ERAHUMED DSS

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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.

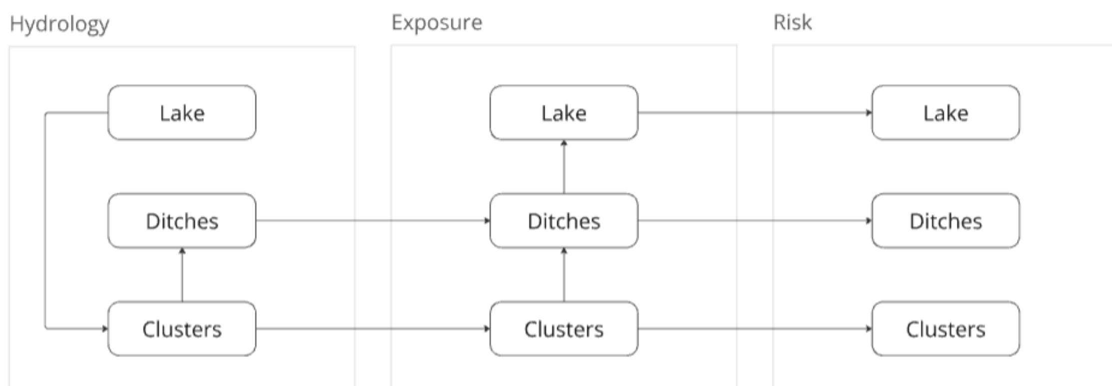

Figure 2.1: Scheme of ERAHUMED model components. Directional arrows indicate the downstream dependencies of the various simulation layers.

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 4.3. 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_cm	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	Hydrolog
\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	Hydrolog
\texttt{storage_curve_intercept_m3}	Storage curve intercept	m^3	Hydrolog
\texttt{petp_surface_m2}	PET surface	m^2	Hydrolog
\texttt{management_df}	Rice paddy management data frame	N/A	Environ
\texttt{ideal_flow_rate_cm}	Ideal flow rate	cm	Hydrolog
\texttt{height_thresh_cm}	Cluster Height Threshold	cm	Hydrolog
\texttt{ditch_level_m}	Ditch water level	m	Hydrolog
\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 variety and type (*tancat* or regular).
- Each cluster is assumed to drain into a single irrigation ditch, selected based on the shortest distance (see Ref. TODO for details).

4.3 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].

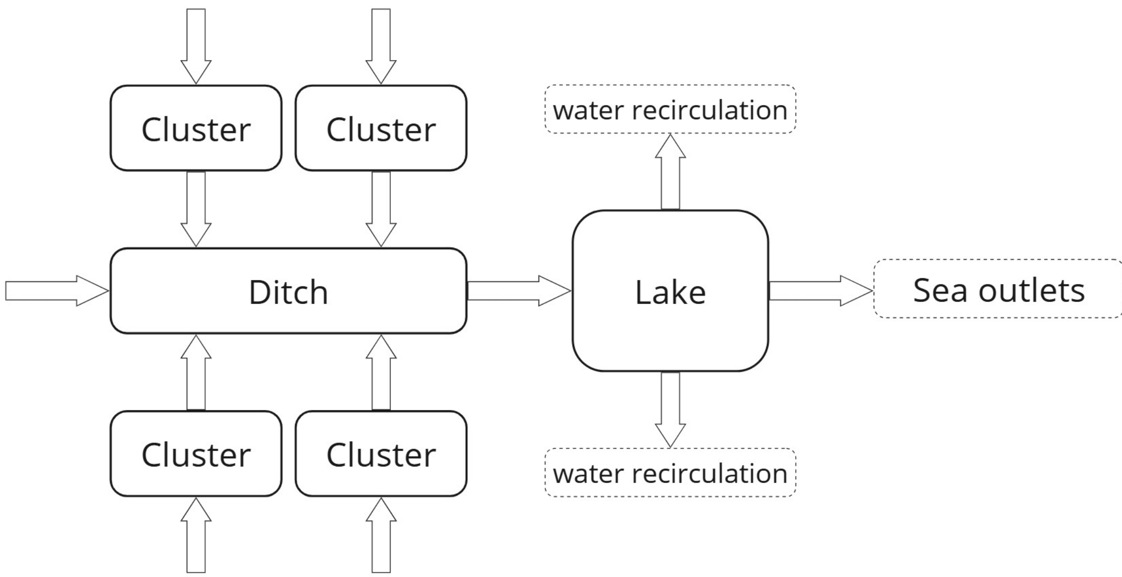

Figure 4.1: Scheme of ERAHUMED hydrological model of the Albufera Natural Park

4.4 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.

4.4.1 Albufera Lake

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

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

In order to start fixing the notation, we define the following variables which 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`).

[1]Further details on this are discussed in Section 4.4.1.

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

In addition we denote:

Variable	Units	Description
V_t	m^3	Lake water volume daily time series
$\Delta V_t \equiv V_{t+1} - V_t$	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 calculated as:

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

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

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

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

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

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

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

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.

4.4.2 Rice field clusters

4.4.3 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