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:

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- Pablo Amador (PhD Researcher)
- Valerio Gherardi (Software Developer)

Software version

This manual corresponds to version 0.20.0.9000 of the `{erahumed}` R package.

1 Introduction

Mediterranean coastal wetlands are exposed to multiple anthropogenic pressures, one of the most significant being pollution from intensive rice production. Among the most critical pollutants associated with rice cultivation are synthetic pesticides, particularly herbicides, insecticides, and fungicides. Once applied in rice production, pesticides can be transported through spray-drift, surface runoff or leaching into nearby water bodies, threatening the structure and functioning of aquatic ecosystems.

The ERAHUMED Decision Support System (DSS) was designed to evaluate the exposure and risks of pesticides used in rice cultivation, focusing on the Albufera Natural Park as a reference and study wetland. The Albufera Natural Park, located near Valencia, Spain, is one of the most important wetlands in the Mediterranean region. It spans an area of 21 hectares, including the Albufera lagoon, surrounding marshlands, rice fields, and sand dunes. The freshwater lagoon is connected to the Mediterranean Sea through a system of canals known as "*golas*." The park is a Ramsar site and hosts a wide variety of flora and fauna, including several endemic and endangered species.

The DSS dynamically calculates the volume of water available in rice fields, canals, and the lagoon throughout the year. Additionally, it can dynamically predict pesticide concentrations in various environmental matrices, including rice crops, surface water, and sediment. Finally, the DSS evaluates the risks associated with each pesticide and their mixtures for aquatic ecosystems, based on Species Sensitivity Distributions (SSDs).

The DSS can be used to predict exposure and risks associated with different pesticides, considering their unique physico-chemical and toxicological properties, at a landscape level. It determines spatially explicit and dynamic variations in concentrations within each water body over time. This makes it a valuable tool for decision-making regarding rice cultivation management and implementing risk mitigation measures at an ecosystem-wide scale. Furthermore, it allows for prospective ecological risk assessments of new substances and the identification of pollution hot-spots and the combined effects of complex contaminant mixtures.

On the practical side, the DSS is implemented as an R package called `{erahumed}`, distributed as open-source software and available for download here. The package includes a Graphical User Interface (GUI), implemented as a Shiny application, which allows users to run the models and analyze the results without directly interacting with the underlying R code.

This documentation provides a comprehensive description of the DSS and is divided into two main parts. The first part, *Technical Description*, outlines the models underlying the DSS,

including the environmental, hydrological, and physico-chemical parameters required for its operation, as well as the processes and equations used to calculate exposure and risks. The second part, *User Manual*, provides step-by-step instructions for using the software, with a particular focus on its GUI. In addition, an *Appendix* details the data used by the DSS.

2 Acknowledgements

The ERAHUMED DSS has been financed by the Talented Researcher Support Programme - PlanGenT (CIDEGENT/2020/043) of the Generalitat Valenciana.

TODO: Based on existing work Martínez-Megías et al. (2024)

Part I

Technical description

3 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 3.1, where arrows indicate downstream dependencies and define the logical computation order.

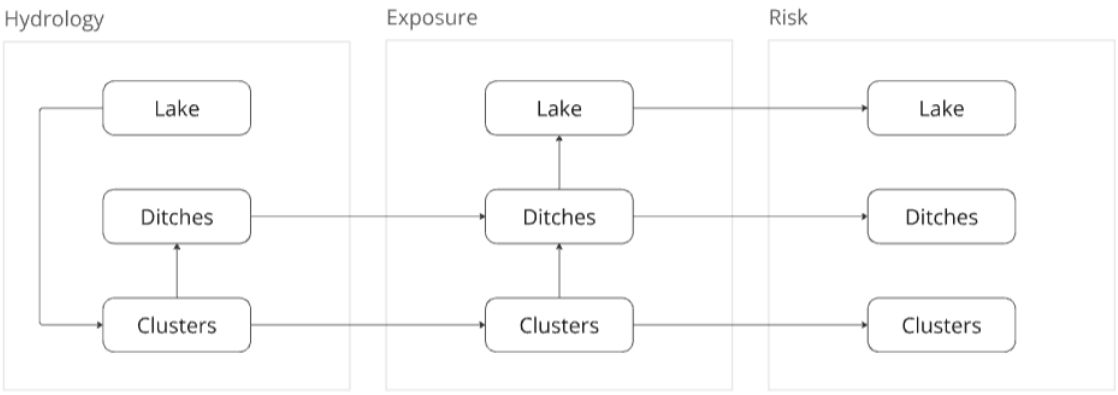

Figure 3.1: Scheme of ERAHUMED model components. Directional arrows indicate the downstream dependencies of the various simulation layers.

To clarify this structure, we can summarize the role of each simulation layer in Figure 3.1 as follows:

[1]The exact definition of "clusters" is discussed in Section 5.3. 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 5.

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 set of differential equations designed to capture the key physical processes driving their spread. These calculations are described in detail Chapter 6.

3. The impact of chemicals across all water bodies is assessed using model-based approaches, currently including Species Sensitivity Distributions (SSDs) and Risk Quotients (RQs). These approaches rely on publicly available toxicity data to estimate ecological risk. Full details of the risk assessment methodology are provided in Chapter 7.

In addition to the default simulation workflow, the ERAHUMED software includes advanced features that allow users to define custom chemical compounds and rice field management systems (RFMSs). While current agrochemical practices in the Albufera Natural Park are already built into the tool, these customization options greatly expand its capabilities. They enable the simulation and comparison of alternative scenarios, making the software a powerful resource for exploring potential changes in management or chemical use. Detailed guidance on how to define and allocate custom chemicals and RFMSs is provided in the following Sections.

The next Section provides a detailed description of all model inputs, including hydrological data, chemical properties, and management practices, which underpin the simulation layers described above.

4 Model inputs

This chapter serves as a central reference for all input parameters used in ERAHUMED simulations. In the tables below, a `numeric(n)` type indicates a numeric vector of `n` components, while `data.frame` inputs have more complex formats, detailed below.

Note: The `Type` column and, to some extent, the `Description` fields in Table 4.1 refer to the internal structures and conventions of the `{erahumed}` *R package*, which is presented in detail in Chapter 9 and references therein. However, the `Description` generally conveys the intended meaning and usage of each parameter, regardless of whether the user is interacting through the R package or the Shiny interface. Users of the Shiny GUI do not need to understand the R-specific details, as the interface provides appropriate input controls and guidance.

The input parameters are grouped into four categories:

- **Landscape parameters** (Table 4.1) define the biophysical and climatic context in which simulations take place. These inputs characterize the structure and behavior of the Albufera system, including the temporal simulation window (`date_start`, `date_end`), the lake's hydrology and geometry, and its interaction with weather and soil processes.
- **Chemical parameters** (Table 4.4) describe the physico-chemical and eco-toxicological characteristics of the pesticide compounds considered in the simulation. These include degradation rates, solubility, partition coefficients, and toxicity distribution parameters used for risk assessment.
- **RFMS parameters** (Table 4.5) specify how different rice field management systems (RFMSs) are configured. These parameters define the timing, frequency, and nature of chemical applications, as well as water management practices such as irrigation and drainage scheduling.
- **Spatial allocation** parameters (Table 4.6) captures how the different RFMSs are spatially distributed across the simulated landscape. This information determines which management practices are applied to which clusters of rice fields, affecting both contaminant fate and risk exposure.

4.1 Landscape parameters

Parameter	Name	Unit	Group
\texttt{date_start}	Start Date	N/A	Genera
\texttt{date_end}	End Date	N/A	Genera
\texttt{seed}	Simulation random seed	N/A	Genera
\texttt{outflows_df}	Lake outflows and levels data frame	N/A	Hydro
\texttt{storage_curve_slope_m2}	Storage curve slope	m^2	Hydro
\texttt{storage_curve_intercept_m3}	Storage curve intercept	m^3	Hydro
\texttt{petp_surface_m2}	PET surface	m^2	Hydro
\texttt{weather_df}	Weather data frame	N/A	Meteo
\texttt{ideal_flow_rate_cm}	Ideal flow rate	cm	Enviro
\texttt{height_thresh_cm}	Cluster Height Threshold	cm	Enviro
\texttt{ditch_level_m}	Ditch water level	m	Enviro
\texttt{covmax}	Max interception potential	1	Enviro
\texttt{jgrow}	Maturation cycle length	day	Enviro
\texttt{dact_m}	Depth of active sediment	m	Enviro
\texttt{css_ppm}	Suspended solid concentration	ppm	Enviro
\texttt{foc_ss}	Fraction of organic content in suspended solid	1	Enviro
\texttt{foc_sed}	Fraction of organic content in sediment	1	Enviro
\texttt{bd_g_cm3}	Bulk density of sediment	$g \cdot cm^{2}$	Enviro
\texttt{qseep_m_day}	Seepage rate	$m \cdot day^{1}$	Enviro
\texttt{porosity}	Porosity	1	Enviro
\texttt{rfms_map}	Map of rice field management systems	N/A	Agroc

4.1.1 Observational inputs: hydrology and weather

Hydrological and meteorological data provide the empirical starting point for ERAHUMED simulations. These observational inputs are supplied as data frames and are used to drive the water balance, pesticide transport, and evapotranspiration dynamics in the model.

Users working with historical scenarios are encouraged to provide real-world data from the corresponding time period, enabling retrospective simulations under observed environmental conditions. Conversely, for future or hypothetical scenarios, users may define synthetic datasets that reflect the expected or desired characteristics of the scenario—e.g., altered rainfall regimes or management-induced changes in outflow patterns.

By default, ERAHUMED includes representative data covering a typical agricultural year in the Albufera Natural Park:

- Hydrological data (`outflows_df`) are derived from continuous measurements of water outflows and lake levels, provided by the *Confederación Hidrográfica del Júcar* (CHJ).

These records can be accessed through the CHJ hydrological data portal.

- Meteorological data (`weather_df`) originate from the *Benifaió* weather station, operated by the *Instituto Valenciano de Investigaciones Agrarias* (IVIA). This station is considered representative of the local climate within the park. Historical meteorological records are publicly available at the IVIA website.

We detail below the format and required fields for each of these data frames.

4.1.1.1 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 4.2: Lake outflows and levels data frame [one row per day in the desired study frame.]

Column	Description
date	Date of measurement
level_m	Lake level (meters above sea level)
outflow_pujol_m3_s	Outflow at Pujol (cubic meters per second)
outflow_perellonet_m3_s	Outflow at Perellonet (cubic meters per second)
outflow_perello_m3_s	Outflow at Perello (cubic meters per second)

4.1.1.2 Weather data frame

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

Table 4.3: Weather data frame [one row per day in the desired study frame.]

Column	Description
date	Date of measurement
temperature_ave	Daily average temperature (degrees Celsius)
temperature_min	Daily minimum temperature (degrees Celsius)
temperature_max	Daily maximum temperature (degrees Celsius).
precipitation_mm	Daily precipitation (millimeters).
evapotranspiration_mm	Daily evapotranspiration (millimeters).

4.2 Chemical parameters

Table 4.4: ERAHUMED inpu

Parameter	Name	Unit	Group
\texttt{display_name}	Chemical display name	N/A	Chemical identity
\texttt{tmoa_id}	Toxic mode of action ID	N/A	Chemical identity
\texttt{MW}	Molecular weight	g/mol	Physicochemical properti
\texttt{ksetl_m_day}	Settling rate	m/day	Transport parameters
\texttt{sol_ppm}	Solubility	ppm	Physicochemical properti
\texttt{koc_cm3_g}	Koc	cm ^{3} /g	Sorption
\texttt{fet_cm}	Foliar extraction term	1/cm	Transport parameters
\texttt{kf_day}	Foliage degradation rate	1/day	Degradation
\texttt{kw_day}	Water column degradation rate	1/day	Degradation
\texttt{ks_sat_day}	Saturated sediment degradation rate	1/day	Degradation
\texttt{ks_unsat_day}	Unsaturated sediment degradation rate	1/day	Degradation
\texttt{kw_temp}	Water degradation reference temp.	$^\circ$ C	Degradation
\texttt{ks_sat_temp}	Sat. sediment degradation ref. temp.	$^\circ$ C	Degradation
\texttt{ks_unsat_temp}	Unsat. sediment degradation ref. temp.	$^\circ$ C	Degradation
\texttt{Q10_kw}	Q10 for water degradation	N/A	Degradation
\texttt{Q10_ks_sat}	Q10 for sat. sediment degradation	N/A	Degradation
\texttt{Q10_ks_unsat}	Q10 for unsat. sediment degradation	N/A	Degradation
\texttt{ssd_acute_mu}	SSD acute mean (log10)	N/A	Toxicity
\texttt{ssd_acute_sigma}	SSD acute std. deviation (log10)	N/A	Toxicity
\texttt{ssd_chronic_mu}	SSD chronic mean (log10)	N/A	Toxicity
\texttt{ssd_chronic_sigma}	SSD chronic std. deviation (log10)	N/A	Toxicity

4.3 RFMS parameters

Table 4.5: ERAHUMED input paran

Parameter	Name	Unit	Group	Type
\texttt{sowing_yday}	Start of sowing season	N/A	Calendar	\texttt{integer(1)}
\texttt{harvesting_yday}	End of sowing season	N/A	Calendar	\texttt{integer(1)}
\texttt{perellona_start_yday}	Start of Perellona	N/A	Calendar	\texttt{integer(1)}
\texttt{perellona_end_yday}	End of Perellona	N/A	Calendar	\texttt{integer(1)}
\texttt{flow_height_cm}	Target water level (sowing)	cm	Hydrology	\texttt{numeric(1)}
\texttt{perellona_height_cm}	Target water level (Perellona)	cm	Hydrology	\texttt{numeric(1)}
\texttt{display_name}	Display name	N/A	Metadata	\texttt{character(1)}

4.4 Spatial allocation parameters

Parameter	Name	Unit	Group	Type
\texttt{map}	Cluster map	N/A	Inputs	\texttt{erahumed_rfms\
\texttt{system}	Management system	N/A	Inputs	\texttt{erahumed_rfms}
\texttt{target_fraction}	Target allocation fraction	1	Allocation settings	\texttt{numeric(1)}
\texttt{ditches}	Ditches	N/A	Allocation settings	\texttt{integer}
\texttt{field_type}	Field type	N/A	Allocation settings	\texttt{character(1)}

5 Hydrological model of the Albufera Natural Park

The first step in assessing toxicological risks in the Albufera Natural Park is to determine the system's hydrology, as water serves as the primary transport medium for the chemicals under study. Specifically, by "hydrology," we refer to the water volumes present in each water body at a given moment and the flow of water between them over a defined time frame (*e.g.*, one day). Since most of these quantities are not directly measurable, they must be estimated through simulation. This Chapter outlines the algorithms used for this process.

5.1 Definition of hydrological elements

Our hydrological model represents the Albufera Natural Park in terms of three main landscape 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).

5.2 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 4.1).
- 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.

5.3 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].

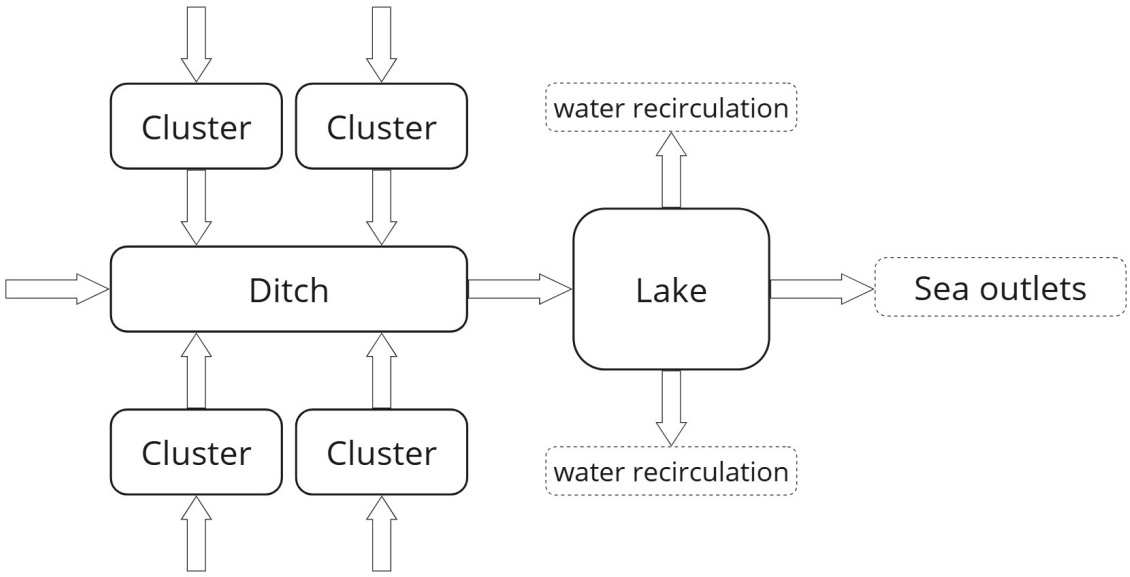

Figure 5.1: Scheme of ERAHUMED hydrological model of the Albufera Natural Park

[1]Further details on this are discussed in Section 5.4.1.

5.4 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.

5.4.1 Albufera Lake

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

$$\text{Volume Change} = \text{Inflow} - \text{Outflow} + \text{Precipitation} - \text{Evapotranspiration}. \tag{5.1}$$

The variables collected into the following table, that enter the balance equation 5.1, have direct correspondence with model input parameters listed in Chapter 4 (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

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

$$V_t = \alpha + \beta \cdot h_t, \tag{5.2}$$

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

$$\Delta V_t^{\mathrm{PET}} = \sigma_{\mathrm{PET}}(\mathrm{P}_t - \mathrm{ET}_t), \tag{5.3}$$

Total inflow and outflow must satisfy Equation 5.1, which we may rewrite explicitly as:

$$\Delta V_t - \Delta V_t^{\mathrm{PET}} = I_t - O_t, \tag{5.4}$$

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:

$$O_t = \max\left[O_t^{\mathrm{Pujol}} + O_t^{\mathrm{Perelló}} + O_t^{\mathrm{Perellonet}},\, \Delta V_t^{\mathrm{PET}} - \Delta V_t\right]. \tag{5.5}$$

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 5.4 itself, due the physical constraint that $I_t \geq 0$.

Once O_t is calculated through Equation 5.5, I_t can be immediately obtained from Equation 5.4. Notice that whenever the aforementioned compensating outflow term due to water recirculation is included (which happens when the maximum in Eq. 5.5 is given by the second term), the total inflow is always estimated to be zero.

5.4.2 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 5.4.1).
- Assumptions about the hydrological connections between the various water bodies in the natural park, detailed in Section 5.3.
- 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 **?@sec-management-df**. 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`	$\text{cm} \cdot \text{day}^{-1}$	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 is:

$$V_{c,t+1} - V_{c,t} = I_{c,t} - O_{c,t} + (\text{P}_t - \text{ETP}_t) \times A_c \tag{5.6}$$

where P_t and ETP_t are the same as in Section 5.4.1.

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 $c = 1, 2, \ldots, N_C$. On the other hand, clusters are assumed to be irrigated from sources external the Albufera system, *i.e.*, not through any of the ditches that eventually flow into the lake. According to our assumptions on the hydrology of clusters and ditches (*cf.* Section 5.3), the sum of cluster outflows is constrained by:

$$\sum_{c=1}^{N_C} O_{c,t} \leq Q_t \tag{5.7}$$

where Q_t denotes the inflow to the relevant ditch. With a small leap in logic, we anticipate from Section 5.4.3, that the water levels in irrigation ditches are assumed to be constant, so that Q_t can also be identified with the ditch outflow, that is in turn estimated as:

$$Q_t = \frac{\text{Area of clusters draining into ditch}}{\text{Area of all clusters}} \times \text{Lake's Inflow}_t \tag{5.8}$$

where the lake's inflow is computed as described in Section 5.4.1.

Qualitatively speaking, the simulation determines daily values of $I_{c,t}$ and $O_{c,t}$ that satisfy Eqs. 5.6 and 5.7, and such that the resulting hydrology aligns as closely as possible with the "ideal" conditions prescribed by the specified management plan. This is accomplished in three steps:

1. Computing ideal inflows and outflows based on current water levels and management plans.
2. Determining actual inflows and outflows, along with the corresponding actual water level changes.
3. Adjusting management plan delays if some clusters were scheduled to be drained but could not be 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 match 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 management plan delays is to ensure that during each year's sowing season, all cluster's are eventually emptied as required for ground applications of chemicals (modeled in subsequent layers of the simulation). This is achieved by postponing the management plan by one day whenever an emptying condition is not met. Outside of the sowing window, delays are reset to zero to prevent them from accumulating indefinitely, which would be 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 $\delta_{c,0} = 0$.

5.4.2.1 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:

$$d_{c,t+1} = d_{t+1} - \delta_{c,t}, \tag{5.9}$$

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

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

In order to compute ideal inflow and outflow, we require (*cf.* Equation 5.6):

$$V^{\mathrm{id}}_{c,t+1} = \max\{V^{\mathrm{id}}_{c,t} + (\mathrm{P}_t - \mathrm{ETP}_t) \times A_c, 0\} + I^{\mathrm{id}}_{c,t} - O^{\mathrm{id}}_{c,t} \tag{5.10}$$

Clearly, Equation 5.10 alone does not individually specify $I^{\mathrm{id}}_{c,t}$ and $O^{\mathrm{id}}_{c,t}$, but only their difference $\Delta^{\mathrm{id}}_{c,t} = I^{\mathrm{id}}_{c,t} - O^{\mathrm{id}}_{c,t}$. In order to fix both these quantities:

$$\begin{aligned} (I^{\mathrm{id}}_{c,t})^{(0)} &= \begin{cases} k_{\mathrm{flow}} & \text{if } \mathrm{Ir}_{c,t} = \mathrm{Dr}_{c,t} = 1 \\ 0 & \text{otherwise} \end{cases}, \\ (O^{\mathrm{id}}_{c,t})^{(0)} &= (I^{\mathrm{id}}_{c,t})^{(0)} - \Delta^{\mathrm{id}}_{c,t}. \end{aligned} \tag{5.11}$$

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

$$\begin{aligned} O^{\mathrm{id}}_{c,t} &= \max\{(O^{\mathrm{id}}_{c,t})^{(0)}, 0\} \\ I^{\mathrm{id}}_{c,t} &= O^{\mathrm{id}}_{c,t} + \Delta^{\mathrm{id}}_{c,t}, \end{aligned} \tag{5.12}$$

which satisfy Equation 5.10 and give rise to positive $O^{\mathrm{id}}_{c,t}$ and $I^{\mathrm{id}}_{c,t}$.

5.4.2.2 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:

$$\begin{aligned} O_{c,t} &= \min\{O^{\mathrm{id}}_{c,t}, Q_t - \sum_{c'<c} O_{c',t}\}, \\ I_{c,t} &= \max\{I^{\mathrm{id}}_{c,t} - O^{\mathrm{id}}_{c,t} + O_{c,t}, 0\} \end{aligned} \tag{5.13}$$

In simple terms, clusters are emptied in a random order within the allowed capacity of the corresponding ditch. Using Equation 5.13, we finally determine the real water level achieved as:

$$V_{c,t+1} = \max\{V_{c,t} + (\mathrm{P}_t - \mathrm{ETP}_t) \times A_c, 0\} + I_{c,t} - O_{c,t} \tag{5.14}$$

to be compared with Equation 5.10.

[2] With some abuse of notation, we assume the indexes c and c' in Equation 5.13 to be sorted according to this random permutation.

5.4.2.3 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 $W = [20\text{th of April, 15th of October}]$, then $\delta_{c,t+1} = 0$. Otherwise, if $h^{\text{id}}_{c,t} > 0$ or $h_{c,t} < h_{\text{thres}}$, the plan delay is unchanged: $\delta_{c,t+1} = \delta_{c,t}$. Finally, if $h^{\text{id}}_{c,t} = 0$ but $h_{c,t} > h_{\text{thres}}$, we add one day of delay: $\delta_{c,t+1} = \delta_{c,t} + 1$.

5.4.2.4 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 $W = [20\text{th of April, 15th of October}]$, then $\delta_{c,t+1} = 0$. Otherwise, if $h^{\text{id}}_{c,t} > 0$ or $h_{c,t} < h_{\text{thres}}$, the plan delay is unchanged: $\delta_{c,t+1} = \delta_{c,t}$. Finally, if $h^{\text{id}}_{c,t} = 0$ but $h_{c,t} > h_{\text{thres}}$, we add one day of delay: $\delta_{c,t+1} = \delta_{c,t} + 1$.

5.4.3 Irrigation ditches

Our approach to the hydrology of irrigation ditches is simplified, with the main assumption being that all ditches have a common, constant water depth h_{ditch} corresponding to the input parameter `ditch_level_m`.

Using the index $D = 1, 2, \ldots, 26$ to enumerate the park's main ditches, ditch outflows to the Albufera lake $O_{D,t}$ are calculated according to Equation 5.8. These outflows also coincide with the total ditch inflows $I_{D,t}$ (due to the constant water volume assumption).

6 Exposure

This Chapter describes how ERAHUMED models pesticide exposure in the Albufera Natural Park. The hydrological simulation discussed in the previous Chapter provides the foundation for this analysis, as water serves as the primary medium for pesticide transport. Here, we outline how ERAHUMED simulates the introduction, dispersion, and fate of pesticides within the system. This includes processes such as deposition, degradation, and transfer between water bodies. By integrating hydrological dynamics with chemical behavior, the model estimates exposure levels over time and space, supporting risk assessment efforts.

6.1 Pesticide applications

The simulation of pesticide applications to rice fields follows a straightforward algorithm that takes as input the scheduled application list and the system's hydrology (Chapter 5). The algorithm outputs a list of actual applications, specifying the application day and the applied mass. Since the application of each pesticide is computed independently of others, we focus on a single pesticide for the present discussion.

The information on scheduled applications is contained in the `ca_schedules_df` data frame, whose structure is described in detail in **?@sec-ca-schedules-df**. For each scheduled application, this data set specifies:

- An application day D, representing the day of the crop cycle when the pesticide is expected to be applied.
- An application amount, expressed in units of mass per unit area.
- An application type, which is either *aerial* or *ground*, that determines the required rice field conditions for the application.

To determine the actual application date, we proceed as follows (for notation related to cluster hydrology, see Section 5.4.2):

1. **Filtering by irrigation and draining states.** For ground applications, we select only those days in which both $\mathrm{Ir}_{c,t} = \mathrm{Dr}_{c,t} = 0$, where $\mathrm{Ir}_{c,t}$ and $\mathrm{Dr}_{c,t}$ are the true (as opposed to ideal) irrigation and draining states time-series, defined after Equation 5.9. Similarly, for aerial applications, we select days according to $\mathrm{Ir}_{c,t} = \mathrm{Dr}_{c,t} = 1$.

2. **Filtering by water depth (ground applications only).** For ground applications, from the days selected in the previous step, we further filter those where the simulated water depth of the cluster satisfies $h_{c,t} < h_{\text{thresh}}$.
3. **Ensuring separation between applications of the same pesticide.** We retain only those days that are at least five days apart from any previous application of the same chemical.
4. **Selecting the final application day.** From the remaining candidate days, we choose the one where the *delayed day* $d_{c,t}$ defined by Equation 5.9 is closest to D, the originally scheduled application day.

These steps are repeated for all subsequent applications of a given pesticide in a given cluster. It is worth noting that the algorithm for simulating the cluster hydrological balance (Section 5.4.2) guarantees that at least one candidate application day will always remain available in the final selection step.

6.2 Pesticide dispersion

As illustrated in our hydrological model (Figure 5.1), pesticides applied to rice field clusters are transported through water flow into ditches, then into the Albufera lake, and ultimately to the sea.

From a mathematical perspective, the fate of these chemicals is governed by a system of differential equations that captures key physico-chemical processes, including transport, diffusion between compartments, and degradation.

The remainder of this chapter describes our approach to pesticide dispersion. We define the simplified differential system used to model these processes in Section 6.2.2, and we present our semi-analytic solution method in Section 6.2.3.

6.2.1 Diagram of physical processes

The schematic diagram below illustrates the processes captured by our model for chemical dispersion. Directional arrows represent the transfer of chemical matter among the three compartments considered—Foliage, Water, and Soil—as well as exchanges with external water bodies (denoted as "Watercourse").

While the overall scheme applies to all landscape elements, specific details vary for clusters, ditches, and the lake (*cf.* the hydrological model of Figure 5.1):

- **Clusters:** Inflow waters originate outside the system and are assumed to be free of pesticides.

- **Ditches and the Albufera lake:** No direct pesticide applications occur in these areas, meaning the foliage compartment plays no role in their dynamics.
- **Ditches:** Receive inflows from two sources—clusters, which contribute pesticide-laden water, and external sources, which are assumed to be free of chemicals.
- **Albufera lake:** Its only inflows come from ditches, which contain nonzero chemical concentrations.

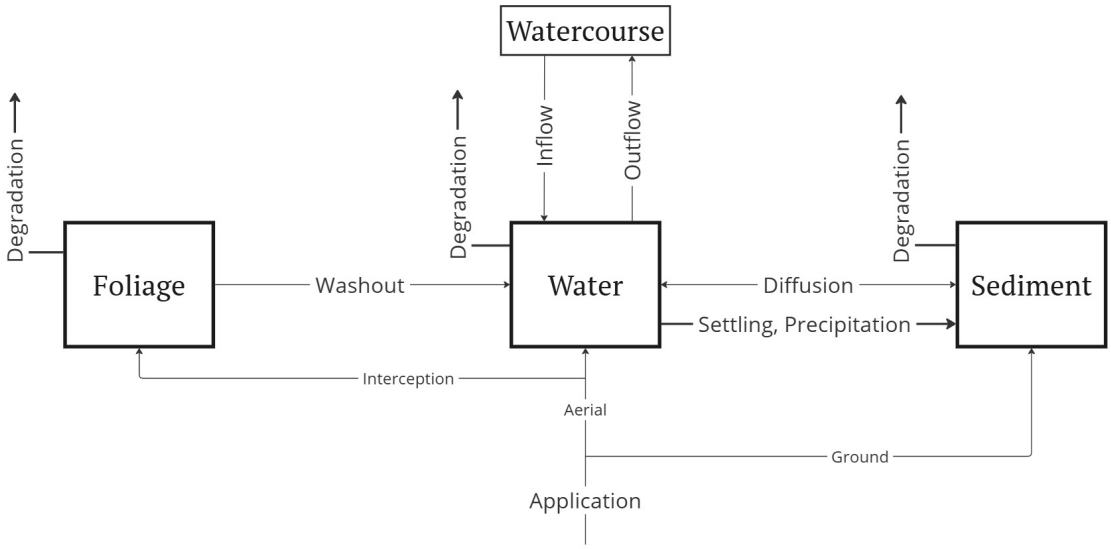

Figure 6.1: Scheme of physical processes considered in ERAHUMED model of chemical dispersion

6.2.2 Evolution Equations

As in Section 6.1, we focus on a single pesticide and a fixed hydrological element (*e.g.*, a cluster). We denote its masses in the three compartments—foliage, water, and sediment—by m_f, m_w, and m_s, respectively. We assume that, at any given time, these masses are fully diluted and homogeneously distributed. In particular, we can meaningfully define spatially constant concentrations c_f and c_s in the water[1] and sediment compartments.

We first describe the differential system that drives the temporal dynamics of m_f, m_w and m_s. The correspondence between the parameters used in this and the following Section is provided in Section 6.2.4.

The fundamental equations describing pesticide diffusion are given as follows:

[1]Provided the water volume is nonzero.

$$
\begin{aligned}
\frac{\mathrm{d}m_f}{\mathrm{d}t} &= -(k_f + w)m_f + a_f \\
\frac{\mathrm{d}m_w}{\mathrm{d}t} &= -(k_w + d_w + s + \frac{O}{V})m_w + d_s m_s + w m_f + a_w - \sigma(\frac{m_w}{\rho V}) \\
\frac{\mathrm{d}m_s}{\mathrm{d}t} &= (d_w + s)m_w - (k_s + d_s)m_s + a_s + \sigma(\frac{m_w}{\rho V})
\end{aligned}
\tag{6.1}
$$

where:

- $a_{f,w,s}$ are the mass income rates of the chemical in the three compartments, that include direct pesticide application and mass coming from inflows.
- $k_{f,w,s}$ are the degradation rates of the chemical in the three compartments,
- d_w and d_s are the water-sediment diffusion rates,
- s is the settling rate,
- w is the washout rate,
- O is the outflow rate of the rice field,
- V is the volume of water in the rice field,
- ρ is the chemical solubility in water,
- $\sigma(x)$ is a function (not further specified, see below) that grows quickly for $x > 1$, and vanishes for $x \leq 1$. This function accounts for solubility.

Strictly speaking, all these terms have instantaneous time dependence[2]. Apart from making the system 6.1 hard to attack by analytic means, such a dependence is troubling because we don't have access to the exact time dependence of the majority of these terms (*e.g.* outflow, volume or chemical applications), our input consisting of simple daily average/cumulative values. On the other hand, if all the terms were constant, and if we could neglect σ, the solution of Equation 6.1 would be immediate, as the corresponding system becomes a linear ODE with constant coefficients, in addition whose eigenvalues and eigenvectors can be computed explicitly.

What we use in practice is an intermediate semi-analytic approach that allows us to compute daily values of $m_{f,w,s}$, which is described next.

6.2.3 Semi-analytic solution of Equation 6.1

The time evolution of $m_{f,w,s}$ in a daily time-step (from t to $t+1$, say, assuming t is measured in days) is obtained through the following four consecutive stages:

[2]This observation also includes pure physico-chemical "constants" such as degradation rates, where the time dependence would stem from *temperature* dependence.

1. We compute the exact evolution of $m_{f,w,s}$ according to the linear ODE obtained by disregarding the processes of outflow, chemical application and solubility, and using daily constant values for all the remaining constants involved (described in more detail below).
2. We compute the m_w losses due to outflow as if they happened instantaneously after the processes computed in the previous step took place, with the water volume of the rice paddy varying from $V(t+1)+O(t)$ to $V(t+1)$.
3. We compute the mass applications again as instantaneous, after the losses in the water compartment due to outflows took place.
4. We compare the resulting m_w with the maximum amount allowed by the solubility in water, that is $m_w^{\max}(t) = \rho V(t+1)$ and transfer any excess to the sediment compartment (m_s).

In the following, we describe in full detail the computations involved in these four steps.

6.2.3.1 Step 1: linear ODE evolution (physico-chemical processes)

Disregarding outflow, mass application and solubility, we get a linear ODE of the form:

$$\begin{aligned} \frac{\mathrm{d}m_f}{\mathrm{d}t} &= \gamma m_f, \\ \frac{\mathrm{d}m_w}{\mathrm{d}t} &= a_{ww} m_w + a_{ws} m_s + w m_f, \\ \frac{\mathrm{d}m_s}{\mathrm{d}t} &= a_{sw} m_w + a_{ss} m_s, \end{aligned} \tag{6.2}$$

with:

$$\begin{aligned} \gamma &= -(k_f + w), \\ a_{ww} &= -(k_w + d_w + s) \\ a_{ws} &= d_s \\ a_{sw} &= d_w + s \\ a_{ss} &= -(k_s + d_s) \end{aligned} \tag{6.3}$$

where the various physico-chemical parameters are assumed to be constant during a daily time-step (*cf.* Section 6.2.4).

The evolution of m_f is easily obtained:

$$m_f(t) = e^{\gamma t} m_f(0). \tag{6.4}$$

Plugging this into the three-dimensional system 6.2 we obtain a reduced two-dimensional system for the water-sediment compartments:

$$\begin{aligned} \frac{\mathrm{d}m_w}{\mathrm{d}t} &= a_{ww}m_w + a_{ws}m_s + we^{\gamma t}m_f(0), \\ \frac{\mathrm{d}m_s}{\mathrm{d}t} &= a_{sw}m_w + a_{ss}m_s, \end{aligned} \tag{6.5}$$

which is solved explicitly with standard methods[3].

6.2.3.2 Step 2: mass losses due to outflow

Mass losses due to outflow are computed as if the outflow process happened instantaneously after the processes discussed in the previous step took place. The amount of mass in the water compartment is affected as follows:

$$m_w \to \frac{V_f}{V_i}m_w, \tag{6.6}$$

where V_i and V_f denote the initial and final volume for the outflow process. Here V_f coincides with the simulated value $V(t+1)$ for the relevant water body and $V_i = V_f + O(t)$, where $O(t)$ denotes the total simulated outflow for day t.

[3] Letting $x = (m_w, m_s)^T$ and $b = w(m_f(0), 0)^T$, the system can be rewritten in the form:

$$\dot{x} = Ax + e^{\gamma t}b$$

where

$$A = \begin{pmatrix} a_{ww} & a_{ws} \\ a_{sw} & a_{ss} \end{pmatrix}$$

The general solution reads:

$$x(t) = e^{At}x(0) + (e^{At} - e^{\gamma t}I)(A - \gamma I)^{-1}b$$

where I is the identity matrix. Notice that the exponential can be computed explicitly from the eigenvalues of A:

$$e^{At} = e^{\lambda_+ t}P_+ + e^{\lambda_- t}P_-,$$

with:

$$\lambda_\pm = \frac{\mathrm{Tr}A}{2}\sqrt{\left(\frac{\mathrm{Tr}A}{2}\right)^2 - \det A}$$

and

$$P_\pm = \pm\frac{1}{\lambda_+ - \lambda_-}(A - \lambda_\mp)$$

6.2.3.3 Step 3: mass income from direct application and inflows

These contributions are computed as instantaneous and subsequent to outflow. Masses in the various compartments ($i = f,\ w,\ s$) are modified as follows:

$$m_i \to m_i + a_i \tag{6.7}$$

As mentioned above, a_i accounts for both direct pesticide applications and water inflow, that is:

$$a_i = a_i^{\text{app}} + a_i^{\text{inflow}}$$

The calculation of direct application rates from input parameters is described below. As to the second term, the amount of incoming mass is exactly given by the amount of outgoing mass in the outflow of the preceding element along the water course chain, which is computed as detailed in the previous Section.

6.2.3.4 Step 4: solubility

The chemical density in the water compartment after Steps 1, 2, and 3 is eventually compared with the chemical's solubility ρ, and any mass excess is instantaneously transferred to the sediment compartment. This implies the following modifications:

$$m_s \to m_s + \max(0,\ m_w - \rho V(t+1)), \quad m_w \to \max(m_w,\ \rho V(t+1)). \tag{6.8}$$

6.2.4 Input parameters (correspondence with Chapter 4)

This Section describes the sources of the various numerical inputs to Equation 6.1.

6.2.4.1 Pesticide application rates

Application rates are given by:

$$\begin{aligned}
a_f^{\text{app}} &= A(t) \cdot (1 - \text{drift}) \cdot c(t), \\
a_s^{\text{app}} &= A(t) \cdot (1 - \text{drift})(1 - c(t)) I(h(t+1) \neq 0), \\
a_w^{\text{app}} &= A(t) \cdot (1 - \text{drift}) \cdot (1 - \text{SNK})(1 - c(t)) I(h(t+1) = 0),
\end{aligned}$$

Here, $A(t)$ is the applied amount on day t, whose computation was described in this chapter; $I(h(t+1) = 0)$ is equal to one if the water level of the cluster $h(t+1) = 0$, and vanishes

otherwise[4]; the quantities drift, SNK correspond to the internal `drift` and `SNK` parameters (*cf.* Chapter 4); finally c is the coverage fraction, computed as:

$$c = \min\left[\frac{d_s(t)}{j_{\text{grow}}}, 1\right] \cdot c_{\max},$$

where $d_s(t)$ is the number of days elapsed from seeding, assumed to be on the 20th of April, while j_{grow} and $c_{\max}$ correspond to the input parameters `jgrow` and `covmax`.

6.2.4.2 Degradation rates

Daily degradation rates $k_{f,w,s}(t)$ for the chemical are modeled through the Arrhenius equation, schematically:

$$k(t) = k_0 \cdot Q_{10}^{\frac{T(t)-T_0}{10}}$$

where k_0 is the degradation rate k_0 at a reference temperature T_0, Q_{10} is a numerical constant, and $T(t)$ is the average temperature on day t. The constants k_0 and Q_10 are internal model parameters, while $T(t)$ is given by `weather_df$temperature_ave`, see Section 4.1.1.1.

6.2.4.3 Diffusion rates

Diffusion rates are given by:

$$d_w(t) = \frac{k_{\text{dif}} \cdot f_{D,w}}{h(t)}, \quad d_s = \frac{k_{\text{dif}} \cdot f_{D,s}}{h_{\text{act}} \cdot \text{pos}}$$

where $h(t)$ is the water depth of the hydrological element; h_{act} is the depth of active sediment, corresponding to the input parameter `dact_m`; *textpos* is the porosity, and is expressed in terms of input parameters as `fc - wilting`; k_{dif} is given by the empirical formula (see TODO):

$$k_{\text{dif}} = \left(\frac{69.35}{365} - \text{pos} \cdot M^{-2/3}\right) \frac{\text{m}}{\text{day}}$$

where M is the molecular weight of the chemical (internal parameter); finally, $f_{D,w}$ and $f_{D,s}$ are given by:

[4]The reason why the height of day $t+1$ is used here is because, as mentioned above, applications are computed using the final water volume of the cluster, as if all daily water flows already took place.

6.2.4.4 Settling rate

The daily settling rate is computed as:

$$s(t) = \frac{k_s(1 - f_{D,w})}{h(t)}$$

where k_s is a (chemical-specific) internal parameter.

6.2.4.5 Washout rate

The daily washout rate is computed as:

$$w(t) = \text{fet} \cdot P(t)$$

where $P(t)$ is the daily precipitation per unit area, while fet is a (chemical-specific) internal parameter.

6.2.4.6 Solubility

The solubility ρ of chemical is an internal parameter.

7 Risk assessment

This Chapter describes how ERAHUMED assesses the toxicological risks associated with pesticide exposure in the Albufera Natural Park. Building on the hydrological and exposure models from the previous Chapters, this step estimates the potential impacts on aquatic organisms and the broader ecosystem. We employ the Species Sensitivity Distribution (SSD) approach, a widely used method in ecological risk assessment [TODO reference]. This approach allows for the identification of high-risk scenarios, supporting management decisions to mitigate adverse effects.

7.1 Calculation of risk using SSDs

The risk calculation follows the approach outlined in [TODO A.Rico Reference], to which we refer the reader for further details. Here, we summarize the key aspects relevant to our model.

SSDs transform the chemical concentrations computed in the previous "Exposure" simulation layer (Chapter 6) into the potentially affected fraction of species (PAF). As described in [TODO], chemicals are grouped by toxic mode of action (TMoA), and different TMoAs are assumed to act independently.

Separate distributions are used to assess acute and chronic risks. In the case of acute risk, we use daily chemical concentration values (computed as described in Chapter 6). For chronic risk, we use a 21-day rolling average of concentrations.

The parameters of each SSD, as well as the TMoA classification for each chemical, are internal to ERAHUMED and are not directly accessible to the user.

Part II

User Manual

8 The ERAHUMED DSS Graphical User Interface

The easiest way to run a simulation with ERAHUMED is through its Graphical User Interface (GUI), which we describe in this chapter. The GUI provides an intuitive way to configure all model inputs described in Chapter 4 and includes predefined visualizations for main model outputs. This makes it an efficient tool for exploring the ecosystem's behavior and analyzing its sensitivity to different scenarios. Additionally, users can export output data for further analysis outside the Decision Support System (DSS).

The GUI is part of a broader software package—an R library—which we describe in detail in Chapter 9. If the screenshots in this chapter differ from the interface you see, check the version number (displayed within the GUI) to ensure you are working with the same release.

8.1 How to run the GUI

At the present moment, the GUI can only be run from R, through the package `{erahumed}`, which is publicly available on Github. Details on R and on the `{erahumed}` package are provided in Chapter 9 and references therein (see, in particular, Sections 9.1 and 9.2 for instructions on how to install R and the `{erahumed}` package). Once you have installed `{erahumed}`, you can access its GUI by running in R the following command:

```
erahumed::launch_dss()
```

8.2 The *Output* tab

Upon launching the GUI, you are greeted by the *Output* tab (Figure 8.1), which serves as the main dashboard for viewing model results through interactive visualizations. Generating the plots may take around 10 to 20 seconds, corresponding to the time required to complete a full simulation for a one-year period.

The dashboard is divided into three sections, each corresponding to a model component:

- **Hydrology** (Chapter 5): Displays water level variations and flow patterns over time.

- **Exposure** (Chapter 6): Shows the concentration of different pesticides in water and sediment.
- **Risk** (Chapter 7): Assesses potential ecological impacts based on pesticide exposure.

Users can explore these components across different hydrological elements of the Albufera Natural Park, including the Albufera lake, irrigation ditches, and rice field clusters. The specific location can be selected using the "Water body" dropdown menu. The interactive plots allow users to zoom, pan, and filter data over specific time periods, facilitating a more detailed analysis of model outputs.

The "Download results" button, located in the top-right corner, exports all raw model outputs as a compressed `.zip` file containing `.csv` data.

Figure 8.1: Graphical User Interface - *Output* tab

The visualizations in this tab reflect the selected input parameters. Adjusting inputs in the Input tab described in the next Section allows users to explore different scenarios and assess their impact on model outcomes.

8.3 The *Input* tab

9 The {erahumed} R package

As mentioned in Chapter 8, the software infrastructure of the ERAHUMED DSS is a library for the R programming language. The {erahumed} R package already has extensive documentation, which you can consult on its main website. In particular, this article provides a step-by-step guide to the package's main functionalities, explaining how to run a simulation.

The rest of this chapter provides brief instructions on installing R and the {erahumed} package. If you are a proficient R user, you may confidently skip this part and simply follow the instructions in the package README to install {erahumed} and launch the Shiny app that provides its GUI.

The {erahumed} R package is open-source software and is hosted on GitHub. If you have a suggestion, want to report a bug, or need help, feel free to open a GitHub issue (you will need to sign in to GitHub with a personal account, which you can create for free). Pull requests with code improvements are also welcome!

9.1 Installing R

R is a free programming language and software environment widely adopted in the scientific community due to its powerful statistical capabilities and user-friendly interface. The {erahumed} package allows users to run simulations, prepare custom inputs, and explore outputs in detail—all from the R command line. Compared to the graphical user interface (GUI), using R directly provides greater flexibility and control over these operations.

To install R, visit the official R project website, where you will find detailed installation instructions for various operating systems. If you are new to R, there are many introductory resources available online, including the official R manual from the R Core Team. However, if your only goal is to run the ERAHUMED GUI on your local machine, you won't need extensive knowledge of R. Simply installing R and running a few commands in the command line will be enough to get started.

9.2 Installing {erahumed}

Once R is installed, setting up the {erahumed} package requires just one or two commands in the R console. Detailed installation instructions are available here.

9.3 Using `{erahumed}`

For a quick start with `{erahumed}`—whether using the GUI or the R command line—refer to the usage guide. For a more in-depth walkthrough of the command-line workflow, see the main package vignette.

9.4 Getting Help

For support and troubleshooting, visit the help section.

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