. 4.5 is given by the second term), the total inflow is always estimated to be zero.

4.5.2 Rice field clusters

Water balance calculations for rice field clusters are complex due to the lack of observational data. The simulation algorithm relies on several key components:

- The hydrology of the Albufera lake (Section 4.5.1).
- Assumptions about the hydrological connections between the various water bodies in the natural park, detailed in Section 4.4.
- An ideal yearly management plan for irrigation and drainage of the rice paddies.

The quantitative inputs for this calculation are collected in the following table; see the definition of the `management_df` input data frame, discussed in Section 3.3.3. Below, v denotes rice variety, and θ denotes the hydrological management system (*tancat* or *regular*).

Variable	Source	Units	Description
$\mathrm{Ir}_{d,v,\theta}$	`management_df$ideal_irrigation`	NA	Boolean expressing whether a cluster of variety v and management system θ is supposed to be irrigated on day of year d
$\mathrm{Dr}_{d,v,\theta}$	`management_df$ideal_draining`	NA	Boolean expressing whether a cluster of variety v and management system θ is supposed to be drained on day of year d
$\mathcal{H}_{d,v,\theta}$	`management_df$ideal_height_eod_cm`	cm	Ideal water depth (in cm) of a cluster of variety v and management system θ on day of year d
k_{flow}	`ideal_flow_rate_cm`	$\mathrm{cm}\cdot\mathrm{day}^{-1}$	Rate of water flow through rice paddies during simultaneous irrigation and drainage, while maintaining a constant overall water level.

Variable	Source	Units	Description
h_{thres}	`height_thresh_cm`	cm	Water height below which a cluster is considered emptied. Used to determine delays in the draining/irrigation plan. Expressed in cm.
A_c	Internal parameter	m^2	Surface area of cluster c

The outputs are collected below, where the indices c and t denotes the cluster and time, respectively:

Variable	Units	Description
$V_{c,t}$	m^3	Cluster's water volume
$I_{c,t}$	m^3	Cluster's inflow
$O_{c,t}$	m^3	Cluster's outflow

The fundamental equation for hydrological balance are:

$$V_{c,t+1} - V_{c,t} = I_{c,t} - O_{c,t} + (\text{P}_t - \text{ETP}_t) \times A_c \tag{4.6}$$

where P_t and ETP_t are the same as in Section 4.5.1, this simulation rests on various simplifications, which we detail in what follows.

In what follows, we will focus on the set of all clusters draining into a given ditch, and we will enumerate clusters through the index $c = 1, 2, ..., N_C$. On the other hand, clusters are assumed to be irrigated from the external of the Albufera system, *i.e.* not through any of the ditches which eventually flow into the lake. According to our assumptions on the hydrology of clusters and ditches (*cf.* Section 4.4), the sum of cluster outflows is constrained by:

$$\sum_{c=1}^{N_C} O_{c,t} \leq Q_t \tag{4.7}$$

where Q_t denotes the relevant ditch's inflow. With a small leap in logic, we anticipate from Section 4.5.3, that the water levels in irrigation ditches are assumed to be constant, so that Q_t can also identified with the ditch outflow, that is in turn estimated as:

$$Q_t = \frac{\text{Area of clusters draining into ditch}}{\text{Area of all clusters}} \times \text{Lake's Inflow}_t \tag{4.8}$$

where the lake's inflow is computed as described in Section 4.5.1.

Qualitatively speaking, the simulation works by finding daily values of $I_{c,t}$ and $O_{c,t}$ compatible with Eqs. 4.6 and 4.7, and such that the resulting hydrology is as close as possible with the "ideal" one prescribed by the specified management plan. This is accomplished in three steps:

1. Computing ideal inflows and outflows, given current water levels and management plans.
2. Computing actual inflows and outflows, and corresponding actual water level changes.

3. Computing required management plan delays, if some clusters were scheduled to be drained, but could not due to insufficient flow through the common ditch (see below for details).

These steps are iterated on a daily basis, starting from some initial time (say $t = 0$) at which all cluster water levels coincide with the ideal ones, and no plan delays are present.

Concerning the last step, a few words may serve to clarify the algorithm described below. The purpose of plan delays is to ensure that during each year's sowing season, all cluster's are emptied at some point, as required for ground applications of chemicals (modeled in subsequent layers of ERAHUMED). This is achieved by delaying by one day the management plan, whenever an emptying condition is not met. When far outside of the sowing window, the delays are reset then to zero, in order to ensure that delays are not carried over indefinitely, which would be quite unrealistic.

In what follows, the conversion between cluster water volumes and depths is provided by $V_{c,t} = A_c \cdot h_{c,t}$, and we denote by $\delta_{c,t}$ the time-series of plan delays for cluster c, which is initialized by $\delta_{c,0} = 0$.

4.5.2.1 Step 1: ideal balance

Ideal balance quantities for each cluster c are obtained from the management plan data-set, whose relevant row is identified by the cluster's rice variety v and field type θ, and the delayed day:

$$d_{c,t+1} = d_{t+1} - \delta_{c,t}, \tag{4.9}$$

where d_{t+1} denotes the day of year corresponding to time $t + 1$, and $\delta_{c,t}$ the accumulated plan delay.

Let $h^{id}_{c,t+1}$ denote the ideal depth for cluster c at time $t + 1$ retrieved in this way, and $Ir_{c,t}$, $Dr_{c,t}$ the corresponding ideal irrigation and draining plans. Furthermore, denote by $V^{id}_{c,t+1} = A_c \cdot h^{id}_{c,t+1}$ the corresponding ideal water volume.

In order to compute ideal inflow and outflow, we require (*cf.* Equation 4.6):

$$V_{c,t+1}^{\mathrm{id}} = \max\{V_{c,t}^{\mathrm{id}} + (\mathrm{P}_t - \mathrm{ETP}_t) \times A_c, 0\} + I_{c,t}^{\mathrm{id}} - O_{c,t}^{\mathrm{id}} \qquad (4.10)$$

Clearly, Equation 4.10 alone does not individually specify $I_{c,t}^{\mathrm{id}}$ and $O_{c,t}^{\mathrm{id}}$, but only their difference $\Delta_{c,t}^{\mathrm{id}} = I_{c,t}^{\mathrm{id}} - O_{c,t}^{\mathrm{id}}$. In order to fix both these quantities:

$$\begin{aligned} (I_{c,t}^{\mathrm{id}})^{(0)} &= \begin{cases} k_{\mathrm{flow}} & \text{if } \mathrm{Ir}_{c,t} = \mathrm{Dr}_{c,t} = 1 \\ 0 & \text{otherwise} \end{cases}, \\ (O_{c,t}^{\mathrm{id}})^{(0)} &= (I_{c,t}^{\mathrm{id}})^{(0)} - \Delta_{c,t}^{\mathrm{id}}. \end{aligned} \qquad (4.11)$$

and, in order to ensure that flows are positive, we finally set:

$$\begin{aligned} O_{c,t}^{\mathrm{id}} &= \max\{(O_{c,t}^{\mathrm{id}})^{(0)}, 0\} \\ I_{c,t}^{\mathrm{id}} &= O_{c,t}^{\mathrm{id}} + \Delta_{c,t}^{\mathrm{id}}, \end{aligned} \qquad (4.12)$$

which satisfy Equation 4.10 and give rise to positive $O_{c,t}^{\mathrm{id}}$ and $I_{c,t}^{\mathrm{id}}$.

4.5.2.2 Step 2: real balance

At each time-step t, the cluster's index set is randomly permuted [2], and the real flows are calculated as:

$$\begin{aligned} O_{c,t} &= \min\{O_{c,t}^{\mathrm{id}}, Q_t - \sum_{c'<c} O_{c',t}\}, \\ I_{c,t} &= \max\{I_{c,t}^{\mathrm{id}} - O_{c,t}^{\mathrm{id}} + O_{c,t}, 0\} \end{aligned} \qquad (4.13)$$

In simple terms, clusters are emptied in a random order within the allowed capacity of the corresponding ditch. Using Equation 4.13, we finally determine the real water level achieved as:

$$V_{c,t+1} = \max\{V_{c,t} + (\mathrm{P}_t - \mathrm{ETP}_t) \times A_c, 0\} + I_{c,t} - O_{c,t} \qquad (4.14)$$

to be compared with Equation 4.10.

---

[2]With some abuse of notation, we assume the indexes c and c' in Equation 4.13 to be sorted according to this random permutation.

4.5.2.3 Step 3: updating the plan delay

The updated value $\delta_{c,t+1}$ is obtained as follows. If d_{t+1} (the *actual* day of year) is outside of the window $W = [$20th of April, 15th of October$]$, then $\delta_{c,t+1} = 0$. Otherwise, if $h^{\mathrm{id}}_{c,t} > 0$ or $h_{c,t} < h_{\mathrm{thres}}$, the plan delay is unchanged: $\delta_{c,t+1} = \delta_{c,t}$. Finally, if $h^{\mathrm{id}}_{c,t} = 0$ but $h_{c,t} > h_{\mathrm{thres}}$, we add one day of delay: $\delta_{c,t+1} = \delta_{c,t} + 1$.

4.5.2.4 Step 3: updating the plan delay

The updated value $\delta_{c,t+1}$ is obtained as follows. If d_{t+1} (the *actual* day of year) is outside of the window $W = [$20th of April, 15th of October$]$, then $\delta_{c,t+1} = 0$. Otherwise, if $h^{\mathrm{id}}_{c,t} > 0$ or $h_{c,t} < h_{\mathrm{thres}}$, the plan delay is unchanged: $\delta_{c,t+1} = \delta_{c,t}$. Finally, if $h^{\mathrm{id}}_{c,t} = 0$ but $h_{c,t} > h_{\mathrm{thres}}$, we add one day of delay: $\delta_{c,t+1} = \delta_{c,t} + 1$.

4.5.3 Irrigation ditches

5 Exposure

5.1 Overview

5.2 Pesticide applications

This should describe how chemical applications are simulated.

5.3 Pesticide dispersion

5.3.1 Diagram of physical processes

Roughly the content of this vignette.

5.3.2 Evolution Equations

5.3.3 Semi-numerical approach

6 Risk assessment

6.1 Overview

6.2 Calculation of risk using SSDs

Part II

User Manual

7 The ERAHUMED DSS User Interface

This chapter should explain how to run ERAHUMED simulations using the Shiny app. It may contain screenshots taken from the app to exemplify the various points.

7.0.1 How to run the DSS?

Describe various options available (which at the moment of writing may as well be "download the package" only - and perhaps a basic deployment on shinyapps.io).

7.0.2 The "Output" tab

7.0.3 The "Input" tab

8 The {erahumed} R package

This should not be an exhaustive description of the R package, but rather mention its existence and giving basic instructions for its installation and refer to the package vignette's and documentation for more details.

References

Martínez-Megías, Claudia, Alba Arenas-Sánchez, Diana Manjarrés-López, Sandra Pérez, Yolanda Soriano, Yolanda Picó, and Andreu Rico. 2024. "Pharmaceutical and Pesticide Mixtures in a Mediterranean Coastal Wetland: Comparison of Sampling Methods, Ecological Risks, and Removal by a Constructed Wetland." *Environmental Science and Pollution Research* 31 (10): 14593–609.

A Input Data

A.1 Hydrological data

A.2 Meteorological data

A.3 Albufera Rice Paddies Management

A.4 Storage curve and P-ETP function

A.5 Definition of rice clusters