



The pesticide fate tool for groundwater vulnerability assessment within the geospatial decision support system LandSupport

Marialaura Bancheri^a, Francesco Fusco^b, Daniele Dalla Torre^{c,d}, Fabio Terribile^{c,e}, Piero Manna^a, Giuliano Langella^{c,e}, Pantaleone De Vita^b, Vincenzo Allocca^b, Harald Loishandl-Weisz^f, Tamás Hermann^g, Carlo De Michele^h, Antonio Coppolaⁱ, Florindo Antonio Mileti^c, Angelo Basile^{a,*}

^a Institute for Mediterranean Agricultural and Forestry Systems (ISAFOM), National Research Council (CNR), Portici, NA, Italy

^b Dipartimento di Scienze della Terra, dell'Ambiente e delle Risorse (DiSTAR), University of Naples Federico II, Naples, Italy

^c CRISP Research Center, Department of Agriculture, University of Napoli Federico II, Portici, Naples, Italy

^d Free University of Bolzano, Faculty of Science and Technology, Bolzano, Italy

^e Department of Agriculture, University of Napoli Federico II, Portici, Naples, Italy

^f Umweltbundesamt – Environment Agency Austria (EAA), Wien, Austria

^g Institute of Advanced Studies (iASK), Kőszeg, Hungary

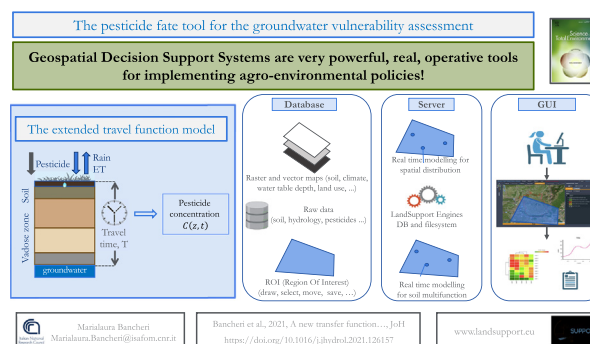
^h ARIESPACE SRL (ARIES), established in Centro Direzionale ISA3, NAPOLI, Italy

ⁱ School of Agricultural, Forestry, Food and Environmental Sciences (SAFE), Hydraulics Division, University of Basilicata, Potenza, Italy

HIGHLIGHTS

- The pesticide fate tool is used for the groundwater vulnerability assessment.
- The tool, dynamical in space and time, is integrated within the LandSupport S-DSS.
- The tool simulates the spatio-temporal distribution of non-point-source solutes.
- The time intervals, crops and pesticides are user-defined and site-specific.
- Three applications of the tool, in different pedoclimatic conditions, are shown.

GRAPHICAL ABSTRACT



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ABSTRACT

The protection of groundwater resources from non-point-source pollutants, such as those coming from agricultural practices, is the focus of several European Directives, including the Water Framework Directive and the Pesticide Directive. Besides the environmental goals to be reached by the single EU member state, these directives clearly underline the role of experts in supporting planners and public authorities to fulfil these objectives. This work presents a new web-based, freely-available dynamical tool, named the *pesticide fate tool*, developed within the geospatial Decision Support system (DSS), LandSupport, for the assessment of groundwater vulnerability, specific for type of pollutant. The tool is based on the extended transfer function model, specifically expanded to consider the transport of reactive solutes, such as pesticides. The work describes the tool implementation for three case studies, with different spatial scales and pedo-climatic conditions: Valle Telesina, IT, Marchfeld, AT, and Zala County, HU. Principal inputs of the tool are: soil physical and hydrological properties, climate, groundwater table depth, type of crops and related pesticides. Results of the model are shown through the LandSupport GUI both as coloured maps, representing the relative concentration of pesticide at the arrival to the water table at the end of the simulation period, and as cumulative charts of the solute arrival at the depth of

* Corresponding author at: Institute for Mediterranean Agricultural and Forestry Systems (ISAFOM), National Research Council (CNR), Piazzale Enrico Fermi, 1, Portici, NA, Italy.
E-mail address: angelo.basile@cnr.it (A. Basile).

interest. The three case studies are shown as examples of application of the LandSupport DSS in supporting the Water and Pesticides directives, demonstrating that it represents a valuable instrument for public authorities, environmental planners, as well as agricultural extension services. For example, large differences are shown by soils in filtering the tetraconazole (99.9% vs 76%), a fungicide used in viticulture, or different percentage of arrival (0.32% and 0.01%) to the groundwater table are shown for two herbicides (Tribenuron and Florasulam) largely used to control annual dicotyledonous weeds.

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1. Introduction

Across the globe, groundwater is an essential source of freshwater for domestic, agricultural and industrial uses, as well as for ecosystems sustainability. However, this resource is often deteriorated by increasing pollution, overexploitation, wrong management, and increasing developmental activities (Machiwal et al., 2018).

All over the world, directives state prioritizing actions to be taken for the protection and the avoidance of pollution of waters. For example, in the European Union, the Directive on the protection of groundwater against pollution and deterioration (Dir. 2006/118/EC), the Nitrate Directive (Dir. 91/676/EEC) and the Pesticide Directive (Dir. 2009/128/EC) are among the most important. Besides, the Water Framework Directive (WFD, Dir. 2000/60/EC) produces a framework which somehow harmonise and includes most of the above regulations.

Despite the huge effort produced in implementing these directives, also through a good governance framework for integrated water management, it is evident from the WFD fitness check (SWD-2019- 440 final) that after 21 years, no substantial progress in improving the quality status of the water bodies has been made (between 1st and 2nd river basin management cycles). In fact, less than a half of the EU's water bodies are in good status, even though the deadline for achieving this goal was 2015. One of the main reasons behind such shortcomings is the weak connections and interactions of water bodies governance with agriculture. Kristensen et al. (2018) highlights that one of the key impediments across Europe to realize the WFD goals are the chemicals coming from agricultural sources. Pollution from non-point sources is considered among the most 'intractable' (e.g., Gunningham and Sinclair, 2005) or 'wicked' (e.g., Patterson et al., 2013; Wiering et al., 2020) problems in the water governance.

Focusing on the Pesticide Directive, one of the main points is the control of the surface water and groundwater pollution, through the reduction of pesticides use and exposure, even based on their substitution, when applicable, with the integrated pest management. This task is demanded, for example, to each individual EU state that, through the National Action Plans (NAPs), to set "the quantitative objectives, targets, measures, timetables and indicators to reduce risks and impacts of pesticide use on human health and the environment". In this framework, quantitative recognition and the role of the experts in supporting users in the selection of crops and crop rotation, and of suitable plant protection measures for specific lands, with particular vulnerability to pollutants, is also crucial.

However, the European Court of Auditors, reports that "the progress towards measuring and reducing risks from pesticide use in the EU has been limited... Several Member States have been late in fully transposing the directive on sustainable use of pesticides, while incentives for farmers to adopt alternative methods remain weak. In addition, the European Commission is unable to precisely monitor the effects or risks resulting from pesticide use, say the auditors.". In the same document, there is also a reference to the new Common Agricultural Policy (CAP), stating that the opportunity to properly address this issue in the forthcoming CAP was unfortunately missed. Eventually, they state that the Commission still lacks a robust evidence base to assess whether the directive has achieved the EU's objective of making pesticide use sustainable and recommend developing better risk, science based, indicators. This opinion is further confirmed in the European Parliament resolution of 13

September 2018 on the implementation of the Plant Protection Products Regulation (EC) No 1107/2009 (2017/2128(INI)).

In such complex and difficult framework, it is self-evident that the availability of freely available operational systems, enabling to connect and manage agriculture in view of water quality, is vital and it may support a better implementation of the above-mentioned water protection directives.

In the last decade, Decision Support Systems (DSS) turn out to be very powerful instruments in the hands of planners/decision-makers, allowing - among many other features - the *on-the-fly* modelling, supporting the what-if scenarios (Yalew et al., 2016; Lindblom et al., 2017; Zaza et al., 2018; Marano et al., 2019; Manna et al., 2020; Nicholson et al., 2020). Between their several applications, DSS can be used, for example, to explicitly simulate the flow of water and the transport of dissolved contaminants, through the saturated and unsaturated zones, at different spatio-temporal scales (Terribile et al., 2015). In this context, the H2020 LandSupport (LS) (www.landsupport.eu) project was implemented with the objective of developing a geoSpatial DSS (S-DSS) - freely available on the web - for the sustainable management of agriculture and forests, under different land uses, with the aim to support and impact about 20 European land policies and selected 2030 UN Sustainable Development Goals, including those related to climate change. Around 100 tools will eventually be available within the platform, among which some, dedicated to the assessment of the groundwater vulnerability, were implemented in the group of land degradation.

The groundwater vulnerability could be defined as its susceptibility to be negatively affected by a contaminant input from the land surface (Foster et al., 2013), through its transport across the unsaturated and saturated zones. The assessment of groundwater vulnerability is a crucial aspect for the management of risk to pollution of groundwater resources as well as for issuing policies aimed at protection of groundwater. Conventionally, a distinction is made between the i) intrinsic vulnerability, and the ii) specific vulnerability. The first can be defined as the vulnerability due to the physical properties of system, i.e., geology, hydrology and hydrogeology, independent from the type of contaminants (Gogu and Dassargues, 2000). Specific vulnerability, on the other hand, is related to particular contaminants, considering their properties (i.e., physical and chemical processes) in addition to the characteristics of saturated and unsaturated zones (Gogu and Dassargues, 2000).

Depending on the scale of analysis and therefore on spatial resolution and quality of data available, groundwater vulnerability can be estimated with different approaches (Civita, 2010). A first group assesses the intrinsic vulnerability at the regional scale by qualitative estimates of hydrogeological and geomorphological features (Albinet and Margat, 1970). A second group includes parametric methods that estimate the intrinsic vulnerability by semi-quantitative approaches based on hydrogeological, topographic, and land use factors affecting the pollutants transport and the attribution to them of scores dependent on their impacts on the aquifer. By a map-overlay procedure, the vulnerability index is estimated as the sum of the previously attributed score values. Among methods included in this group: GOD (Foster, 1987), DRASTIC (Aller, 1985), SINTACS (Civita and De Maio, 2000; Tufano et al., 2020) or EPIK (Doerfliger et al., 1999). Applying a similar approach, with empirical corrections, some methods - among others -

assess the specific vulnerability for pesticides (Saha and Alam, 2014) and for nitrates (Javadi et al., 2011). Finally, a third group of methods includes quantitative approaches based on numerical modelling or analytical solutions of pollutant transport. Among the most used indicators of groundwater vulnerability is the travel time of a pollutant through the unsaturated zone, which can be estimated by analytical advective-dispersive transport models (e.g., Connell and Van den Daele, 2003), finite element models (e.g., Holman et al., 2004; Fusco et al., 2020) or type transfer functions (TTFs) (e.g., Coppola et al., 2013a; Bancheri et al., 2021).

This work deals with the evaluation of the groundwater specific vulnerability through the application of the TFM-ext model (Bancheri et al., 2021), an operational model for policy applications, not computationally demanding, combining the research-scientific world and the everyday real-life applications. In S-DSS context, in fact, the use of models based on CPU-demanding numerical solutions (e.g., Richards combined with Advective-Dispersion equation) may not be advisable, because the end-users typically require real-time answers that are effective, easily interpretable, on a dynamical map and, ideally, freely available on the web.

The main aim of this work is to present the *pesticide fate tool* for assessing the groundwater specific vulnerability to pesticides through its application in three different case studies.

The *Pesticide fate tool* aims at supporting public authorities, spatial planners, agricultural extension services, farmers, and scientists to better relate agricultural activities to groundwater preservation, by a dynamical estimation, both in time and space, of specific groundwater

vulnerability, based on the analysis of the natural filtering capacity of the soils, under different crop and pesticide use conditions. It allows the identification of most vulnerable areas, at different spatial scales, given a specific crop and specific management activities. In this sense, the tool represents a valuable instrument in view of a better implementation of both WFD and Pesticide Directive not only for the zoning of the most vulnerable areas, but also for the evaluation of the trade-off between different pesticide uses, within a specific user-defined region of interest.

The *Pesticide fate tool* - thanks to its combined statistically and physically-based approach and its on-the-fly modelling features - represents a great novelty in the panorama of available tools for agro-environmental issues, specifically for pesticides management; definitely, a tool like this, simply does not yet exist.

2. The LandSupport platform

2.1. LandSupport GCI

LandSupport S-DSS allows the users to interact in real-time with digital maps and geo-spatial data through an open-source web-platform. It is designed to operate for different classes of users (public authorities/policymakers; farmers; urban planners; scientific community and so on) and deployed at different scales (European, National, Regional and Local). It is mainly devoted to (i) Support sustainable Agriculture and Forestry; (ii) Evaluate interaction and trade-off with other land uses,

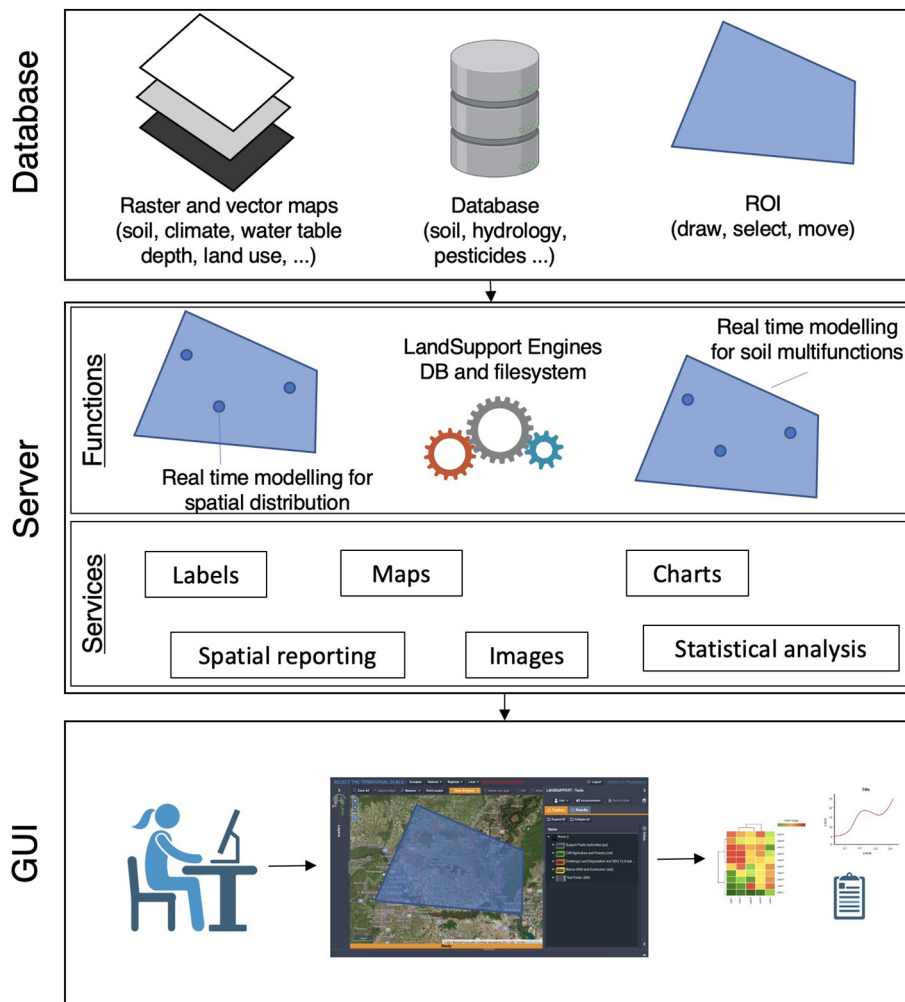


Fig. 1. Synthetic workflow of the basic structure of the LandSupport GCI architecture: functions and technological components.

including spatial planning and (iii) Support the achievement of selected policies, including 2030 SDG's land policies.

The system is built on a Geospatial Cyber-Infrastructure (GCI), which is based on free and open-source libraries and programs, and supports the acquisition, storage, management, integration and visualization of data (both static and dynamical) and on-the-fly modelling applications (Fig. 1). Through the Graphical User Interface (GUI), the users can select the Region of Interest (ROI), launch the DSS tool according to his/her defined specifics and obtain the results as tables, graphs, maps and pdf informative files.

On the server side, a control and management layer called middleware is implemented. This is the component of the GCI where the requests submitted by the end-users are solved. The middleware, in fact, includes services, processes, flows and functionalities to ensure the overall execution of the system, and calls the proper modelling chain, according to the two following cases:

- when the process chain involves models, which are developed on top of COMPSs (Badia et al., 2015) - a runtime system for parallel execution of applications in a set of distributed resources - the last takes care of scaling the calculations according to the computational demand and to the available hardware;
- when the chain requires only structured queries on databases, depending on the data, it makes the right requests to Rasdaman datacube (where raster data are managed) or to PostgreSQL/PostGIS (where vector data are stored and managed).

Eventually, the middleware notifies the user when output data are produced and can be returned to the GUI.

More details on the functionalities and methodological issues can be found in Terribile et al. (2015) and at <https://cordis.europa.eu/project/id/774234/results/it>.

2.2. The LandSupport dashboard and pesticide fate tool implementation

The LandSupport dashboard layout and the *pesticide fate tool* panel, as shown in Fig. 2, are the result of multiple interactions between experts, end-users and stakeholders. One of the most important features

is the choice of the scale of interest that allows the end-user to zoom in/out to the desired area and to access to a scale-dependent toolbox. In fact, tools are activated/deactivated according to the chosen spatial scale, since not all the tools are going to be available/used for all the possible scales (European, National, Regional and Local).

The dashboard consists of five sections (Fig. 2):

- selection of the scale, which allows the users to be directed to the area of interest. This choice automatically activates/deactivates the available tools;
- tools for drawing/selecting/measuring the ROI;
- toolbox/results tabs, to navigate through the tools and through the results of the runs;
- visualization of pre-loaded layers and simulation results;
- layer manager, to activate/deactivate pre-loaded layers and output maps.

The right panel of Fig. 2 shows the pop-up panel of the pesticide tool. It can be accessed both at regional and at local scales, enabling the three implementations for the Valle Telesina, Marchfeld and Zala County. Once the tool is selected, the end-user can choose a pre-defined ROI or draw his/her own ROI in which to perform his/her on-the-fly simulations. Other inputs are i) the start and end dates of simulation; ii) the land use, intended as the type of crop and iii) the pesticide. Then, by clicking on the "evaluate" button, the end-user will get the simulation results.

The "evaluate" button, as described in Fig. 3 and in Section 2.1, will actually activate the middleware workflow: firstly, the soil polygons within the ROI and involved in the simulation will be detected. Then, the middleware takes care of data retrieval both from Rasdaman (for water table depth info and climate data) and from PostgreSQL/PostGIS database for vector layers and tables (soil units, soil data, crop and pesticide lists). At this stage, COMPSs will take care of the model runs. The first model to be launched is for the computation for the mean daily net precipitation. It takes as input the climatic variable for all the simulation points, computes the annual cumulated rainfall, the annual cumulated actual evapotranspiration and eventually, the mean daily net precipitation, which is an input of the TFM-ext model. Then, the TFM-ext model



Fig. 2. Five sections can be distinguished within the LS dashboard: i) the scale selection, ii) the tools for the ROI, iii) the toolbox/results, iv) the layer visualization and v) layer management. The *pesticide fate tool* panel consists of five entries: the ROI, the start and end dates of simulation, the crop and pesticide selections.

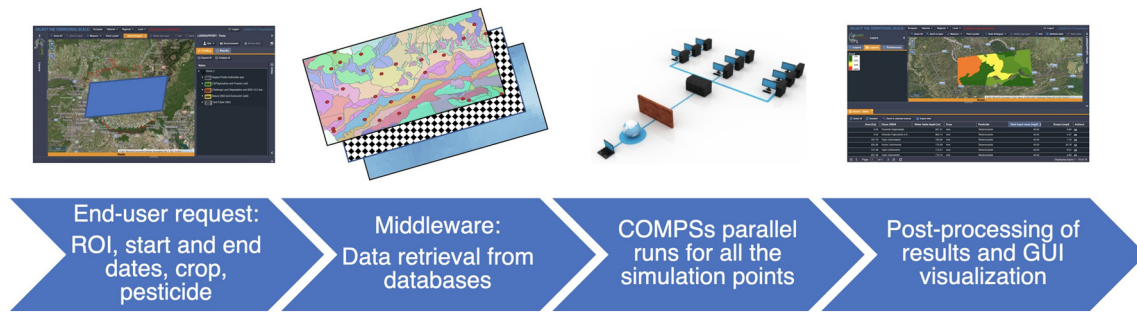


Fig. 3. Implementation of the *pesticide fate tool* within the LandSupport GCI.

is launched for each soil polygon and each year of simulation, according to the user-defined crop and pesticide. Finally, its results are processed to be represented as vector maps or cumulative charts, as shown in the 4.1 Application sections.

3. Materials and methods

3.1. TFM-ext model description

The *pesticide fate tool* is based on the TFM-ext model, fully described in Bancheri et al. (2021). The model computes the output solute flux concentration $C_z(z, t)$ [ML^{-3}], at specified depth z and time t , according to the following equation (Jury et al., 1990):

$$C_z(z, t) = \int_0^T C_0(0, t') f_f(z, t-t') dt' \quad (1)$$

where $C_0(t)$ [ML^{-3}] is the solute input concentration, $f_f(z, t)$ is the Travel Times probability density function (TT-pdf) for a travel distance z , conditional to time t and t' is a dummy variable.

According to Scotter and Ross (1994), TFM-ext derives the TT-pdf for each horizon of a defined soil profile starting from the corresponding hydraulic conductivity curve, $k(\theta)$, and a given steady-state flow rate q . Where no information about the transport properties are available, e.g., between the bottom of the soil profile and the top of the groundwater table level, the model uses the Generalized Transfer Function (GTF) (Zhang, 2000), which describes the travel times distribution with a log-normal form.

In the case of reactive solutes, the model considers:

- the mass decay, due to the natural process by which the solute spontaneously transforms itself (decays) for a radioactive activity, biodegradation, or a chemical process;
- the retardation factor, which, for adsorbed solutes, where sorption is linear, rapid and reversible, describes the ratio between the average linear velocity of the water and the average linear velocity of the reactive solute.

In particular, the mass decay, considering a first order decay process, is computed according to the following equation:

$$\frac{dC(z, t)}{dt} = -\mu C(z, t) \quad (2)$$

where μ [T^{-1}] is the decay constant, computed from the half-life of the considered reactive solute (DT50). The retardation factor R , considering a linear adsorption model, is:

$$R = 1 + \frac{B_d}{\theta} K_d \quad (3)$$

where B_d [M L^{-3}] is the bulk density, θ [$\text{L}^3 \text{L}^{-3}$] is the water content and K_d [$\text{L}^3 \text{M}^{-1}$] is the distribution coefficient of the considered solute.

The model was implemented as a Java application and integrated within the LandSupport platform to be run on-the-fly according to the user specifications, as described below.

3.2. Study sites

Three implementations of the *pesticide fate tool* to Valle Telesina, in Italy, Marchfeld region, in Austria and Zala County in Hungary are presented in this work (Fig. 4). In LandSupport project the three areas were selected because they represent a variety of different climates, morphologies, soil types and spatial extensions, as detailed later in the text. The latter characteristic is particularly relevant in the project, because at different spatial scales correspond different Public Authorities with specific responsibilities and competences.

The Valle Telesina site is located in southern Italy, has an area of about 200 km^2 , characterized by a hilly topography with an altitude from 50 to 1200 m.a.s.l. The climate is typically Mediterranean, with a mean annual rainfall of about 1000 mm and mean annual reference evapotranspiration of around 900 mm, mainly distributed between autumn and winter, and a mean annual temperature of around 15 $^{\circ}\text{C}$ (Alferi et al., 2019). Five different landscape systems (Fig. 4) can be classified in different hydrological complexes (De Vita et al., 2018): carbonate mountains, with volcanic ash deposits covering slopes; hills, comprised of marl arenaceous flysch series; pediment zone, comprised of colluvium material from the slope fan of the limestone reliefs; ancient alluvial terraces; actual alluvial plain. Such complexity is represented by 60 soil typological units, which were aggregated into 46 soil mapping units, as shown in the left panel of Fig. 4.

Marchfeld area is located in Lower Austria, north east of Vienna, has an area of about 1000 km^2 and it is characterized by a flat topography, with an altitude of about 160–180 m.a.s.l. The climate is typically semi-arid, with a mean annual precipitation of about 500–550 mm. The average temperature is between 9 and 10 $^{\circ}\text{C}$ and mean annual reference evapotranspiration is about 800 mm. The dominant soil types are Chernozem and Fluvisol, characterized by humus-rich surface horizons and sandy deep horizons, followed by fluvial gravel from the former river bed of the Danube. 205 soil mapping units were recognized, as shown in the upper right panel of Fig. 4. Although Marchfeld is one of the driest regions in the country (minimum annual precipitation of 300 mm), it is one of the primary sources of agricultural products in Austria, thanks to the use of irrigation to compensate low precipitation.

Zala County is one of the nineteen counties of Hungary. It has an area of about 3800 km^2 and is characterized by varied landscape of hills and valleys. The climate is characterized by an annual mean temperature of about 9–10 $^{\circ}\text{C}$ and by an annual precipitation of 660–800 mm. The geology of the area is characterized by mainly young, Tertiary, clayey or sandy sediments (Pannon deposition) and Pleistocene loess. Its largest river is the Zala that is encompassed by drained swamps along its way to lake Balaton, Central-Europe largest lake (Adhikari et al., 2009). The dominant soil types are brown forest soils, texture differentiated meadow and peat bog soils and less developed (or eroded) soils. 11

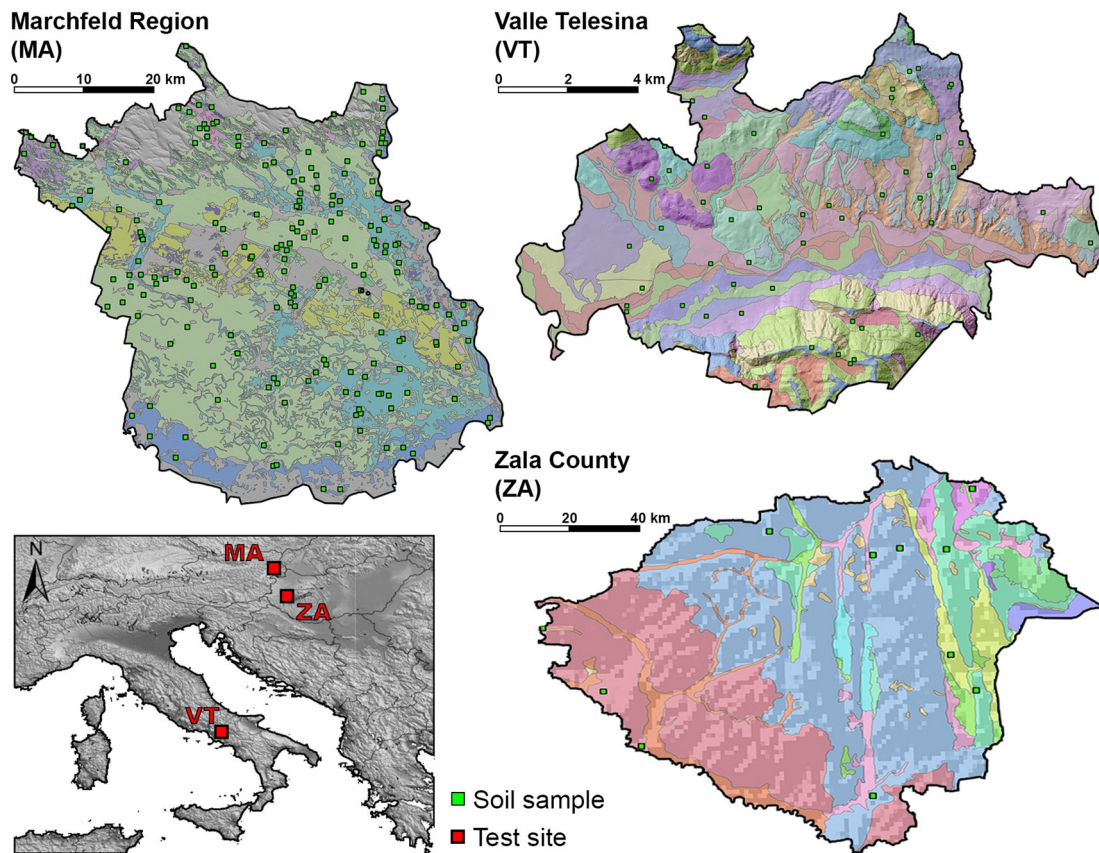


Fig. 4. Localization of the Valle Telesina, Italy (upper right panel), of Marchfeld region, Austria (upper left panel) and of Zala County, Hungary (lower right panel). The plots show the soil units (coloured polygons) and the associate representative soil profile (green dots). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

soil mapping units were recognized, as shown in the lower right panel of Fig. 4.

3.3. Input datasets for Valle Telesina, Marchfeld and Zala

Input datasets for the three case studies are synthetically described in Table 1 that reports, for each theme, the source database and the spatio-temporal resolution, the type of file, the data contained, the parameters obtained by the dataset, the model applied to process the data and the example of model outputs. Eventually, in the following sections, a brief description of the used dataset is reported, while more details are reported in Appendix A.

3.3.1. Soil datasets

The soil datasets for the three case studies contain both information on the hydraulic properties of the representative soil profiles and on the geospatial features of the soil polygons, such as the location and their spatial extent. At the end of the homogenization process, the three datasets contained exactly the same data: horizon depths, hydraulic conductivity curve parameters, textures, organic matters, bulk densities, referred to representative soil profiles linked to polygons or map units in the soil map.

3.3.2. Climate

The dataset of climatic variables contains two different sources of data: reanalysis data, for past climate and climatic scenarios Representative Concentration Pathways (RCP 4.5 e RCP 8.5), for future climate. Reanalysis data (Hersbach et al., 2020; Pelosi et al., 2020) come from the ERA5-Land hourly dataset that has a global coverage from 1981 to present. Available variables are: wind, temperature, surface pressure, solar radiation, precipitation. Future climate data are retrieved from

the EURO CORDEX and CMCC-COSMO-CLM models at daily time-step and cover the time-interval 2006-2100. Available variables are: mean, maximum and minimum temperature, and total precipitation.

3.3.3. Crop type

For all case studies the list of most-commonly crops was populated according to the local farmers/agronomists suggestions. For the Valle Telesina the following 5 crops were considered: vine, olive, wheat, maize and alpha alpha. For Marchfeld: potatoes, sunflower, soya, rape, sugarbeet, maize and wheat. For Zala County: rape, sunflower, wheat and maize.

3.3.4. Water table depth

In this study, maps of groundwater table depth for the three study areas were reconstructed considering piezometric data of existing boreholes and wells, including points of natural surfacing of groundwater circulation (such as springs, rivers, etc.).

3.3.5. Pesticides

The local farmers/agronomists gave - with respect to specific crops - information on the most-commonly used pesticides and management practices related to the dose and the time-span of application. This information was integrated with the ones detailed in the technical sheets associated to commercial formulates. (Pesticide Properties Database (PPDB): <https://sitem.herts.ac.uk/aeru/ppdb/en/index.htm> (Lewis et al., 2016)); The final lists of pesticides for the three case studies is reported in Appendix A and contain 16 active principles for the Valle Telesina, 27 for Marchfeld and 38 for Zala County, including herbicides, fungicides, insecticides both of synthetic and natural origins.

Table 2 reports the details about crops and pesticides used in the three applications shown in the present work.

4. Results and discussion

4.1. Applications

Three example applications are reported in this Section to show the possible use of the tool for i) groundwater vulnerability assessment under different climatic conditions; ii) alternative pesticide uses; iii) protected areas zoning. The three applications, main functionalities, required activities, example of input parameters and example of outputs are reported in Table 3. Then, in the following, results of each are fully described and discussed. It is important to stress that the actual version of the tool, presented in this work, is the result of multiple interactions made, during many months, between developers and end-users/stakeholders involved in the project (Italian, Austrian and Hungarian partners). These interactions mainly concerned the definition of the interface features of the tool, such as how to show the results (maps, graphs and related legends), the layouts of the interfaces of the input and output of the tool (data format, tables organization, preferred units, preferred headers and more). Moreover, from the modelling side, interactions were made to obtain the detailed inputs of the model for each case study (common crops and managements, type of pesticides, doses, day of applications) and to improve the results, considering new equations and relationships to better simulate the pesticide fate.

4.1.1. Groundwater vulnerability assessment

In the first application, the use of the tool for the groundwater vulnerability assessment, under different climatic conditions, is shown (Fig. 5). Once the end-user, e.g., an environmental planner, drew the ROI, selected the start and end dates, the crop and the pesticide, he/her will get the results through the GUI both in a map format and as cumulative charts of pesticide arrival. The example of Fig. 5 shows a ROI selected in the Valle Tesesina, an area devoted to high-quality vine production. For this crop a commonly-used fungicide is the tetraconazole, used for the powdery mildew between April and June, while the simulation period covered the entire year 2009.

The map shows the output mass of pesticide at the end of simulation period, at the groundwater table depth, expressed as a percentage with respect to the total mass injected in the soil over the entire period of simulation (0.04 kg ha^{-1}). The map gives an immediate idea of the soil

response to the pesticide load: greener colours mean that a smaller percentage of mass arrived at the groundwater table depth at the end of 2009, compared to redder polygons. In this case, for example, the soil unit coloured in orange showed a mass arrival at the end of 2009 of about 4% while the soil units coloured in dark green presented a mass arrival of about 0%. To make a more comprehensive analysis, starting from the results obtained with the previous simulation, we also performed 4 runs considering a past climate (1980-2005) and 3 future datasets (2020-2045; 2045-2070; 2070-2095), considering two different climate change scenarios, RCPs 4.5 and 8.5, for the same ROI and under the same crop and pesticide conditions. Given the features of the LS GUI, it is possible to see the evolution of the percentage of mass arrival at the groundwater table depth in time (Fig. 6). Each panel shows the results obtained for three different soils, which were selected because they presented three very different % of mass arrival (orange, yellow and green colours in the map of Fig. 5). We only show the results for the worst-case scenarios (RCPs 4.401 and 8.5 for 2070-2095).

The three soils are classified as *Typic Calciustolls*, *Humic Haplustand* and *Humic Ustivitrands*, according to the soil map dataset. In general, the *Typic Calciustolls* shows the lowest arrival of pesticide, between 0% and 0.004%. The *Humic Haplustand* shows an intermediate behavior (up to 0.1% of mass arrival), while the faster response is shown by the *Humic Ustivitrands*, where in two years after the injection we have that up to the 24% of the input pesticide will likely arrive at the groundwater table depth of 1.70 m. The main reasons behind these different behaviours are both the soil characteristics and, most importantly, the groundwater table depth that varies from 45 m for the *Typic Calciustolls* to the 1.70 m of the *Humic Ustivitrands*.

Comparing, for each soil, the responses under different climate change conditions, it is clear that passing from the past climate (1980-2005) to the RCP 8.5 (2070-2095), we have lower % of pesticide arrivals at the groundwater table depth due to a decrease in the mean net daily precipitation. In fact, the climatic scenario RCP 8.5 shows an increasing trend of the reference evapotranspiration and a decreasing trend of precipitation that, obviously, affect the water balance. Eventually, because the TFM-ext model considers constant input fluxes in time, the variability, in forecasted precipitations and temperatures, shown by the climate change scenarios, both at monthly and at early time scales, resulted to be dumped.

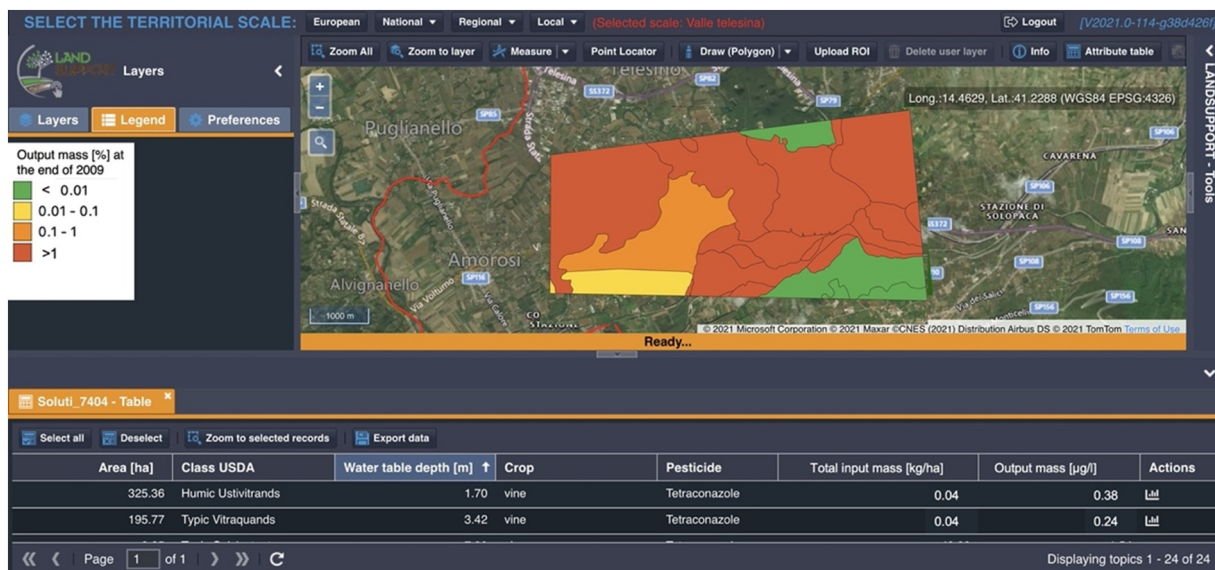


Fig. 5. First example of tool usage: groundwater specific vulnerability assessment. The map shows each soil polygon with a colour associated to its vulnerability: green colour → low vulnerability; red colour → high vulnerability. The result table shows, for each soil polygon: i) the area, ii) the USDA classification, iii) the depth of the water table, iv) the crop and v) the pesticide, vi) the total mass of the pesticide in input during the entire simulation period; vii) the output mass of the pesticide at the end of the simulation period and viii) the action buttons, to show the cumulative charts. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

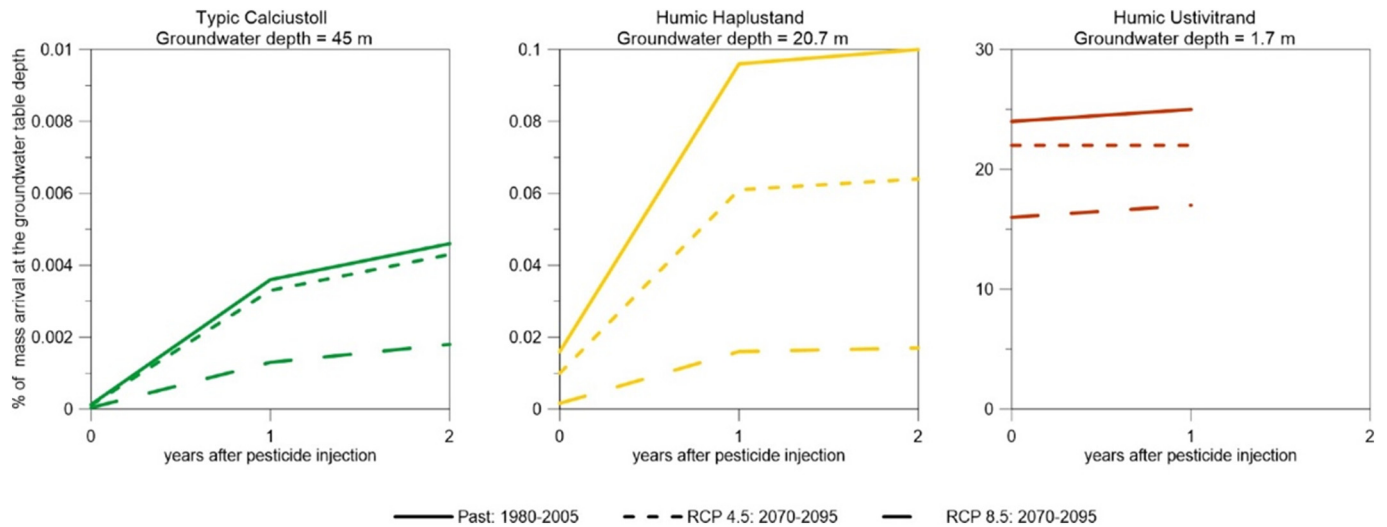


Fig. 6. The charts show the percentage of mass arrival at the groundwater table depth in time for three soil profiles, with very different behaviours. The colours are associated to the polygons shown in the map and consider 3 climatic conditions (past, future RCPs 4.5 and 8.5). Note that the magnitude of the y-axes is different.

The previous results give the end-user an immediate and complete idea of the specific groundwater vulnerability and allows the easy detection of the most vulnerable zones within the selected ROI, under different climatic datasets.

Obviously, depending on the specific needs, public authorities, can choose different time spans of simulations to measure the effects, for example, of a longer time load of a specific pesticide. Moreover, multiple ROIs can be simultaneously chosen, to assess the specific groundwater vulnerability under different spatial conditions. This last example,

could be useful to public authorities for the detection of the most vulnerable zones to be subjected to prioritizing actions.

4.1.2. Alternative pesticide use

In the second application, the use of the tool for the choice of alternative pesticides is shown (Fig. 7). The cumulative charts of the percentage arrival in time are also particularly useful in this case, to compare the behaviours of the two pesticides. The example shows a ROI selected in Zala County, considering wheat, one of the mostly cultivated crops in

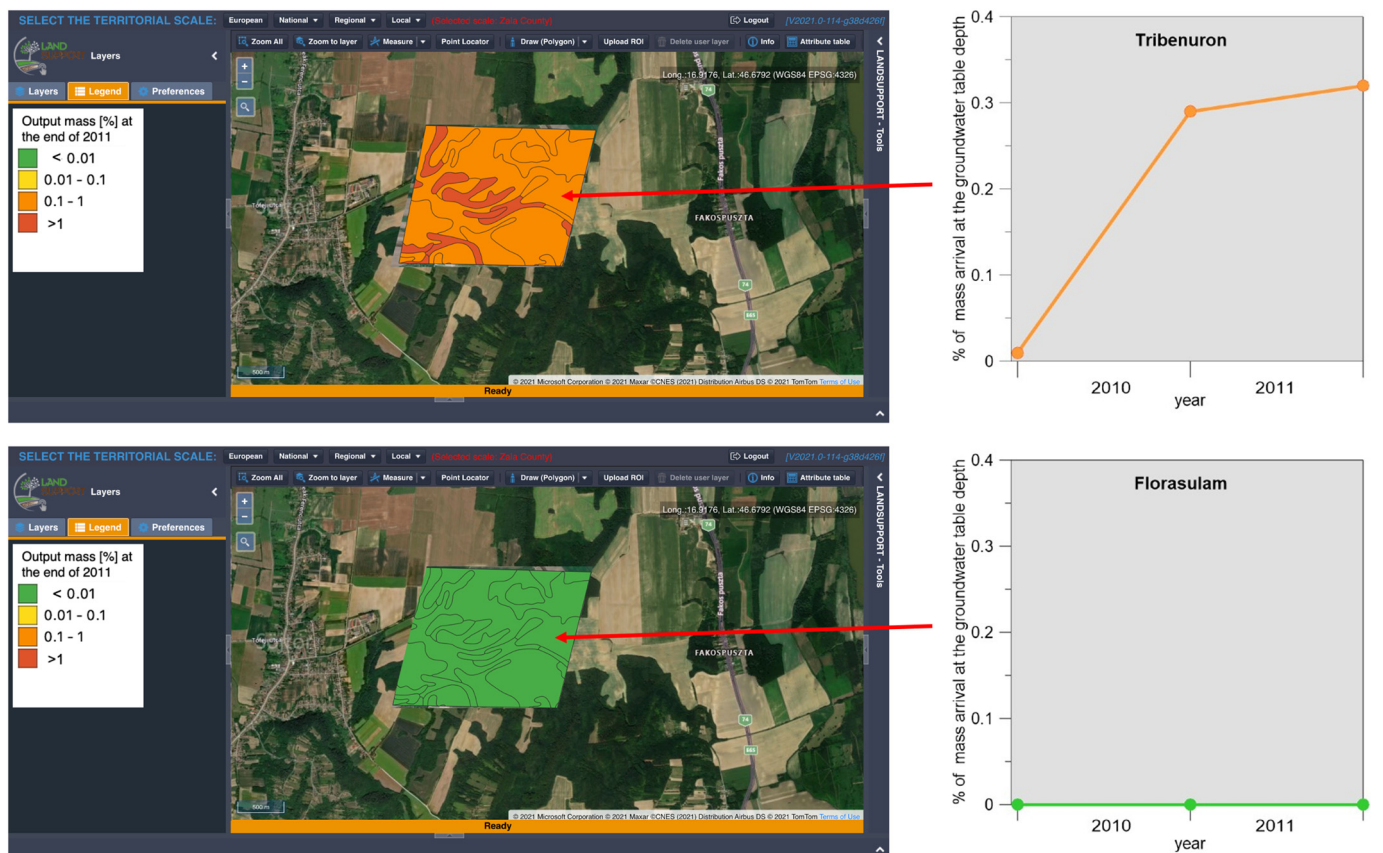


Fig. 7. Second example of tool usage: alternative pesticide use. For the same ROI, it is possible to evaluate the different specific vulnerability associated to the 2 pesticides. The cumulative charts complete the information of the estimated pesticide arrival at the WT depth.

the area and a simulation period of two years (2010–2011). Two commonly-used herbicides are Tribenuron and Florasulam, which are used for annual dicotyledonous weeds.

The two maps immediately help the user, e.g., a farmer, to check the differences of the arrival between the two herbicides. In particular, the Tribenuron shows a map (upper box) with orange to red colours, while the Florasulam (lower box) shows a completely green map. The charts complete the information about the expected % of mass arrival: for the Tribenuron case, due to its lower decay, the maximum mass arrival is about 0.32% of the total input and it would likely arrive at WT depth at the end of 2012, while, for the Florasulam, nothing is expected to arrive. Therefore, this simulation suggests that the careful farmer should prefer the use of the Florasulam herbicide.

This second application is also useful for a Public Authority to estimate the effects of alternative land uses for the definition of Best Practices, thus fulfilling the goals of the new green deal, e.g., the reduction of the overall use of chemical pesticides of 50% by 2030 (https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal/actions-being-taken-eu/farm-fork_en).

4.1.3. Protected areas zoning

In the third application, the use of the tool in special areas for the protected areas zoning is shown (Fig. 8). When the directives request to reduce the use of pesticides within protected sites, such as Natura 2000, the planner should take in mind that not all the areas have the same specific groundwater vulnerability. In this case, the tool helps to zone the most vulnerable areas, allowing better support for an informed reduction of pesticide use. The example shown (Fig. 8) shows a ROI drawn for the Marchfeld area case study in the areas covered by Natura 2000, as shown in the upper-right box of the Figure. With the LandSupport platform, in fact, it was possible to activate the layer showing the Natura 2000 sites and then draw the ROI in the lower Marchfeld, because it is a particularly intensively-cultivated area. The simulation of the *pesticide fate tool* covered two years (2013–2014), considering soya, one of the mostly cultivated crops in Marchfeld and the Dimethenamid-

p pesticide, a pre-emergence herbicide often used to control annual grasses, annual broad-leaved weeds and sedges.

The results show a map predominantly green, with orange polygons on the right of the ROI, with some yellow spots. The higher percentage of solute arrival at the end of simulation period, which caused the yellow and orange polygons, mainly depends on the shallower water table depth, which, for the orange spots, is between 1 m and 3 m. In the greener parts, instead, the water table depth is deeper (more than 10 m). Given the feature of the LS GUI, it is possible to download all the simulation results, thus letting the interested end-users have a deeper analysis of the results. For example, in the lower part of the ROI, for the same water table depth of about 4 m, we can distinguish some green polygons, associated to loamy soils, where the solute arrival at the end of the 2014 is around the 0.001%. The yellow spots in the same area are, on the other hand, associated to loamy-sandy soil, where the solute arrival at the end of the 2014 is around 0.05%. In this particular case, the use of the tool makes the planner aware of the different specific vulnerability and he/she could perform more informed decisions on which area should be primarily treated with other pest management (IPM or organic agriculture) and/or in which area the pesticide needs to be significantly reduced. In this case the tool represents a strong support for the environmental planner to help increase total farmland used for organic farming by 2030 as required by the new green deal.

4.2. Future developments

Future developments of the *pesticide fate tool* are foreseen, principally regarding upgrading of the inputs detailed in Table 1. Due to the flexibility of the LandSupport GCI it is easily possible, as soon as new detailed datasets are available, to integrate them in the databases. This allows a continuous upgrade of the platform and of the tools, keeping them always updated with the latest improvements. In particular, new detailed maps of the soils will be integrated for the present and new case studies. Moreover, the climate database is also easily adaptable, as soon as new climatic models furnish more precise data, and the groundwater table depth could be made dynamical in time to take into account its temporal

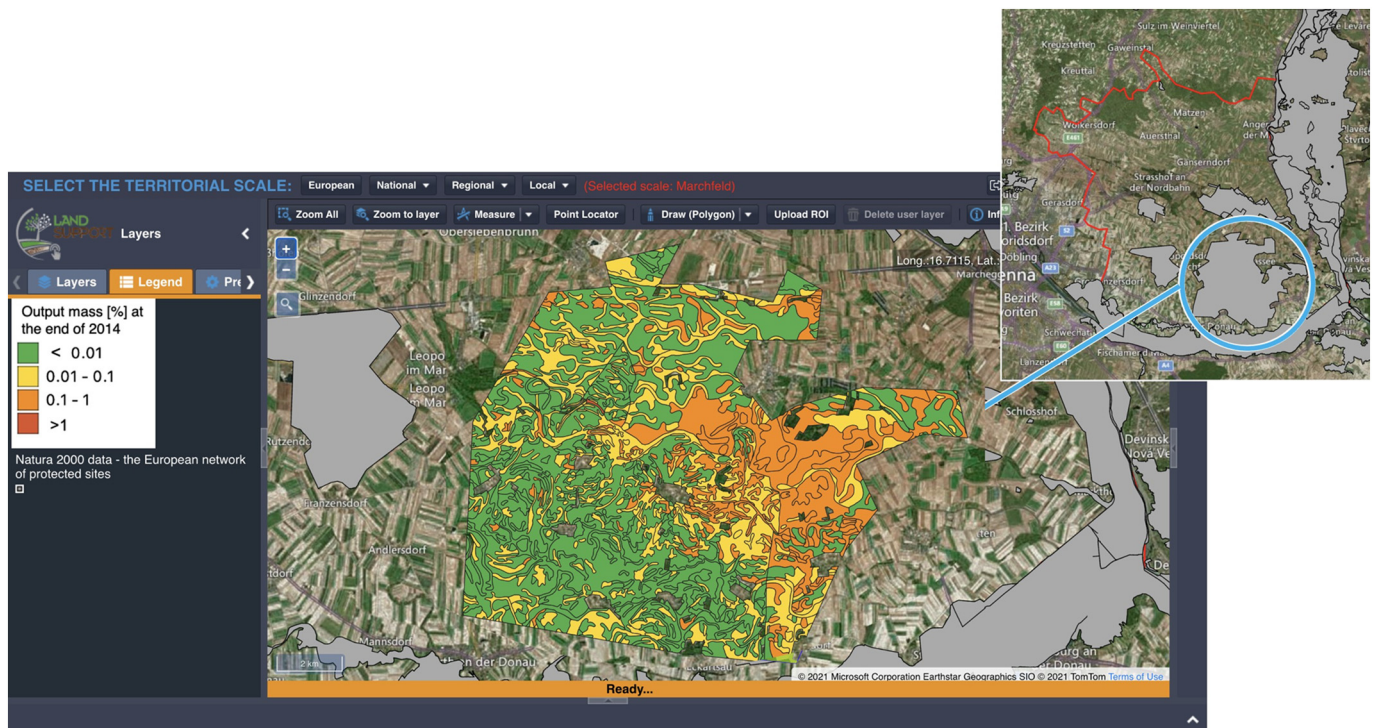


Fig. 8. Third example of tool usage: protected areas zoning. The tool in this case can support the detection of the most vulnerable zones in light of a reduction of pesticide use in special sites, such as Natura 2000 (grey polygons in the map).

Table A.4
Detailed pesticide inputs used for the three case studies (VT, MA, ZA).

	Crop	Pesticide	Type	DT50 [d]	k_d	dose [g ha ⁻¹]	BBCH	
Valle Telesina	Maize	Chlorantraniliprole	Insecticide	597	3.2	41.2	20-39/40-89	
	Maize	Deltamethrin	Insecticide	58.2	-	8.6	40-89	
	Maize	Lambda-cyhalothrin	Insecticide	175	3709	23.7	0	
	Olive	Copper oxychloride	Fungicide	10,000	-	40.6	71-89	
	Olive	Dimethoate	Insecticide	2.5	-	149.6	13-15	
	Olive	Phosmet	Insecticide	3.2	6.78	182.2	16-55	
	Wheat	Azoxystrobin	Fungicide	78	8.9	67.0	80-90	
	Wheat	Deltamethrin	Insecticide	58.2	-	7.0	80-90	
	Grapevine	Benalaxyl	Fungicide	33.2	71	54.7	53-69	
	Grapevine	Dimethomorph	Fungicide	72.7	-	485.4	53-69	
	Grapevine	Copper oxychloride	Fungicide	10,000	-	876.0	53-69	
	Grapevine	Folpet	Fungicide	4.7	-	700.8	53-69	
	Grapevine	Sulphur	Fungicide	30.0	-	2336.0	53-69	
	Grapevine	Tau-fluvalinate	Insecticide	4.0	3000	219.0	53-69	
	Grapevine	Tetraconazole	Fungicide	61.0	-	40.0	53-69	
	Grapevine	Zoxamide	Fungicide	5.5	-	485.4	53-69	
	Marchfeld	Maize	Dicamba	Herbicide	4	-	35.8	10-19
		Maize	Mesotrione	Herbicide	19.6	1.62	80.7	10-19
		Maize	Nicosulfuron	Herbicide	26	-	135.0	10-19
		Maize	Tefluthrin	Insecticide	37	1088	80.0	0
Potatoes		Diflufenican	Herbicide	94.5	134.3	58.0	0	
Potatoes		Metribuzin	Herbicide	7.03	-	230.0	0	
Potatoes		Prosulfocarb	Herbicide	11.9	-	2151.6	10-21	
Potatoes		Tefluthrin	Insecticide	37	1088	80.0	0	
Rape		Azoxystrobin	Fungicide	78	8.93	74.5	14-29	
Rape		Clopyralid	Herbicide	23.2	0.07	73.3	up to 50	
Rape		Difenoconazole	Fungicide	130	-	74.5	14-29	
Rape		Halauxifen-methyl	Herbicide	1.3	72.7	3.0	up to 50	
Soya		Dimethenamid-p	Herbicide	11	-	480.0	0	
Soya		Imazamox	Herbicide	200.2	-	16.4	12-18	
Soya		Metobromuron	Herbicide	34.3	-	1025.0	0	
Sugarbeet		Azoxystrobin	Fungicide	78.00	8.9	155.4	39-49	
Sugarbeet		Difenoconazole	Fungicide	130	-	155.4	39-49	
Sugarbeet		Ethofumesate	Insecticide	21.6	-	352.0	10-19	
Sugarbeet		Phenmedipham	Fungicide	12	35.2	352.0	10-19	
Sunflower		Imazamox	Herbicide	200.2	-	40.5	12-18	
Wheat		Carfentrazone	Herbicide	1	-	22.5	31-59	
Wheat		Cyprodinil	Fungicide	37	-	560.0	31-32	
Wheat		Florasulam	Herbicide	1.85	0.46	5.2	13-32	
Wheat		Isopyrazam	Herbicide	244	-	63.2	31-59	
Wheat		Metsulfuron-methyl	Herbicide	10	-	4.2	13-32	
Wheat		Prothioconazole	Fungicide	14.1	15	63.2	31-59	
Wheat		Tribenuron	Herbicide	14	-	16.6	13-32	
Zala		Maize	Azoxystrobin	Fungicide	78	8.93	102.0	30-69
		Maize	Cyprosulfamide	Herbicide	-	-	9.7	00-14
		Maize	Foramsulfuron	Herbicide	25.4	-	56.2	13-15
		Maize	Mesotrione	Herbicide	19.6	1.62	122.0	00-14
		Maize	Nicosulfuron	Herbicide	26	-	38.4	13-15
		Maize	Propiconazole	Fungicide	71.8	33.7	88.4	30-69
		Maize	S-metolachlor	Herbicide	51.8	-	1017.0	00-14
		Maize	Terbuthylazine	Herbicide	72	-	610.0	00-14
		Maize	Thiencarbazone-methyl	Herbicide	11.6	-	24.7	00-14
		Rape	Aminopyralid	Herbicide	35	-	35.1	00-14
		Rape	Dimethenamid-P	Herbicide	11	-	166.1	00-14
		Rape	Difenoconazole	Fungicide	130	-	90.4	14-16/30-31
		Rape	Fluroxypyr-meptyl	Herbicide	1	188.75	142.6	00-14
	Rape	Mepiquat chloride	Herbicide	13.3	-	279.9	14-16/21-22	
	Rape	Metazachlor	Fungicide	8.6	0.78	544.5	00-14	
	Rape	Metconazole	Fungicide	142.2	-	39.7	14-16/21-22	
	Rape	Paclbutrazol	Fungicide	112	-	45.4	14-16/30-31	
	Rape	Quinmerac	Herbicide	30	-	181.5	00-14	
	Sunflower	Boscalid	Fungicide	484.4	-	105.0	16-18/61-69	
	Sunflower	Dimoxystrobin	Herbicide	210	-	105.0	16-18/61-69	
	Sunflower	Fluopyram	Herbicide	309	-	350.0	16-18/61-69	
	Sunflower	Flurochloridone	Fungicide	53	-	625.0	0	
	Sunflower	Imazamox	Herbicide	200.2	-	24.3	12	
	Sunflower	Prothioconazole	Fungicide	14.1	15.2	350	16-18/61-69	
	Sunflower	S-metolachlor	Herbicide	51.8	-	1300.0	0	
	Sunflower	Terbuthylazine	Herbicide	72	-	783.0	0	
	Sunflower	Tribenuron-methyl	Herbicide	9.1	1.1	20.6	12	
	Wheat	Diflufenican	Herbicide	94.5	134.3	100.0	11-23	
	Wheat	Cloquintocet-mexyl	Herbicide	5	-	7.5	39	
	Wheat	Florasulam	Herbicide	1.85	0.46	18.3	11-23/39	
	Wheat	Penoxsulam	Herbicide	32	1.4	3.7	11-23	
	Wheat	Prochloraz	Fungicide	120	-	170.7	65	

Table A.4 (continued)

Crop	Pesticide	Type	DT50 [d]	k_d	dose [g ha ⁻¹]	BBCH
Wheat	Proquinazid	Fungicide	45	–	21.4	65
Wheat	Prothioconazole	Fungicide	14.1	15.2	25.2	65
Wheat	Spiroxamine	Fungicide	25	–	106.6	69
Wheat	Tebuconazole	Fungicide	63	–	155.2	65/69
Wheat	Thifensulfuron-methyl	Herbicide	1.39	0.74	8.3	32
Wheat	Tribenuron-methyl	Herbicide	9.1	1.1	8.3	32

variation. Eventually, the possibility to upload user-defined pesticide practices is foreseen. All the above features of the *pesticide fate tool* can be lumped in a single word: flexibility. This - in contrast with other tools such as the static maps provided by the applications of models such as DRASTIC - is a key feature of a geoSpatial-DSS that must survive to its developers in order to be a concrete, practical tool in the hands of deciders.

5. Conclusion

The aim of this work was to present the *pesticide fate tool* in the LandSupport platform for the assessment of specific groundwater vulnerability.

Despite the clear objective stated in many European directives about the overall reduction of non-point source pollutant sources, such as pesticides, a comprehensive understanding of the

transport processes underling groundwater vulnerability, based on measured and simulated data, is still lacking. Moreover, there is a lack of operational tools enabling to connect such transport processes understanding to real practice. As a result, it is not surprising that the European Parliament resolution of 13 September 2018 states that, as regards agricultural production and innovation, the objectives of the regulation on plant protection products are still not being achieved in practice. Moreover, the European Court of Auditors states that the Commission still lacks a robust evidence base to assess whether the directive has achieved the EU's objective of making pesticide use sustainable and recommend developing better risk indicators.

In this context, the role of the expert in supporting both environmental planners and farmers is clearly crucial. The *pesticide fate tool*, integrated within the geospatial decision support system LandSupport, aims at

Table 1

Main databases employed in LandSupport-GCI for the *pesticide fate tool*: description of data type and examples of their use in modelling.

Theme	Source database-(spatial/time) resolution-years of production	Type of file	Data	Parameters (obtained by dataset)	Applied model	Example of model outputs
Soil	VT Soil mapping dataset-1:50000-2018 MA Soil mapping dataset-1:10000-2018 ZA Soil mapping dataset-1:100000-2018	Polygon and table	Main soil morphological, chemical, physical parameters	Soil hydraulic properties soil depth,	Clipping spatial data from database; zonal statistics	Soil data within the ROI
Climate	ERA5 land reanalysis data-9 km/hourly-1980/2021 EURO-CORDEX/CMCC-COSMO-CLM data-12 km/daily-2020/2021 Local info-punctual-2021	GRIB NetCDF	Rainfall, temperature, rel. Humidity, radiation, etc.	Annual precipitation, annual evapotranspiration	Fao-Penman Monteith (Allen et al., 1998)	Mean daily net precipitation for each soil unit
Crop type	Local info-punctual-2021	List	Most-commonly grown crops, seeding and harvesting dates	Crop coefficient	none	Actual evapotranspiration
Pesticides	Local info-punctual-2021	List	Most-commonly used pesticides, dose and time of application	Input concentration	Actual dose model (EFSA, 2017)	Net pesticide dose arriving at the ground
Legal restriction to land use	Natura 2000; hydrogeology restriction-punctual-2019	Polygon	Legal boundaries	Limit and type of restriction	Presence/absence of restriction	Surfaces under restriction
Geology	VT: local info and geological maps-1:50000; 1:100000; 1:250000-1990 MA: local info and geological maps-1:50000-2010 ZA: bibliography-1:100000-2005	Raster	Stratigraphy; Geological Units; Geomorphology	Stratigraphic and geological setting at small scale	Clipping spatial data from database	Geological, stratigraphic and geomorphological data
Hydrogeology	VT: local info, bibliography and hydrogeological maps-1:100000; 1:300000-2020 MA: local info, bibliography and hydrogeological maps-1:50000; 500,000-2020 ZA: hydrogeological map-1:100000-2005	Raster	Geological Units; Geomorphology Hydro-stratigraphy; Hydrogeology; Hydrology	Geological setting at large scale Hydrogeological and hydro-stratigraphic setting at small scale	Clipping spatial data from database	Main geological and geomorphological data Hydrogeological, hydro-stratigraphic and hydrological data
Water table depth	VT: local info and bibliography-20 m resolution; high detail-2021 MA: local info and bibliography-50 m resolution; high detail-2021 ZA: bibliography-1 m resolution; low detail-2021	Raster	Hydrogeology; Geomorphology Groundwater table depth	Hydrogeological setting at large scale Piezometry and water table depth at small scale Piezometry at large scale	Clipping spatial data from database	Main hydrogeological data Water table depth

Table 2
Detailed pesticide inputs of the three applications shown in this work.

Application	Crop	Pesticide	Type	DT50 [d]	k_d	dose [g ha ⁻¹]	BBCH
1	Grapevine	Tetraconazole	Fungicide	61.00	–	40	53–69
2	Wheat	Florasulam	Herbicide	1.85	0.46	18.32	39
		Tribenuron-methyl	Herbicide	9.10	1.10	8.3	32
3	Soya	Dimethenamid-p	Herbicide	11	–	480	0

being an operative instrument to be used for the definition of these quantitative measures, taking into account the great spatial variability of soil pedo-climatic conditions. It proved to have a great flexibility of usage for different spatial scales, from the local case of the Valle Telesina to the regional case of Zala County, with very different pedo-climatic conditions, as well as for different crops and pesticide managements. The work details the tool implementations for the three case studies, which are the results of multiple interactions with several project partners and stakeholders, in order to obtain the best compromise between the research-scientific world and everyday real-life applications.

The three application examples practically show how the tool can be managed and used by different users, for groundwater vulnerability assessment, under different climatic scenarios, the evaluation of alternative pesticide uses and the zoning of protected areas, supporting the previously cited directives.

Finally, the integration of the tool within the solid and flexible LS infrastructure, opens the road to future implementations for new regions and applications, as soon as new datasets are available.

CRedit authorship contribution statement

Marialaura Bancheri: Conceptualization, Methodology, Software, Writing – original draft, Writing – review & editing. **Francesco Fusco:** Data curation, Writing – review & editing. **Daniele Dalla Torre:** Software. **Fabio Terribile:** Writing – review & editing, Supervision. **Piero Manna:** Data curation. **Giuliano Langella:** Software, Data curation. **Pantaleone De Vita:** Data curation, Writing – review & editing. **Vincenzo Allocca:** Data curation, Writing – review & editing. **Harald Loishandl-Weisz:** Data curation, Validation. **Tamás Hermann:** Data curation. **Carlo De Michele:** Software. **Antonio Coppola:** Methodology. **Florindo Antonio Mileti:** Data curation. **Angelo Basile:** Conceptualization, Writing – review & editing, Visualization, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Table 3
Details for modelling implemented in LandSupport-GCI for the Pesticide fate tool functionalities.

Application	Main functionalities	Required activity	Example of input parameters	Example of output
GW vulnerability assessment	Assessing the specific groundwater vulnerability for a user-defined ROI	i) select a ROI ii) select time iii) select land use iv) select pesticide	– vector and tabled data related to soil type – climate data – land use and management – raster of the GW table depth	– vector map of the percentage of pesticide – arrival at the end of simulation – period for the selected ROI
Alternative pesticide use	Providing support for the most environmentally-safe pesticide	i) select a ROI ii) select time iii) select land use iv) select different pesticides	– vector and tabled data related to soil type – climate data – land use and management – raster of the GW table depth	for each simulated pesticide, vector maps of the percentage of arrival at the GW table depth to compare the specific vulnerabilities
Protected areas zoning	Supporting the zoning of the most vulnerable areas within very sensitive sites such as Natura 2000	i) select multiple ROIs ii) select time iii) select land use iv) select pesticide	– vector and tabled data related to soil type – climate data – land use and management – raster of the GW table depth	within very sensitive areas, comparison of the solute arrivals to identify the most vulnerable zones

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Appendix A. Detailed description of the input datasets for Valle Telesina, Marchfeld and Zala

Input datasets of the *pesticide fate tool* are described in detail in the following subsections for the three case studies.

A.1. Soil datasets

The soil datasets for the three case studies contain both information on the hydraulic properties of the representative soil profiles and on the geospatial features of the soil polygons, such as the location and their spatial extent.

The soil dataset of the Valle Telesina case study contains the main soil morphological, chemical and physical parameters, together with van Genuchten-Mualem parameters of 46 georeferenced soil profiles, on a 1:50,000 scale. The hydraulic parameters were determined in laboratory by the Wind's method (Arya, 2002; Basile et al., 2012) and then scaled to field condition for taking into account field incomplete saturation (Basile et al., 2006) and stoniness (Coppola et al., 2013b). The dataset is fully described in Bancheri et al. (2021) and can be found at <https://doi.org/10.5281/zenodo.3701360>.

As regards the soil dataset of Marchfeld, since only information of the depths and textures of the representative soil profiles were available, on a 1:10000 scale, the parameters of the hydraulic conductivity curves, always represented by the van Genuchten-Mualem model, were derived using the HYPRES pedotransfer (Wösten et al., 2001) for each horizon within the profiles.

Eventually, Zala County soil dataset contains the main soil parameters, such as the thickness, the USDA textures, the bulk densities, the organic matters for each soil horizon of the representative profile, together with van Genuchten-Mualem parameters of 11 georeferenced soil profiles obtained from $h(\theta)$ and saturated hydraulic conductivity measurements, on a 1:100000 scale measured.

At the end of the homogenization process, the three datasets contained exactly the same data: horizon depths, hydraulic conductivity curve parameters, textures, organic matters, bulk densities, referred to representative soil profiles linked to polygons or map units in the soil map.

A.2. Climate

The database of climatic variables contains two different sources of data:

- reanalysis data, for past climate;
- climatic scenarios Representative Concentration Pathways (RCP) 2.6, RCP 4.5 e RCP 8.5, for future climate.

Reanalysis data (Hersbach et al., 2020; Pelosi et al., 2020) come from the ERA5-Land hourly dataset that has a global coverage from 1981 to present. Their native resolution is 9 km, in GRIB format and are delivered monthly with a delay of about three months relatively to actual date. To fill this gap, data retrieved from a Numerical Weather Prediction model (Marsigli et al., 2005) are continuously stored in the database, until the newest release of reanalysis data. Available variables are: 10 m u-component of wind [m s^{-1}]; 10 m v-component of wind [m s^{-1}]; 2 m dew-point temperature [K]; 2 m temperature [K]; surface pressure [Pa]; surface solar radiation downwards [J m^{-2}]; total precipitation [m].

Eventually, for the future climate data are retrieved from the EURO-CORDEX and CMCC-COSMO-CLM models at daily time-step with a native resolution of 12 km, in NetCDF format. Future data cover the time-interval 2006–2100. Available variables are: mean temperature [K]; maximum temperature[K]; minimum temperature[K]; total precipitation [m].

The actual evapotranspiration is computed at run time from the potential evapotranspiration, considering the specific crop coefficients and the actual water content on the soils, according to the model of Allen et al. (1998). Therefore, the mean daily net precipitation value, computed from the mean daily precipitation and mean daily actual evapotranspiration, varies in time and space, according to the soil polygons within the selected ROI. It is worth reminding, as fully specified in Bancheri et al. (2021), that the TFM-ext model and, therefore, the tool, work at yearly time scale, since the assumption on the steady state fluxes could be reasonably true only at this time scale. Thus, the simulations carried out considering future climatic scenarios, over fixed time spans, e.g., 25 years, consider the same mean daily net precipitation over the entire chosen period.

A.3. Crop type

For all case studies the list of most-commonly crops was populated according to the local farmers/agronomists suggestions. The type of crop affects both the computation of the mean daily net precipitation, as previously described, and the type of pesticides that can be chosen. Besides, it allows to simulate alternative scenarios, analysing both the actual crop management and a potential one. For the Valle Telesina 5 crops were considered: vine, olive, wheat, maize and alpha alpha; for Marchfeld: potatoes, sunflower, soya, rape, sugarbeet, maize and wheat; for Zala County: rape, sunflower, wheat and maize.

A.4. Water table depth

In this study, maps of groundwater table depth (GWTD) for the three study areas were reconstructed considering piezometric data of existing boreholes and wells, including points of natural surfacing of groundwater circulation (such as springs, rivers, etc.). For such a scope, extended bibliographic research and consultations of archives allowed the implementation of a comprehensive and unpublished database. Moreover, resulting maps were obtained through statistical approach, interpolating piezometric levels, as for Telesina Valley and

Marchfeld study areas, or simply digitalizing GWTD maps, as for Zala County area. Thus, resolution and detail scale of GWTD maps was strongly affected by availability and both distribution and quality of source data. In detail:

- map for the Telesina Valley study area has both high spatial resolution (20×20 m) and detail, and derives by processing of:
 - data from boreholes (BHs) including wells (Ws) from Municipalities archives and Institutional ones (Italian Geological Society, public bodies (Italian National Institute for Environmental Protection and Research - ISPRA) and scientific associations (Italian Geological Society);
 - bibliographic data (Guadagno et al., 1998; Allocca et al., 2014; De Vita et al., 2018).
- map for the Marchfeld study area has both high spatial resolution (50×50 m) and detail, and derives by processing of:
 - data from BHs including Ws deriving from HADES archive (HADES-Bohrungsdatenbank der Niederösterreichischen Landesregierung);
 - bibliographic data (Geologische Bundesanstalt web service; Fank et al., 2008).
- map for the Zala County study area has high spatial resolution (1×1 m) while low detail, and derives by processing of:
 - bibliographic data (<https://map.mbfisz.gov.hu>).

A.5. Pesticides

The local farmers/agronomists gave - with respect to specific crops - information on the most-commonly used pesticides and on some management practices related to the dose and the time-span of application. This information was integrated with the ones detailed in the technical sheets associated to commercial formulates, for the computation of the actual dose in mg l^{-1} for each treated hectare. In particular, the following procedure was applied:

1. we considered all active principles within the commercial formulates and calculated its concentration;
2. for each active principle, we got the chemical information on the molecular weight, the typical half-life DT50 in soil and the distribution coefficient from the Pesticide Properties Database (PPDB: <https://sitem.herts.ac.uk/aeru/ppdb/en/index.htm> (Lewis et al., 2016));
3. according to time of application, defined through the BBCH (Hess et al., 1997), we computed the fraction of the dose reaching the soil as the sum of the fraction of the dose washed-off from the leaves and the fraction of the dose that directly reaches the soil (EFSA, 2017);
4. to obtain the concentration in mg l^{-1} for each treated hectare, we took from technical sheet of each pesticide, the suggestions on the mean water volume in which the pesticide should be dissolved for its usage.

The final lists of pesticides for the three case studies is reported in the following Table A.4. For each case study and crop, the list of the most commonly-used herbicides, insecticides and fungicides are reported, together with the chemical parameters, the effective dose and the BBCH of their applications.

References

- Adhikari, K., Guadagnini, A., Toth, G., Hermann, T., 2009. Geostatistical analysis of surface soil texture from zala county in western hungary. International Symposium on Environment, Energy and Water in Nepal: Recent Researches and Direction for Future, Citeseer, pp. 219–224.
- Albinet, M., Margat, J., 1970. Cartographie de la vulnérabilité à la pollution des nappes d'eau souterraine. Bull. BRGM 2, 4.
- Alfieri, S., Riccardi, M., Menenti, M., Basile, A., Bonfante, A., De Lorenzi, F., 2019. Adaptability of global olive cultivars to water availability under future Mediterranean climate. Mitig. Adapt. Strateg. Glob. Chang. 24, 435–466.

- Allen, R.G., Pereira, L.S., Raes, D., Smith, M., 1998. Crop evapotranspiration guidelines for computing crop water requirements. *Fao Irrigation and Drainage Paper*. 56. Fao, Rome, p. 300 D05109.
- Aller, L., 1985. In: Kerr, Robert S. (Ed.), *DRASTIC: A Standardized System for Evaluating Groundwater Pollution Potential Using Hydrogeologic Settings*. Environmental Research Laboratory, Office of Research and Development, US Environmental Protection Agency.
- Allocca, V., Manna, F., De Vita, P., 2014. Estimating annual groundwater recharge coefficient for Karst aquifers of the southern Apennines (Italy). *Hydrol. Earth Syst. Sci.* 18, 803–817.
- Arya, L., 2002. Wind and hot-air methods. *methods of soil analysis: part 4 physical. Methods* 916–926.
- Badia, R.M., Conejero, J., Diaz, C., Ejarque, J., Lezzi, D., Lordan, F., Ramon-Cortes, C., Sirvent, R., 2015. Comp superscalar, an interoperable programming framework. *SoftwareX* 3, 32–36.
- Bancheri, M., Coppola, A., Basile, A., 2021. A new transfer function model for the estimation of non-point-source solute travel times. *J. Hydrol.* 126157. <https://doi.org/10.1016/j.jhydrol.2021.126157> (URL:<https://www.sciencedirect.com/science/article/pii/S0022169421002043>).
- Basile, A., Coppola, A., De Mascellis, R., Randazzo, L., 2006. Scaling approach to deduce field unsaturated hydraulic properties and behavior from laboratory measurements on small cores. *Vadose Zone J.* 5, 1005–1016.
- Basile, A., Buttafuoco, G., Mele, G., Tedeschi, A., 2012. Complementary techniques to assess physical properties of a fine soil irrigated with saline water. *Environ. Earth Sci.* 66, 1797–1807.
- Civita, M., 2010. The combined approach when assessing and mapping groundwater vulnerability to contamination. *Journal of Water Resource and Protection* 2010.
- Civita, M., De Maio, M., 2000. In: Pitagora (Ed.), *Sintacs r5 a new parametric system for the assessment and automatic mapping of groundwater vulnerability to contamination*. 226 Bologna.
- Connell, L., Van den Daele, G., 2003. A quantitative approach to aquifer vulnerability mapping. *J. Hydrol.* 276, 71–88.
- Coppola, A., Comegna, A., Dragonetti, G., De Simone, L., Lamaddalena, N., Zdruli, P., Basile, A., 2013a. A stochastic texture-based approach for evaluating solute travel times to groundwater at regional scale by coupling GIS and transfer function. *Procedia Environ. Sci.* 19, 711–722.
- Coppola, A., Dragonetti, G., Comegna, A., Lamaddalena, N., Caushi, B., Haikal, M., Basile, A., 2013b. Measuring and modeling water content in stony soils. *Soil Tillage Res.* 128, 9–22.
- De Vita, P., Allocca, V., Celico, F., Fabbrocino, S., Mattia, C., Monacelli, G., Musilli, I., Piscopo, V., Scalise, R.A., Summa, G., Tranfaglia, G., Celico, P., 2018. Hydrogeology of continental southern Italy. *J. Map* 14, 230–241.
- Doerfliger, N., Jeannin, P.Y., Zwahlen, F., 1999. Water vulnerability assessment in karst environments: a new method of defining protection areas using a multi-attribute approach and GIS tools (Epik method). *Environ. Geol.* 39, 165–176.
- EFSA, 2017. EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil: this guidance published on 19 October 2017 replaces the earlier version published on 28 April 2015. *EFSA Journal* 15.
- Fank, J., Rock, G., Dalla Via, A., Polting, W., Draxler, J., Plieschnegger, M., 2008. Grundwasserströmungsmodell marchfeld. Studie im Auftrag der Niederösterreichischen Landesregierung. 117. unvöffentlichlicher Bericht, St. Polten.
- Foster, S., 1987. Fundamental concepts in aquifer vulnerability. *Pollution Risk and Protection Strategy*.
- Foster, S., Hirata, R., Andreo, B., 2013. The aquifer pollution vulnerability concept: aid or impediment in promoting groundwater protection? *Hydrogeol. J.* 21, 1389–1392.
- Fusco, F., Allocca, V., Coda, S., Cusano, D., Tufano, R., De Vita, P., 2020. Quantitative assessment of specific vulnerability to nitrate pollution of shallow alluvial aquifers by process-based and empirical approaches. *Water* 12, 269.
- Gogu, R.C., Dassargues, A., 2000. Current trends and future challenges in groundwater vulnerability assessment using overlay and index methods. *Environ. Geol.* 39, 549–559.
- Guadagno, F., Ilesce, M., Piscopo, V., Vecchiarelli, R., Acquino, S., 1998. Caratterizzazione idrogeologica e potenzialità dell'acquifero della bassa valle del f. Calore (Campania). *Gunningham, N., Sinclair, D., 2005. Policy instrument choice and diffuse source pollution. J. Environ. Law* 17, 51–81.
- Hersbach, H., Bell, B., Berrisford, P., Hirahara, S., Nicolas, J., Peubey, C., Radu, R., Schepers, D., 2020. The ERA5 global reanalysis. *Quarterly Journal of the Royal Meteorological Society* 146, 1999–2049.
- Hess, M., Barralis, G., Bleiholder, H., Buhr, L., Eggers, T., Hack, H., Stauss, R., 1997. Use of the extended BBCH scale—general for the descriptions of the growth stages of mono and dicotyledonous weed species. *Weed Res.* 37, 433–441.
- Holman, I.P., Dubus, I.G., Hollis, J., Brown, C.D., 2004. Using a linked soil model emulator and unsaturated zone leaching model to account for preferential flow when assessing the spatially distributed risk of pesticide leaching to groundwater in England and Wales. *Sci. Total Environ.* 318, 73–88.
- Javadi, S., Kavehkar, N., Mousavizadeh, M., Mohammadi, K., 2011. Modification of DRASTIC model to map groundwater vulnerability to pollution using nitrate measurements in agricultural areas. *J. Agric. Sci. Technol.* 13, 239–249.
- Jury, W.A., Roth, K., et al., 1990. Transfer functions and solute movement through soil: theory and applications. *Birkhäuser Verlag AG*.
- Kristensen, P., Whalley, C., Zal, F.N.N., Christiansen, T., 2018. European waters assessment of status and pressures. *EEA Report*.
- Lewis, K.A., Tzivilakis, J., Warner, D.J., Green, A., 2016. An international database for pesticide risk assessments and management. *Human Ecol. Risk Assess. Int. J.* 22, 1050–1064.
- Lindblom, J., Jung, M., Jonsson, A., 2017. Promoting sustainable intensification in precision agriculture: review of decision support systems development and strategies. *Precision Agriculture* 18, 309–331.
- Machiwal, D., Jha, M.K., Singh, V.P., Mohan, C., 2018. Assessment and mapping of groundwater vulnerability to pollution: current status and challenges. *Earth Sci. Rev.* 185, 901–927.
- Manna, P., Bonfante, A., Colandrea, M., Di Vaio, C., Langella, G., Marotta, L., Mileti, F.A., Minieri, L., Terribile, F., Vingiani, S., et al., 2020. A geospatial decision support system to assist olive growing at the landscape scale. *Comput. Electron. Agric.* 168, 105143.
- Marano, G., Langella, G., Basile, A., Cona, F., De Michele, C., Manna, P., Teobaldelli, M., Saracino, A., Terribile, F., 2019. A geospatial decision support system tool for supporting integrated forest knowledge at the landscape scale. *Forests* 10, 690.
- Marsigli, C., Boccanera, F., Montani, A., Paccagnella, T., 2005. The cosmo-leps mesoscale ensemble system: validation of the methodology and verification. *Nonlinear Process. Geophys.* 12, 527–536.
- Nicholson, F., Krogshave Laursen, R., Cassidy, R., Farrow, L., Tendler, L., Williams, J., Surdyk, N., Velthof, G., 2020. How can decision support tools help reduce nitrate and pesticide pollution from agriculture? A literature review and practical insights from the EU fairway project. *Water* 12, 768.
- Patterson, J.J., Smith, C., Bellamy, J., 2013. Understanding enabling capacities for managing the 'wicked problem' of nonpoint source water pollution in catchments: a conceptual framework. *J. Environ. Manag.* 128, 441–452.
- Pelosi, A., Terribile, F., D'Urso, G., Chirico, G.B., 2020. Comparison of ERA5-land and uerra mescan-surfex reanalysis data with spatially interpolated weather observations for the regional assessment of reference evapotranspiration. *Water* 12, 1669.
- Saha, D., Alam, F., 2014. Groundwater vulnerability assessment using DRASTIC and pesticide DRASTIC models in intense agriculture area of the Gangetic plains, India. *Environ. Monit. Assess.* 186, 8741–8763.
- Scotter, D., Ross, P., 1994. The upper limit of solute dispersion and soil hydraulic properties. *Soil Sci. Soc. Am. J.* 58, 659–663.
- Terribile, F., Agrillo, A., Bonfante, A., Buscemi, G., Colandrea, M., D'Antonio, A., De Mascellis, R., De Michele, C., Langella, G., Manna, P., et al., 2015. A web-based spatial decision supporting system for land management and soil conservation. *Solid Earth* 6, 903.
- Tufano, R., Allocca, V., Coda, S., Cusano, D., Fusco, F., Nicodemo, F., Pizzolante, A., De Vita, P., 2020. Groundwater vulnerability of principal aquifers of the Campania region (southern Italy). *J. Maps* 16 (832), 565–576.
- Wiering, M., Lieferink, D., Boezeman, D., Kaufmann, M., Kurstjens, N., 2020. The wicked problem the water framework directive cannot solve. *Water* 12, 1240.
- Wösten, J., Pachepsky, Y.A., Rawls, W., 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. *Journal of Hydrology* 251, 123–150.
- Yalew, S., Van Griensven, A., van der Zaag, P., 2016. Agrisuit: a web-based gis-mcda framework for agricultural land suitability assessment. *Comput. Electron. Agric.* 128, 1–8.
- Zaza, C., Bimonte, S., Facciglione, N., La Sala, P., Gallo, C., 2018. A new decision-support system for the historical analysis of integrated pest management activities on olive crops based on climatic data. *Comput. Electr. Agric.* 148, 237–249.
- Zhang, R., 2000. Generalized transfer function model for solute transport in heterogeneous soils. *Soil Sci. Soc. Am. J.* 64, 1595–1602.