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Environmental decision support systems (EDSS) for risk management of chemicals in agriculture

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Introduction

Since 1960, the world population has more than doubled, from approximately 2.9 billion in 1960 to more than 7.4 billion today. The demands placed on global agricultural production arising out of population and income growth almost tripled.

Agricultural growth contributes directly to food security. It also supports poverty reduction. And it acts as an engine of overall economic growth in much of the developing world. The success of the agricultural sector has not been shared uniformly across regions and countries, however, and it is unclear whether this success can be sustained much less extended to those left behind. Many of the least developed countries, particularly in sub-Sahara Africa and in marginal production environments across the developing world, continue to experience low or stagnant agricultural productivity, rising food deficits, and high levels of hunger and poverty. By 2050, world population is projected to grow to between 9 and 10 billion people (World Bank, 2007).

Several factors concurred to the increased yields of the last decades and are expected to provide even more growth in the future. The introduction of modern crop varieties, namely high yielding crop varieties such as rice and wheat in mid 1960s; for example, in developing countries the production growth in the 1960-2000 period ranged from 17% to 40%. Irrigation became the most important productivity factor for expanding agriculture in developing countries or introduce high yielding crop in developed countries; irrigated areas has increased from 50 million hectares in 1900 to about 270 million hectares today. Labour productivity growth rates seem to have increased, with a strong growth in the middle of last century in developed countries and after 1980s in developing countries. Finally, the introduction of chemicals, in some cases at the beginning of the last century, could be considered the main productivity factor in the modern intensive farming, firstly in developed countries since the 1950s and in developing countries since 1970s.

This PhD thesis focuses on the adverse factors related to the use of chemicals in agriculture looking at the fate of substances in the environment and in particular into groundwater since, as an example, 65% of the whole drinking water in Europe comes from groundwater stocks (Bouraoui, 2007). Our first objective was the design and development of an Environmental Decision Support System for the evaluation of territorial vulnerability to chemical substances with couples environmental models with a geographical information system (GIS). VULPES (Vulnerability to Pesticides) has been developed originally for evaluating the environmental fate of plant protection products (PPPs) and then adapted to evaluate veterinary medicine products (VMPs) as well. In particular the transition between these two different chemicals evaluation introduced some novelties that made it the first tool for the evaluation of territorial vulnerability to VMPs. At same time we dedicated our effort to the definition of another EDSS called ValorE which addresses all the major components of manure management in Lombardy region (Northern of Italy). ValorE provides a picture of the current flows of manure in the entire region and provide advices to policy makers (regional system) and to farmers (farm system) for the correct management and distribution of manure and mineral fertilisers. At last, we dedicated our efforts for the realisation of an indicator (called Vigneto) of environmental impact of agronomic operations in vineyard, in order to evaluate the sustainability of such operations within a comprehensive project of sustainability of the Italian viticulture. The PhD course and the main part of the work has been done at the University of Milano-Bicocca, but we established collaboration with other university for the realisation of ValorE (University of Milan) and Vigneto (Catholic University of Piacenza).

This introduction foresee a description of the three types of chemical substances we evaluated with our EDSSs, evidencing the actual load in the European environment, the main regulations in Europe and Italy, the potential impacts on the environment. Then we describe the concept of environmental decision support system with a particular focus to its three main features: spatial representation of environmental variables and parameters, use of mathematical modelling and dynamicity. Then the introduction continues with a description of the evolution of environmental fate modelling through time and it ends with a short description of the next five chapters.

Chemicals in agriculture

Chemicals in agriculture relate to three main compartments: organic and mineral fertilisers, pesticides and veterinary pharmaceuticals; other chemical substances such as additives are frequently used in other sectors of the food production chain, but could be considered outside the direct agriculture sector.

Organic and mineral fertilisers

Use of organic and mineral fertilisers is intended to provide an adequate supply of all essential nutrients for a crop throughout the growing season. If the amount of any nutrient is limiting at any time, there is a potential for loss in production. As crop yields increase and as increasing amounts of nutrients are exported from the fields where crops are grown, the nutrient supply in the soil can become depleted unless it is supplemented through application of fertilizers.

When fertilizers were introduced, they have been used to supply the primary nutrients nitrogen (N), phosphorous (P) and potassium (K). In fields where primary nutrients are no longer the most limiting factor, fertilizers are used to supply secondary and micronutrients as well.

Loads on the environment

Use of fertilisers in Europe reached high levels during 1970s and 1980s for all countries and especially where agriculture is historically an intense activity. The introduction of European regulations (adopted subsequently by Member States) aimed to reduce and control the use of mineral and organic fertilisation for preventing environmental pollution, in particular in surface and groundwater (Eurostat, 2013).

Inputs of gross nitrogen balance consists of nitrogen supplied in mineral fertilisers and manure, other organic fertilisers (excluding manure), seeds and planting material, atmospheric deposition and biological nitrogen fixation (see). In particular, the biggest amount of nitrogen in Italy is provided by manure spreading.

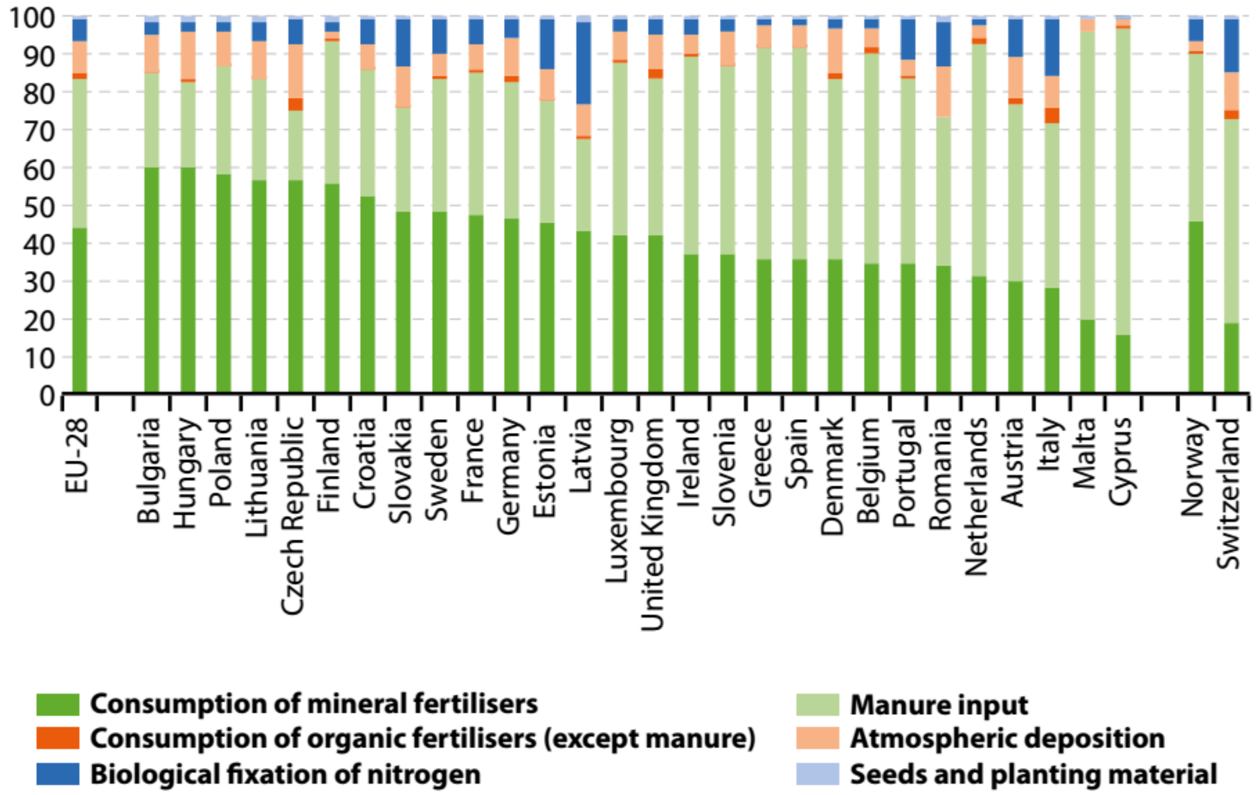

Figure 1 - Share of the different nitrogen inputs in total nitrogen inputs, average 2009–14 (%). Source: Eurostat

The vast majority (93.2 %) of phosphorus input in the EU-28 between 2009 and 2014 comes from manure and mineral fertilisers. The rest was supplied with other organic fertilisers (5.4 %) and seeds and planting material.

Rules and regulations

Legislative initiatives through the Nitrates Directive (European Commission, 1991) and the Water Framework Directive (European Commission, 2000) have sought to limit nutrient losses to water bodies through more careful management of agricultural land. In the case of the Nitrates Directive, this has included the designation of nitrate vulnerable zones (NVZs), establishment of Code(s) of Good Agricultural Practice to be implemented by farmers on a voluntary basis, establishment of Action Programmes to be implemented by farmers within NVZs on a compulsory basis, and national monitoring and reporting every 4 years. In the legislative text of the Water Framework Directive, an indicative list of pollutants includes organophosphorous compounds and substances that contribute to eutrophication (in particular nitrates and phosphates).

Environmental impacts

Keeping the focus on maintaining soil fertility, which is the most important goal for sustaining the future world population, excessive use of mineral fertilizers has roused environmental concerns. Stated that half of the applied fertiliser reaches the crop (Bockman et al., 1990), losses of nitrogen and phosphates occur through leaching and run–off while nitrogen loss also occurs through volatilization. The amount lost varies widely depending upon the crop, method of application, type of fertilizer, soil factors and environmental factors. The main environmental problem is the contribution of phosphate and nitrogen compounds to the eutrophication of surface waters, and the excessive concentration of nitrogen compounds in water and the atmosphere. Fertilizers are also significant contributors to anthropogenic sources of greenhouse gases, which contribute about 90% of all nitrous oxide, about 2% of the annual additions of CO2 to the atmosphere of about 8.5 billion tonnes and global ammonia emission of about 4.5 million tonnes (Snyder, 2009, Robertson et al., 2000).

Moreover, there are concerns about the production and manufacturing of mineral fertilisers. Phosphorus is mostly obtained from mined rock phosphate and is often combined in mineral fertilizers with sulphuric acid, nitrogen, and potassium. Existing rock phosphate reserves could be exhausted in the next 50–100 years. The fertilizer industry recognises that the quality of reserves is declining and the cost of extraction, processing and shipping is increasing. (Cordell et al., 2009).

Pesticides

Farmed crops would suffer from pests and diseases causing a large loss in yield: even today with advances in agricultural sciences losses due to pests and diseases range from 10-90%, with an average of 35% in pre-harvest for all potential food and fibre crops (Popp, 2013). A **pesticide** is something that prevents, destroys, or controls a harmful organism ('pest') or disease, or protects plants or plant products during production, storage and transport. Pesticides could be divided into several categories, depending on the target: herbicides, fungicides, insecticides, acaricides, nematicides, molluschicides, rodenticides, growth regulators, repellents, rodenticides and biocides. **Plant protection products** (PPP) are pesticides that protect crops or desirable or useful plants. They are primarily used in the agricultural sector but also in forestry, horticulture, amenity areas and in home gardens. They contain at least one active substance and have one of the following functions:

- protect plants or plant products against pests/diseases, before or after harvest
- influence the life processes of plants (such as substances influencing their growth, excluding nutrients)
- preserve plant products
- destroy or prevent growth of undesired plants or parts of plants

EU countries authorise plant protection products on their territory and ensure compliance with EU rules.

An **active substance** is any chemical, plant extract, pheromone or micro-organism (including viruses), that has action against pests or on plants, parts of plants or plant products. Before an active substance can be used within a plant protection product, it must be approved by the national or international regulatory institution. For example, in EU substances undergo an intensive evaluation and peer-review by Member States and the European Food Safety Authority before a decision can be made on approval.

Loads on the environment

Taking the year 2014 as the last reference (Eurostat, 2016) the total quantity of pesticide sales in the EU-28 amounted to close to 400 000 tonnes. Spain (19.8 %), France (18.9 %), Italy (16.1 %), Germany (11.6 %) and Poland (5.9 %) were the Member States in which the highest quantities of pesticides were sold, and together they made up 72.3 % of the EU-28's pesticide sales.

Table 1 – Pesticides sales (active ingredients - kg) by major groups, 2014. Source: Eurostat.

	Fungicides and bactericides	Herbicides	Insecticides and acaricides	Molluscicides	Plant growth regulators	Other	Total	Perc.
Belgium	3,095,003	2,519,651	555,844	47,691	261,248	521,620	7,001,057	**1.8%**
Bulgaria	186,142	652,446	163,439	:	:	:	1,002,027	**0.3%**
Czech Republic	1,788,321	2,755,332	337,679	15,487	350,315	416,247	5,663,381	**1.4%**
Denmark	530,223	1,242,544	38,291	15,382	114,239	33,903	1,974,582	**0.5%**
Germany	12,739,857	17,876,678	977,198	255,457	2,171,262	12,058,009	46,078,461	**11.6%**
Estonia	88,227	425,845	25,283	:	56,636	:	595,991	**0.1%**
Ireland	635,509	2,039,237	51,430	9,850	:	-	2,736,026	**0.7%**
Greece	1,866,378	1,194,605	588,794	1,162	148,483	107,670	3,907,092	**1.0%**
Spain	38,379,663	14,908,032	7,515,055	66,211	156,383	17,792,964	78,818,308	**19.8%**
France	34,430,575	30,965,455	2,610,867	870,246	2,802,877	3,607,514	75,287,534	**18.9%**
Croatia	1,004,779	889,121	143,098	5,411	72,157	4,485	2,119,051	**0.5%**
Italy	37,907,115	7,864,438	2,251,888	75,017	367,432	15,605,228	64,071,118	**16.1%**
Cyprus	698,083	153,359	180,623	1,001	1,202	12,458	1,046,726	**0.3%**
Latvia	224,735	847,474	63,998	36	274,510	6,642	1,417,395	**0.4%**
Lithuania	604,845	1,394,236	43,566	-	502,943	:	2,545,590	**0.6%**
Luxembourg	:	:	:	:	:	:	-	**0.0%**
Hungary	3,634,091	4,011,143	916,538	3,528	203,314	190,869	8,959,483	**2.2%**
Malta	97,370	7,632	2,946	480	-	:	108,428	**0.0%**
Netherlands	4,869,128	3,266,403	252,034	45,106	452,039	1,780,842	10,665,552	**2.7%**
Austria	1,641,052	1,375,815	240,220	16,180	53,529	46,419	3,373,215	**0.8%**
Poland	7,442,470	12,073,411	1,479,165	35,280	2,127,974	392,283	23,550,583	**5.9%**
Portugal	8,244,381	2,410,804	732,935	35,733	1,406	1,463,967	12,889,226	**3.2%**
Romania	4,131,916	5,025,373	569,046	1,199	270,600	23,091	10,021,225	**2.5%**
Slovenia	723,695	238,502	33,453	2,241	580	10,523	1,008,994	**0.3%**
Slovakia	567,191	1,215,096	106,509	:	179,808	129,406	2,198,010	**0.6%**
Finland	198,523	1,305,390	12,839	:	88,646	1,974,465	3,579,863	**0.9%**
Sweden	302,337	2,103,771	34,185	:	29,302	17,134	2,486,729	**0.6%**
United Kingdom	7,128,108	12,418,936	779,422	179,441	2,156,812	:	22,662,719	**5.7%**
Norway	121,834	692,015	4,822	1,331	39,114	675	859,791	**0.2%**
Switzerland	1,002,208	745,403	83,063	55,886	30,727	323,594	2,240,881	**0.6%**

Fungicides and bactericides and herbicides are the most sold pesticide, making together a figure of 77% of the total. The highest quantity of the three groups Fungicides, Insecticides and Other pesticides are sold in Spain, while the largest quantity of Herbicides has been sold in France.

If we compare quantities with each country utilised agricultural areas (UAA), a rough estimate of the load of pesticides per hectare can be done (Figure 2).

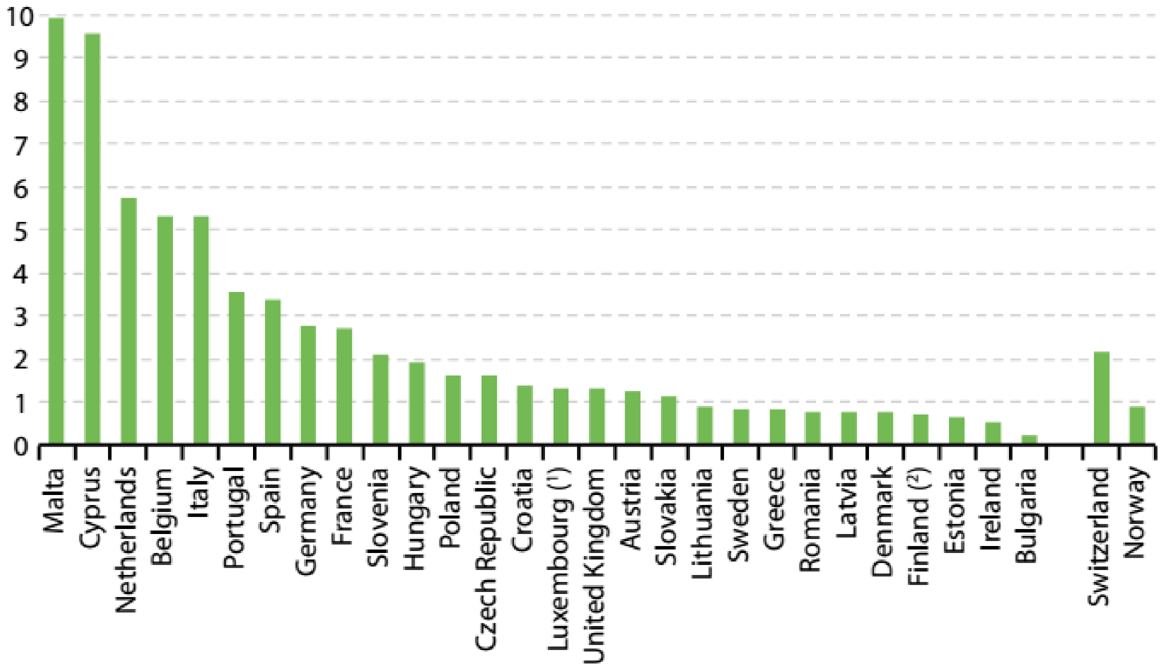

Figure 2 – Pesticide sales by utilised agricultural area (kg/ha), 2014.

As it can be seen, none of the top four countries having the highest pesticides sales, ranked in the top four of pesticide sales per ha of UAA. With a value of 9.97 kg/ha, Malta recorded the highest quantity of pesticides per hectare, while Bulgaria has the lowest load (0.22 kg/ha). Italy shows a figure of about 5.3 kg/ha.

Rules and regulations

At European level, several legislative acts strictly regulate the release of active ingredient and plant protection product (PPPs) into the market and the maximum residue limits (MRLs) in food.

Moreover, to prevent the risks of groundwater contamination, the European Commission issued several Directives which directly and indirectly regulate the use of PPPs in EU. For instance, the Council Directive 80/778/EEC (Council of the European Union, 1980), amended by Directive 98/83/EC (Council of the European Union, 1998) has set to 0.1 µg/l and 0.5 µg/l the maximum allowable concentrations in drinking water for each individual pesticide and for their total sum, respectively.

Council Directive 91/414/EEC (Council of the European Union, 1991), repealed and replaced by Regulation (EC) No 1107/2009 on 21 October 2009 (European Commission, 2009a), laid down the authorisation procedures of new active substances and PPPs to be marketed within the European Union.

More recently, the Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009, commonly referred to as “the Sustainable Use of Pesticides Directive” (European Commission, 2009b), established a framework for Community action to achieve the sustainable use of PPPs. Among the requirements of the Directive, it obliges Member States to adopt a National Action Plan (NAP). The plan should define a national strategy to set down objectives, quantifiable measures and timeframes to reduce the risks associated with the use of pesticides.

Regulation EC 396/2005 and its amendments (European Commission, 2005) harmonises and simplifies pesticide MRLs, and sets a common EU assessment scheme for all agricultural products for food or animal feed.

Environmental impacts

Depending on their mechanisms of action, main areas of concern about use (and abuse) of pesticide relates to water pollution, human toxicity, environmental toxicity.

Water pollution, particularly by herbicides, has been recognised as a problem since the 1970s. One area of concern is the extent to which pesticides reach rivers and lakes by leaching and runoff, since this may lead to impacts on aquatic life, and on humans if contamination extends to drinking waters.

Toxicity of different pesticides to **humans** probably varies greatly, but there is a general lack of epidemiological data on the impact of pesticides on human health. Pesticide uptake occurs through the skin, eyes, lungs or intestinal tract, and toxicity is influenced by the dose, type of chemical and its metabolites, the health of the individuals and their genetic susceptibility. Ingestion can also occur via contaminated food and the pesticide may be metabolised or stored in body fat. Synergistic effects can result in combinations of pesticides being more toxic than their individual components.

The effects of pesticide spray drift on **fauna and flora** seem to cause measurable short-term impacts to wildlife, but the time scale and long-term effects are uncertain. There are considerable differences in pesticide sensitivity among microbial species and that the use of an uncertainty factor is necessary to provide an acceptable margin of safety in evaluating the hazard of pesticides.

Veterinary pharmaceuticals

Veterinary medicinal products (VMP) are used to treat diseases and protect animal health, other than as growth promoters. The main categories of VMP (Crane et al., 2008) are:

- paraciticides, used to control parasites either externally and internally the livestock;
- antibacterials, used in treatment and prevention of bacterial diseases;
- antifungals, generally used topically and orally to treat fungal and yeast infections;
- growth promoters, mainly antibiotic compounds added to animal feedstuffs to improve the efficiency of food digestion;
- coccidiostats and antiprotozoals, used for the prevention of coccidiosis and swine dysentery.

Other therapeutic groups are interested by VMP such as anesthetics, analgesics, tranquilisers.

VMP are used in several productivity compartments, i.e. aquaculture, livestock production, domestic animals, each of them presenting different route of administration and pathways to the environment. In our PhD, we focused on the environmental fate of VMPs used in livestock production.

Loads on the environment

At the time being, the only category of veterinary medicine products (VMP) sales monitored at European level refers to the antimicrobial class, meanwhile it is not possible to obtain a complete data set not for the used quantities of all the other categories (parasiticides, hormones, antifungals and so on), nor about the geographic distribution and pattern of use of VMPs in the European territory. This is a big issue because every evaluation using statistical or modelling analysis could not disregard quantities and load of every VMP class (or any other impacting substance) on the territory.

The European Medicine Agency (EMA) edited in 2015 the first ESVAC report (European Surveillance of Veterinary Antimicrobial Consumption – EMA, 2015) based on data from sales or prescription during 2013.

Table 2 reports the total sales of veterinary antimicrobial agents and the sales expressed as mg sold per population correction unit (PCU). PCU is used to estimate sales corrected by the animal population in individual countries and across countries. In the report, 1 PCU = 1 kg of different categories of livestock and slaughtered animals.

Table 2 - Sales, in tonnes of active ingredient, of veterinary antimicrobial agents marketed mainly for food-producing animals, including horses, population correction unit (PCU) and sales in mg/PCU, by country, for 2013. Source: European Medicine Agency.

Country	Sales (tonnes)	PCU (1,000 tonnes)	mg/PCU
Austria	54.7	957	57.2
Belgium	259.5	1,657.50	156.6
Bulgaria	46.5	400.9	116.1
Cyprus	47.9	112.5	425.8
Czech Rep.	57.2	696.8	82.1
Denmark	108.5	2,418.40	44.9
Estonia	8.5	137.2	62.2
Finland	12.5	514.4	24.3
France	681	7,165.40	95
Germany	1,527.20	8,525.60	179.1
Hungary	175.7	763.1	230.2
Iceland	0.6	115.2	5.3
Ireland	99.6	1,761.60	56.5
Italy	1,318.40	4,371.90	301.6
Latvia	6.2	167.1	37
Lithuania	12.4	339.5	36.6
Luxembourg	2.7	51	53.6
Netherlands	225.6	3,226.30	69.9
Norway	6.6	1,788.60	3.7

Poland	575.6	3,806.20	151.2
Portugal	179.4	958.2	187.2
Slovakia	15.5	247.8	62.5
Slovenia	4	180.2	22.4
Spain	2,201.90	6,943.60	317.1
Sweden	10	795.6	12.6
UK	422	6,799.10	62.1

One important conclusion of the ESVAC report is that for the 20 countries that delivered sales data for four years (2010-2013) the data analysis indicates that the overall sales (mg/PCU) for these countries continues to decline; for this period, the overall reduction was 11.1%. Explanation for this reduction could include the implementation of responsible-use campaigns, changes in animal demographics, restrictions on use, increased awareness of the threat of antimicrobial resistance, and/or the setting of targets, testifying that the antimicrobial resistance is a increasingly considered problem.

Rules and regulations

In the last two decades, there have been significant developments in the regulatory requirements for placing in the market new VMPs in consideration of their potential negative environmental impacts. Nowadays, the European Framework Directive 2001/82/EC (European Commission, 2001) regulates the production, placing on the market, labelling, marketing, and use of veterinary pharmaceuticals in the European Union. According to this Directive, the potential impact on the environment of such products must be assessed before granting a marketing authorisation. Currently in EU, the environmental risk assessment (ERA) procedures for VMPs are based on technical guidance documents (CVMP/VICH, 2000; CVMP/VICH, 2005; CVMP, 2008) which are coordinated and continuously updated by the European Medicine Agency (EMA).

Environmental impacts

Veterinary antibiotics were studied in a comprehensive paper by Sarmah et al. (2006). Authors affirm that antimicrobials are designed to affect mainly microorganisms and bacteria found in animals but this therefore makes them potentially hazardous to other such organisms found in the environment. On release into the environment through manure application, antibiotics may end up on arable land and can be taken up by plants. Batchelder (1981) tested the effects of chlortetracycline and oxytetracycline on pinto bean plants gown in aerated nutrient media and showed that relatively low antibiotic concentrations can markedly affect the plant growth and development in nutrient solution.

Reproductive effects and adverse impacts on early life stages of different aquatic organisms may be caused by the presence of antibiotic residues in the environment (Kümpel et al., 2001)

The frequent use of antibiotics either to treat diseases or as animal feed supplements has raised concerns about the potential for to the rise of populations of new strains of bacteria resistant to antibiotics (antibacterial resistance).

Models as a representation of environmental processes

This PhD thesis illustrates a three years' work focused on the evaluation of environmental fate of chemical substances used in agriculture. The final aim has been the realisation of software prototype tools to be used by regulatory and quality managers (primarily from the public authorities), hence by technicians well-aware of the context but not necessarily used to dealing with the scientific background. Some of the tools in fact make use of complex mathematical models which describe the environmental processes and other modules which provide the spatialisation of the results on the territory.

A model could be identified as a simplified and idealised representation of the underlying physical (in our case) system. In particular, reality is almost always too complex to be satisfactory described by a set of mathematical equations, and therefore there is need to simplify the context and focus the attention to the process under investigation. Modelling implies the concept of simulation, intended as way a model describes a process behaviour; environmental processes could be described by dynamic simulations, which provide information over time.

Environmental models could be divided in two main sectors: scale models, which are basically down-sized or enlarged copies of their target systems (a sort of replica) and idealised models, often based on the Galilean idealisation which introduces simplifications whenever a situation is too complicated to tackle. Models used in this thesis refers to the latter branch.

Models could be also classified in deterministic and probabilistic. The former intends that every process has a precise definition and a clear output while the latter describes models with variables and output characterised by a probabilistic function.

At last, environmental models could be divided into four main categories:

- Indices, where attribute data controlling environmental processes are combined following logical and mathematical rules. In most cases, the process is broken up in several sub-processes that can be combined using different weight (and different weighting techniques);
- Analytical models, which are mathematical models that have a closed form solution, i.e. the solution to the equations used to describe changes in a system can be expressed as a mathematical analytic function. Use of closed-form equation could provide a concise preview of a model's behaviour but it is true as long as its mathematical description does not become too complex;
- Numerical models, which are mathematical models that use some sort of numerical time-stepping procedure to obtain the models behaviour over time. The mathematical solution is represented by a generated table and/or graph which has to be interpreted by modeller. Numerical models are used in software for the realisation of computer simulations, which

are computer programs that can be either small, running almost instantly on small devices, or large-scale programs that run for hours or days on network-based groups of computers, depending on the context and the sort of processes to be studied;

- Meta-models, which are models of the model: if a model is an abstraction of phenomena in the real world a metamodel is yet another abstraction, highlighting properties of the model itself. In many decision support systems (DSS) where responsiveness is a mandatory condition, metamodels could provide rapidly an output querying a regression line built from an analysis of many model runs on sensitive conditions.

Leaching models

Leaching models identified by the FOCUS (Forum for the Coordination of Pesticide Fate Models and their Use) workgroup (FOCUS, 2000) are a set of numerical models to be used in the frame of the regulatory approval of new or expired plant protection products to evaluate the leaching behaviour of their active ingredient, following a tiered approach. At the first tier, nine realistic worst-case environmental scenarios (a combination of soil, climate and crop parameters), which should collectively represent agriculture in the EU, are used in combination with a set of pesticide leaching models, namely PEARL (Tiktak et al., 2000), PRZM (Suarez, 2005), PELMO (Klein, 2000), and MACRO (Jarvis, 1994). The models all report concentrations at 1 m depth for comparative purposes, under the assumption that groundwater is unlikely to be affected by pesticides at concentrations exceeding 0.1 µg/l if those concentrations are not encountered at a shallow depth. Higher tier (more refined) modelling approaches are classified as Tier 2 (parameter refinements for modelling or scenario refinements) or Tier 3 (advanced spatial modelling).

The Plant Protection Products and their Residues (PPR) panel of the European Food Safety Authority (EFSA) considers the Tier 3 which makes use of advanced spatial modelling as the more accurate way of identify the pesticide fate in groundwater (EFSA PPR, 2013).

The EDSS Vulpes couples PELMO and PEARL models with GIS and a complex simulation manager in order to comply with the advanced spatial modelling requested by Tier 3. VULPES has been designed and implemented to transfer the actual scientific knowledge in terms of environmental risk assessment of pesticide to the risk assessors. It allows applying consolidated models and methodologies used in standardised scenarios for regulatory purposes to real data (pedology, weather and agronomic management) following the recent trend hoped by EFSA for the next generation of pesticide evaluations. Other model systems (GEO PEARL, GEO PELMO, FITOMARCHE) has been developed to evaluate groundwater leaching of pesticide at territorial scale, but they use simplified data and/or they are metamodels.

Territorial vulnerability

Territorial vulnerability is a way to evaluate the impact of chemical substance at a spatial scale.

Vulnerability assessment is a mean to identify areas (at different spatial scales, depending on the granularity of data) sensible to external inputs. Referring to groundwater, US Environmental Protection Agency (1993) divide between aquifer sensitivity and groundwater vulnerability.

- **Aquifer sensitivity** is the relative ease with which a contaminant applied on or near a land surface can migrate to the aquifer of interest; Aquifer sensitivity is a function of the intrinsic characteristics of the geologic materials in question, any overlying saturated materials and the overlaying unsaturated zone. Sensitivity is not dependent on agronomic practices or pesticide characteristics.
- **Groundwater vulnerability** is the relative ease with which a contaminant applied on or near a land surface can migrate to the aquifer of interest under a given set of agronomic management practices, contaminant characteristics and aquifer sensitivity conditions.

Expanding the above definitions, Dixon (2005) called the aquifer sensitivity as "**intrinsic vulnerability"** (with the word "intrinsic" related to the inner characteristics of the site under study) and the groundwater vulnerability as "**specific vulnerability**" where "specific" refers to the contaminant (and its physico-chemical characteristics) applied.

In recent years, many approaches have been developed to evaluate both the intrinsic and specific aquifer vulnerability and comprehensive reviews of groundwater vulnerability assessment methods are present in literature (Zhang et al., 1996; Worrall and Besien, 2005; Pavlis et al., 2010)

Modelling and monitoring for vulnerability assessment

At the time being, the approach used by water quality managers to evaluate territorial vulnerability and therefore implement risk mitigation measures for chemical substances on the territory falls within two categories:

a) monitoring studies, as a mean to disclose the present contamination status and assess the impact of newly implemented measures;
b) use of models to predict the environmental distribution and fate of chemical substances.

Both approaches show pros and cons. For instance, monitoring campaigns are very useful for regulatory purposes to verify whether the concentration of a chemical (or more) exceeds predetermined trigger values (e.g. 0.1 µg/L in groundwater for PPPs). On the other hand, the main limitation of the monitoring approach is referred to the informative content of the obtained data. As matter of fact, they represent a snapshot of what is happening (in terms of concentrations) while sampling.

In other words, they represent a single point in space and time (static), in a situation in which different dynamic processes act at the same time; consequently, the future state of the environment cannot be forecasted from monitoring data (Suzuki et al., 2004). Furthermore, they do not provide information on the origin of contamination (point and non-point source pollution). Finally, a preliminary set of information are needed to plan monitoring campaigns, both for selecting pesticides to be included in the list of monitored substances (leaching potential, loading rates, availability of analytical techniques) and to define the number and the spatial distribution of sites to be monitored and the sampling frequency (hydrogeology, agronomic practices, climate and soil properties). However, such information is not always easily available. In addition, the high economic costs of monitoring often limit the density of monitoring sites and influence a proper implementation of monitoring plans.

In alternative to monitoring, water quality managers can use modelling approaches. As already described, some spatially distributed fate and transport models of PPPs have been realised in recent years. Advent of GIS has facilitated the development of spatially explicit representations (maps) of contaminants from a given spatial distribution of sources. Spatially explicit models provide a valuable analytical tool to identify vulnerable areas and to forecast the probable consequences of risk mitigation actions taken from risk managers on a territory but if the input data are incorrect or uncertain, the resulting outputs can be wrong or debatable. This leads to the introduction of biases and uncertainties in the spatial estimation of pesticide transport toward water resources; consequently, this could hamper the correct implementation of risk mitigation actions on the territory, even if the model has been previously validated in another geographical context.

One of the findings of the doctorate is new approach which couples modelling evaluations with existing monitoring data, taking advantage of both the approaches. It provides risk assessors with a complete methodology to investigate the groundwater vulnerability to pesticide, raising the knowledge of the active substance presence and movement in the considered territory. It combines vulnerability maps from pesticide fate models with monitoring data analysis in order to identify areas where mitigation measure or limitation of use of the investigated active ingredient should apply. Moreover, it could be useful to verify the appropriateness of the current monitoring network or to suggest its repositioning. At last, it could identify areas where simulation models could not represent the correct substance transport in the groundwater, probably due to an incorrect parameterisation of the pedo-climatic characteristic of the area.

Environmental Decision Support Systems

As stated by Rizzoli and Young (1997), modelling allows prediction of an expected future state, and thus is an important part of informed decision making in natural resources management. While single models can (and do) directly support this decision-making process, often the complexity of environmental systems, and the multi-faceted nature of many environmental problems, means that decision makers commonly require access to a range of models, data and other information. Software systems that integrate models, or databases or other decision aids, and package them in a way that decision makers can use are commonly referred to as Decision Support Systems (DSS). Those that are developed for use in environmental domains are referred to herein as Environmental DSS (EDSS).

Environmental systems have several attributes which make their formal representation different from that of other systems (Guariso and Werther, 1989):

- dynamics, they evolve over time;

- spatial coverage, physical processes behind environmental processes are often in a 2-D if not 3-D world, hence the ability to represent territorial coverage with geographical information systems (GIS) and spatial databases is a required feature;
- complexity, since they involve interactions between physico-chemical and biological processes;
- stochastic behaviour, many environmental processes are inherently stochastic, hence they should be studied using statistical analysis;
- periodicity of most environmental variables.

Environmental systems are generally used by three classes of users, depending that by the intrinsic complexity of environmental processes and the wide interest that they claim:

- the environmental scientist, which develop models and test them in the system; he/she defines the problem domain of the application;
- the environmental manager (or decision maker), which "uses" the systems with the help of the scientist and need to obtain answers to environmental impact or new policies;
- the environmental stakeholder, which is generally interested to some parts of the environmental process and often could not enter in technical details as the decision maker; For these users, the functions of education, demonstration and explanation are very important.

To be representative of the environmental process they would analyse, EDSS should be designed to acquire and structure the knowledge available in the domain under study, for example in databases. They should provide expert knowledge for the specific domain and deal with spatial data (through GIS). They are substantially multi-purpose tools, because they should be used in planning, management and optimisation, i.e. in the past, present and future analyses of the environmental matter take into consideration.

Since its the early definition, in the last decades of the XXth century, several examples of EDSS have been developed and applied; for a representative analysis and evaluation readers could refer to McIntosh et al. (2011).

Overview

The three years PhD was intended to study, design and develop Environmental Decision Support Systems aiming at addressing some of the challenges that the introduction of chemical substances in agriculture poses to the environment and ultimately to human beings. Developed tools contain many of the EDSS features described above: they define a finite domain where main environmental variables and parameters are described at the finest level; they rely on expert knowledge which describe the environmental processes by the means of expert judgements or environmental models; they represent processes at territorial level by the means of geographical information systems (GIS) and linked spatial databases; they can be used for planning, evaluating and optimising scenarios, hence they could be used to test the efficacy of policies, to evaluate the actual scenarios or to evaluate situations in the past.

The first EDSS developed was ValorE (Valorizzazione degli Effluenti), an expert system for the valorisation of manure from livestock with the clear objective to reduce the high values of nitrogen at the field in Lombardy region (Acutis et al., 2014). Subsequently, the EDSS VULPES (Vulnerability to Pesticide) for the identification of groundwater vulnerable areas to chemical substances has been implemented, taking advantage of current modelling tools from the FOCUS workgroup (FOCUS, 2000) coupled with GIS (Di Guardo and Finizio, 2015). Moreover, we developed a new methodology (moni-modelling approach) for the identification of vulnerable areas to chemical substances which couples modelling results from VULPES EDSS and existing monitoring data from public authorities (Di Guardo and Finizio, 2016). Again, VULPES has been coupled with the ValorE expert system in order to analyse the environmental fate of veterinary medicine products in the groundwater (Di Guardo and Finizio, 2017). Finally, we developed a new indicator (VIGNETO) to evaluate the impact of vineyard management practices in a perspective of farm sustainability (Lamastra et al., 2016).

ValorE – Valorisation of livestock effluent

ValorE is an integrated decision support system to be used in the Lombardy region to address all the major components of manure management (production, storage, treatment and land application) for a variety of livestock types. The DSS allows an integrated assessment at farm and territorial scale using two different tools aimed at two different stakeholders. The EDSS ValorE helps stakeholders (i) to find the best option for minimising the risk of environmental pollution (mainly N), (ii) improving the value of manure from different livestock in Environmental, technical, agronomic and economic terms, (iii) planning manure treatment plants, and (iv) evaluating the effects of new technologies on farm management as well as checking, ante factum, possible impacts of new policies.

To carry out comparative analysis, the software offers the possibility to analyse the current perspective in terms of manure management system at farm or territorial scale by interrogating the available databases. Then, it is possible to modify the farm management by generating different alternative scenarios both at farm and territorial scale thanks to an extensive choice of options. Changes can be focused on manure management system and on cropping system features. Current and alternative scenarios sustainability can be evaluated and compared through indicators. Moreover ,a specific tool of the DSS allows the investigation of effects due to policy measures.

VULPES – Vulnerability to pesticide

The EDSS VULPES (VULnerability to PESticides) is the first tool completely developed during the doctorate. VULPES is a regional exposure assessment tool for evaluating the groundwater impact of the use of pesticide at regional level (currently it works at NUTS 2 level). VULPES responds to this specific need, providing a simple tool which couples environmental models to GIS representation of the territory in order to identify vulnerable areas to PPPs. VULPES applies the same pesticide fate models of the FOCUS group to real environmental data (pedology, weather, irrigations, crops) thus likely approaching to the real impact on the area.

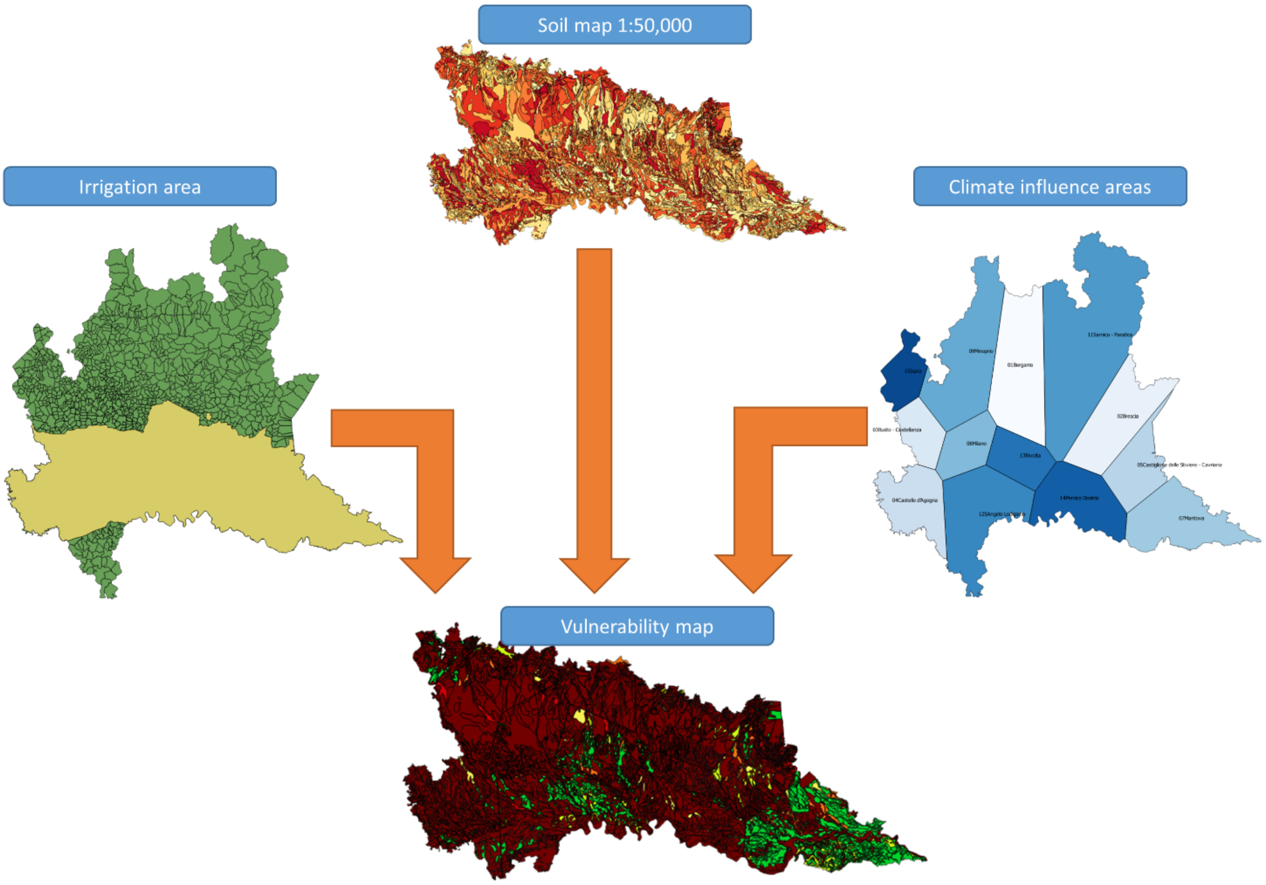

Figure 3 – Maps used in the system. Vulnerability map is calculated making use of spatial data from soil, weather, irrigation and administrative unit maps

VULPES stores a set of alphanumeric data linked to cartographic layers, i.e. influence areas of relevant weather stations, the pedology map and areas where irrigation is allowed. These layers are overlaid each other in order to obtain a new map in which every new polygon (called Uniform Geographical Unit – UGU) has a unique set of environmental data, i.e. one type of weather, one map unit of soil types, the presence or not of irrigation. Other databases in VULPES contain crop parameters and plant protection products data (in particular physical-chemical properties for each active ingredients) which complete the set of data needed by pesticide fate models. Results are then collected on a vectorial GIS map, where the value of substance concentration of each polygon is aggregated into six classes according to the potential risk, with the clear characterisation of the worst case (concentration values > 0.1 µg/l, corresponding to the regulatory limit for drinking water) in red colour.

VULPES has been applied to the PO plain of Lombardy region, calculating the vulnerability maps to Terbuthylazine (Figure 4).

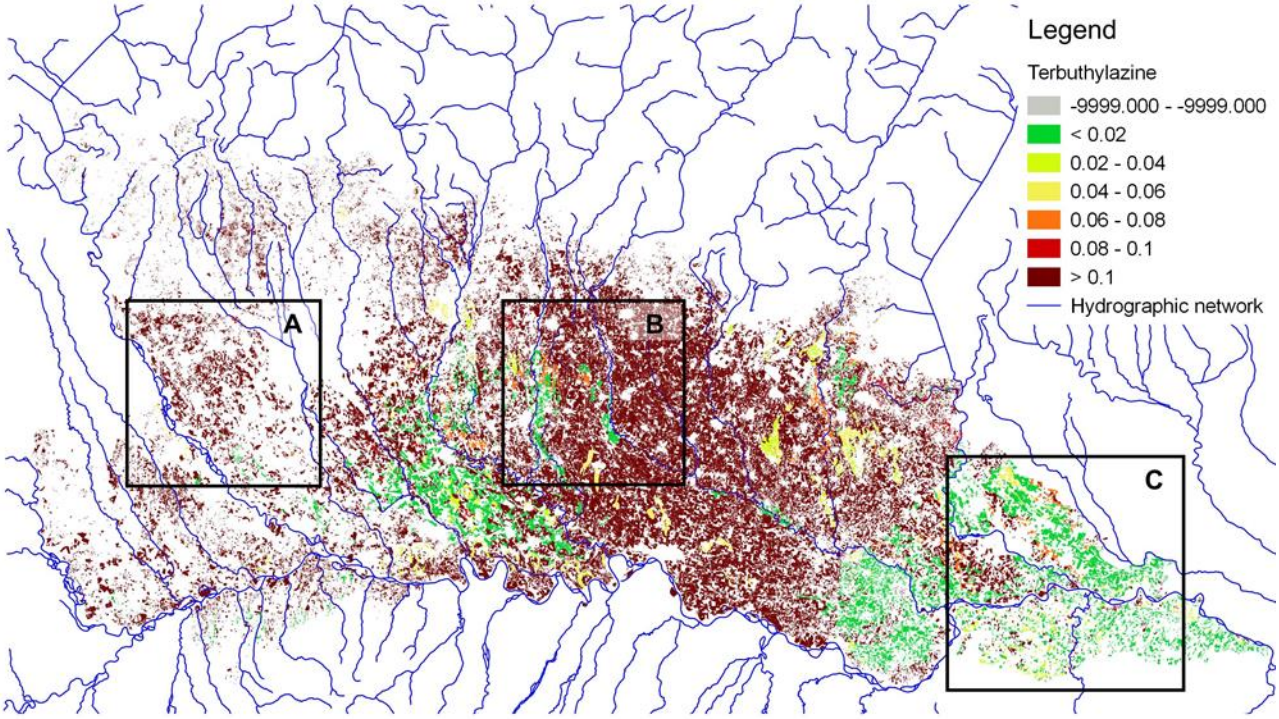

Figure 4 – Vulnerability map of Lombardy region to terbuthylazine substance filtered with maize cropped fields. Boxes A, B and C depict respectively the Lomellina area, the lower Adda-Ticino basin and the East province of Mantua.

The resulting map allowed us to identify areas of the Lombardy region cropped with Maize with a high potential risk of terbuthylazine percolation towards groundwater and other areas with less permeable soils to the substance.

The moni-modelling approach

The moni-modelling approach, here briefly described (Figure 5), is based on coupling spatial modelling of environmental fate and long term monitoring data of plant protection products (PPPs) occurrence in wells. A methodology of comparison between the results of the two types of information permits to take valuable conclusions on the effective vulnerability of the area.

In the first instance, it foresees the definition of vulnerability maps at regional scale using GIS-coupled models for predicting the potential pesticide concentrations in groundwater at regional scale. In this study, we used the EDSS VULPES. On the other side, another brick of information for decision making is given by the availability of long term monitoring data of PPPs residues in groundwater. Considering the availability of long term data on PPPs residues in groundwater it is possible to create a map of 95th percentile of each PPP observed in each monitoring site. This map can be used as input for a geostatistical analysis (we used an ordinary block kriging interpolation method) to produce a new map highlighting the influence areas of different wells in the territory.

By evaluating both monitoring and modelling results, decision makers will have a powerful tool to identify specific areas at risk where implement risk mitigation measures. In addition, decision maker will have useful information to plan better monitoring networks and/or better calibrations of predictive models.

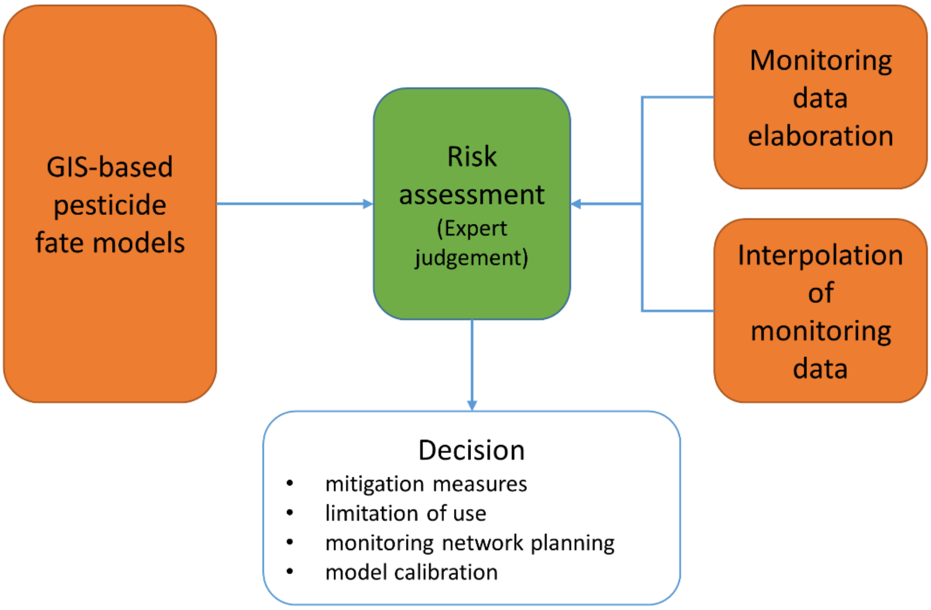

Figure 5 - Flux diagram of the proposed methodology. Colours represent different spatial levels of each action (in orange at regional level, in green at local level).

The moni-modelling approach has been applied to the Po plain of Lombardy region studying six different pesticide active ingredients; VULPES simulation results were coupled with monitoring data provided by regional monitoring agency. Results of the study, pointed out six typical situations where monitoring and modelling data could easily integrate themselves providing new information for the correct evaluation of territorial vulnerability.

Sust-PHarm

SUST-Pharm is a new tool for evaluating the impact of veterinary medicine products (VMP) usage on groundwater at a spatial scale; it tries to fill the gap of knowledge on the territorial implementation of appropriate risk mitigation measures for VMPs in order to protect groundwater resources quality. The methodology shares the same overall philosophy and underlying science actually used for modern risk management of pesticides on the territory. Therefore, provides coherent and integrated solutions to VMP risk assessment and risk reduction for groundwater on a territorial basis. However, there are a number of relevant differences with the approach used for pesticides that gives to the proposed approach its own originality.

In our study, data about livestock farms, their typologies and geographic distribution along the Lombardia Region have been taken from the EDSS ValorE. Information about manure management practices at farm level were extrapolated from ValorE and linked to the EDSS VULPES.

Sustainable wine production – VIGNETO model

Sustainable agriculture could be defined as a set of agronomic practices that are economically viable, environmentally safe, and socially acceptable with the aim to create a system that is capable of persisting preserving the same characteristics. In 2004, OIV (Organization Internationale de la Vigne et du Vin - OIV, 2004), defined sustainability as a "global strategy on the scale of the grape production and processing systems, incorporating at the same time the economic sustainability of structures and territories, producing quality products, considering requirements of precision in sustainable viticulture, risks to the environment, products safety and consumer health and valuing of heritage, historical, cultural, ecological and aesthetic aspects".

A new fuzzy expert system connected to web GIS software has been developed; it is a useful instrument for measuring the environmental impact of viticulture in a holistic way. The easy-to-use software could be used by farmers and other decision makers to perform a sustainability assessment at vineyard scale, and help to improve their performance, adopting effective measures to improve the sustainability of the wine estate.

"Vigneto" was developed in the framework of the "V.I.V.A. sustainable wine" project, launched in 2011 by the Italian Ministry for the Environment, Land and Sea. The final output of the project is a sustainability label that signals to the consumers the sustainability attributes of the products and provides easily interpretable information about four selected indicators. The wine label shows the V.I.V.A. logo and through a QR code it is possible to consult the results obtained in the four selected indicators: in addition to "vigneto" the other indicators are "Aria" (Carbon Footprint), "Acqua" (Water Footprint, Lamastra et al., 2014), and "Territorio" (a selection of quality indicators to evaluate the socioeconomic aspects of sustainability).

References

Acutis, M., Alfieri, L., Giussani, A., Provolo, G., Di Guardo, A., Colombini, S., Bertoncini, G., Castelnuovo, M., Sali, G., Moschini, M., Sanna, M., Perego, A., Carozzi, M., Chiodini, M.E., Fumagalli, M., 2014, ValorE: an integrated and GIS-based decision support system for livestock manure management in the Lombardy region (northern Italy), Land Use Policy, 41, 149–162

Batchelder, AR, 1981. Chlortetracycline and oxytetracycline effects on plant growth and development in liquid cultures. J. Environ. Qual., 10, 515–518

Bockman, OC, Kaarstad O, Lie, OH, Richards, I. 1990. Agriculture and Fertilizers. Agricultural Group, Norsk Hydro a.s, Oslo, Norway

Bogaard A., Fraser R., Heaton T. H. E., Wallace M., Vaiglova P., Charles M., Jones G., Evershed R. P., Styring A. K., Andersen N. H., Arbogast R., Bartosiewicz L., Gardeisen A., Kanstrup M., Maier U., Marinova E., Ninov L., Schäfer M., Stephan E., 2013, Crop manuring and intensive land management by Europe’s first farmers, PNAS, 110 (31) 12589-12594

Bouraoui, F., 2007. Testing the PEARL model in The Netherlands and Sweden. Environ. Model Softw. 22, 937–950

CVMP, 2008. Environmental Impact Assessment for Veterinary Medicinal Products in Support of the VICH Guidelines GL6 and GL38. European Medicines Agency, London. EMEA/CVMP/418282/2005-Rev.1.

CVMP/VICH, 2000. CVMP/VICH Topic GL6 (Ecotoxicity Phase I). Guideline on Environmental Impact Assessment (EIAs) for Veterinary Medicinal Products - Phase I. European Medicines Agency, London. CVMP/VICH/592/98-FINAL.

CVMP/VICH, 2005. CVMP/VICH Topic GL38. Guideline on Environmental Impact Assessment for Veterinary Medicinal Products - Phase II. European Medicines Agency, London. CVMP/VICH/790/03-FINAL.

Cordell, D., Drangert, J., White, S., 2009. The story of phosphorus: Global food security and food for thought, Global Environmental Change, 19, 2, 292-305

Council of the European Union, 1980. Council Directive 80/778/EEC of 15 July 1980 relating to the quality of water intended for human consumption. OJ L 229 pp. 11–29 (30.8.1980)

Council of the European Union, 1991. Council Directive 91/414/EEC of 15 July 1991 concerning the placing of plant protection products on the market. OJ L 230 pp. 1–32 (19.8.1991)

Council of the European Union, 1998. [98/83/EC] Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. OJ L 330, pp. 32–54 (5.12.1998)

Crane, M., Boxall, A.B.A., Barrett, K., 2008. In: Crane, M., Boxall, A.B.A., Barret, K. (Eds.), Veterinary Medicines in the Environment. Taylor & Francis/CRC Press, Boca Raton, FL, USA/London, UK, p. 224.

Di Guardo, A., Finizio, A., 2015. A client–server software for the identification of groundwater vulnerability to pesticides at regional level. Sci. Tot. Environ., 530–531, 247–256

Di Guardo, A., Finizio, A., 2016. A moni-modelling approach to manage groundwater risk to pesticide leaching at regional scale. Sci. Tot. Environ., 545, 200-209

Di Guardo, A., Finizio, A., 2017. Sustainable use of Veterinary Pharmaceuticals on the territory (SUSTPharm): linking available database of manure management and environmental fate models, Sci Total Environ, 575, 1014–1026

Dixon, B., 2005. Groundwater vulnerability mapping: a GIS and fuzzy rule based integrated tool. Appl. Geogr. 25 (4), 327–347

EFSA Panel on Plant Protection Products and their Residues (PPR) 2013. Scientific Opinion on the report of the FOCUS groundwater working group (FOCUS, 2009): assessment of higher tiers. EFSA Journal 2013;11(6):3291.

European Commission, 2001. Directive 2001/82/EC of the European Parliament and of the Council of 6 November 2001 on the Community code relating to veterinary medicinal products. OJ L 311, 1–66 28.11.2001.

European Commission, 2005. Regulation (EC) No 396/2005 of the European Parliament and of the Council of 23 February 2005 on maximum residue levels of pesticides in or on food and feed of plant and animal origin and amending Council Directive 91/414/EEC. OJ L 70, 16.3.2005, p. 1–16

European Commission, 2009a. Commission Regulation (EC) No 1107/2009 of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L 309 pp. 1–50 (24.11.2009)

European Commission, 2009b. Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009 establishing a framework for Community action to achieve the sustainable use of pesticides. OJ L 309 pp. 71–86 (24.11.2009)

European Medicines Agency, European Surveillance of Veterinary Antimicrobial Consumption, 2015. 'Sales of veterinary antimicrobial agents in 26 EU/EEA countries in 2013'. (EMA/387934/2015)

Eurostat, 2013 - http://ec.europa.eu/eurostat/statistics-explained/index.php/Agri-environmental_indicator_-_mineral_fertiliser_consumptio (visited: 03/01/2017)

Eurostat, 2016 - http://ec.europa.eu/eurostat/statistics-explained/index.php/Pesticide_sales_statistics (visited: 03/01/2017)

Eurostat, 2016 – Eurostat, 2016. Agriculture, forestry and fishery statistics. 2016 edition. Luxembourg: Publications Office of the European Union

FOCUS Groundwater Scenarios Workgroup, 2000. FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup 2000. EC Document Reference Sanco/321/2000 rev.2, pp. 1–202

Guariso, G. and Werthner, H. 1989. Environmental Decision Support Systems. Ellis Horwood Wiley, New York

Jarvis, N.J., 1994. The MACRO model (Version 3.1). Technical description and sample simulations. Reports and Dissert 19. Dept. Soil Sci., Swedish Univ. Agric. Sci, Uppsala, Sweden

Klein, M., 2000. PELMO: Pesticide Leaching Model, User Manual Version 3.0.2. Fraunhofer-Institut für Umweltchemie und Ökotoxikogie

Kümpel, R. Alexy, Kümmerer What do we know about antibiotics in the environment? K. Kümmerer (Ed.), Pharmaceuticals in the Environment: Sources, Fate, Effects and Risks, Springer-Verlag (2001)

Lamastra, L., Suciu, N.A., Novelli, E., Trevisan, M., 2014. A new approach to assessing the water footprint of wine: an Italian case study. Sci. Total Environ. 490, 748–756.

Lamastra, L., Balderacchi, M., Di Guardo, A., Monchiero, M., Trevisan, M., 2016. A novel fuzzy expert system to assess the sustainability of the viticulture at the wine-estate scale, Sci Total Environ, 572, 724–733

McIntosh, B.S., Ascough, J.C. II, Twery, M., Chew, J., Elmahdi, A., Harou, J.J., Hepting, D., Cuddy, S., Jakeman, A.J., Chen, S., Kassahun, A., Lautenbach, S., Matthews, K., Merritt, W., Quinn, N.W.T., Rodriguez-Roda, I., Sieber, S., Stavenga, M., Sulis, A., Ticehurst, J., Volk, M., Wrobel, M., van Delden, H., El-Sawah, S., Rizzoli, A., Voinov, A. 2011. Environmental decision support systems (EDSS) development—challenges and best practices. Environ Model Softw, 26:1389–1402

OECD series on pesticide, Number 8, Report of the OECD/FAO Workshop on Integrated Pest Management and Pesticide Risk Reduction, April 1999

OIV, 2004. Resolution OIV/CST 1/2004. Definition of Sustainable Vitiviniculture

Pavlis, M., Cummins, E., McDonnell, K., 2010. Groundwater vulnerability assessment of plant protection products: a review. Hum. Ecol. Risk. Assess. 16 (3), 621–650

Popp, J., Pető, K. & Nagy, J. 2013. Pesticide productivity and food security. A review. Agron. Sustain. Dev. 33: 243

Rizzoli, A. E., and Young, W. J., 1997. Delivering environmental decision support systems: software tools and techniques. Environ. Modell. & Soft., 12, 2-3, pp. 237-249

Robertson, G.P., Paul, E. A., Harwood, R. R., 2000. Greenhouse Gases in Intensive Agriculture: Contributions of Individual Gases to the Radiative Forcing of the Atmosphere. Science, 289, 5486, 1922-1925

Sarmah, A.K., Meyer, M.T., Boxall, A.B.A., 2006. A global perspective on the use, sales, exposure pathways, occurrence, fate and effects of veterinary antibiotics (VAs) in the environment, Chemosphere, 65, 5, 725-759

Smith A.E., Secoy, D.M., 1975 Forerunners of Pesticides in Classical Greece and Rome, J. Ag. Food Chem. 23 (6) 1050 (1975)

Snyder, C.S., Bruulsema, T.W., Jensen, T.L., Fixen, P.E., 2009. Review of greenhouse gas emissions from crop production systems and fertilizer management effects, Agriculture, Ecosystems & Environment, 133, 3–4, 247-266

Suarez, L.A., 2005. PRZM-3, A Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 3.12.2. U.S. Environmental Protection Agency, Washington, DC (EPA/600/R-05/111 (NTIS PB2006-101105))

Suzuki, N., Murasawa, K., Sakurai, T., Nansai, K., Matsuhashi, K., Moriguchi, Y., Tanabe, K., Nakasugi, O., Morita, M., 2004. Geo-referenced multimedia environmental fate model (G-CIEMS): model formulation and comparison to the generic model and monitoring approaches. Environ. Sci. Technol. 38 (21), 5682–5693.

Tiktak, A., van den Berg, F., Boesten, J.J.T.I., Leistra, M., van der Linden, A.M.A., van Kraalingen, D., 2000. Pesticide Emission Assessment at Regional and Local Scales: User Manual of FOCUS Pearl Version 1.1.1. RIVM Report 711401008Alterra Report

28. RIVM, Bilthoven (142 pp.).Tilman D., Balzer C., Hill J., Befort B. L., 2011. Global food demand and the sustainable intensification of agriculture. PNAS, 108, (50), 20260-20264

US Environmental Protection Agency, 1993. A Review of Methods for Assessing Aquifer Sensitivity and Ground Water Vulnerability to Pesticide Contamination. USEPA, Office of Water, Washington, DC

World Bank. 2007. World Development Report 2008: Agriculture for Development. Washington, DC. https://openknowledge.worldbank.org/handle/10986/5990.

Wik, M., Pingali, P., Broca, S., 2008. Global Agricultural Performance: Past Trends and Future Prospects. Background paper for the world development report 2008.

Worrall, F., Besien, T., 2005. The vulnerability of groundwater to pesticide contamination estimated directly from observations of presence or absence in wells. J. Hydrol. 303, 92–107

Zhang, R., Hamerlink, J.D., Gloss, S.P., Munn, L., 1996. Determination of non-point source pollution using GIS and numerical models. J. Environ. Qual. 25, 411–418

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ValorE: An integrated and GIS-based decision support system for livestock manure management in the Lombardy region (northern Italy)

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ABSTRACT

Intensive agriculture and livestock breeding represent critical factors in the Lombardy region since the nitrate vulnerable zones are 62% of utilised agricultural plain area. The aim of reducing the environmental risk caused by agriculture activities (e.g. nitrogen losses into groundwater and atmosphere) can be only achieved through a critical and scientific analysis of livestock manure management in a whole-farm perspective. Keeping in mind this objective, the decision support system (DSS) ValorE was developed. It can be described as a tool able to evaluate from the environmental, technical, agronomic and economic points of view the main components of manure management (production, storage, treatment and land application) for a variety of livestock types (i.e., cattle, swine, poultry, sheep, goats and horses), under different scenarios adopted at farm and territorial scale. ValorE consists of three main components: data management subsystem, model management subsystem and two versions of user-interface, both for farm and territorial scale. Most of the inputs to the DSS comes from external databases, while a software tool developed in the .NET environment and implemented using object oriented programming (C# language), provides the logic to manage the scenario simulation of agronomic and environmental farm-scale models. Users and stakeholders can carry out comparative analysis, starting from the knowledge of the current perspective, in terms of manure management system at farm or territorial scale by interrogating the available databases. Moreover, they can generate different alternative scenarios thanks to different options for the manure handling and cropping system simulation. Then they can finally evaluate and compare different scenarios through multidisciplinary and synthetic indicators but also visualise spatial effects exploiting the coupled webGIS. ValorE is therefore an attempt to offer a comprehensive tool for improving both farm strategy and decision making process, which is particularly important in a very intensive agricultural area, with one of the highest livestock density in the world, as Lombardy.

Introduction

Livestock production, responsible of a big part of agricultural land use for grazing and feed production, determine serious environmental problems such as greenhouse gas emissions (Steinfeld et al., 2006) and emissions of reactive nitrogen (N) in atmosphere and water (Oenema, 2006). These problems are getting much

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0264-8377/

importance due to the environmental targets required by the agricultural policies and regulations for preventing pollution of land, air and water. The core of the livestock production is the manure management from the animal excretion to the land spreading, because it affects both the quality of soil, air, water and the crop growth, and consequently it bears on the farm income. The selection of livestock manure management options is becoming a strategic task that farmers and public policy makers have to handle properly. As presented by Karmakar et al. (2010), several options for manure collection, storage and land application are available. Moreover, as discussed by Petersen et al. (2007) a variety of manure treatments with a specific target has been developed as well as improvements in animal nutrition to control manure production and composition. Consequently, before investing money, it is of paramount importance to get a support tool that could assist stakeholders and farmers on identification, evaluation, and selection of the more suitable option of the manure management for a specific area and aim. In fact, each management strategy has its advantages and disadvantages when considering environmental, agronomic, technical, energetic, cost and labour issues (Fumagalli et al., 2012).

A decision support system (DSS) is an interactive computer-based system intended to help decision makers in using communication technologies, data, documents, knowledge and/or models to identify and solve problems, hence completing the decision process tasks with the overall objective of making well-informed decisions (Power, 1997). Multiple examples of the development and application of DSSs in agriculture addressing a variety of domains, such as pest management (Perini and Susi, 2004; Riparbelli et al., 2008; Calliera et al., 2013), water management (Fassio et al., 2005; Pallottino et al., 2003; Giupponi, 2007; Acutis et al., 2010), agricultural land management (Mazzocchi et al., 2013) and nutrient management (Djodjic et al., 2002; Forsman et al., 2003; De et al., 2004), are available. As reviewed by Karmakar et al. (2007) DSSs for manure management are available but most of them are addressed to the nutrient management in the agronomic planning with regard only to timing, amount and spreading method (De et al., 2004; De and Bezuglov, 2006). Only few DSSs consider the whole-farm manure management from the production to the land application providing support towards the choice of the more suitable option. Among these Karmakar et al. (2010) developed a specific DSS for swine farms of the Canadian Praires region: multiple combinations of management options can be evaluated considering different decision criteria such as environmental, agronomic, social and health, greenhouse gas emission, and economic factors, whilst the software MLCONE4 (Ogilvie et al., 2000) allows to evaluate manure-handling systems of a greater number of livestock types (i.e., swine, dairy and poultry) and it was specifically designed for Ontario Province's conditions. Similarly, Sørensen et al. (2003) developed a model to evaluate different manure handling systems for pig and dairy farms.

The use of DSSs considering manure management in a whole-farm perspective becomes a priority in areas with nutrient surplus and where farmers should define optimal strategies to reduce environmental impact at a sustainable cost. In fact, in these conditions solutions often include the implementation of treatment technologies to remove nutrient surplus that entails high investment and operating costs. A good example of this condition is represented by the plain area of the Lombardy Region (northern Italy) in which the Government have developed regional legislation including implementation of the requirements of Nitrates (91/676/EEC) and Water Framework (2000/60/EC) Directives and of Italian Regulations, such as the Ministerial Decree of 19 April 1999 approving the Code of good agricultural practices and that of 7 April 2006 regarding criteria for manure management. Specific Action Programmes for both nitrate and non-nitrate vulnerable zones (D.g.r. VIII/5868/2007 and D.g.r. IX/2208/2011) together with several measures funded through the Rural Development Programme (RDP) have been implemented to control nutrient pollution of water from agricultural sources. Moreover from 2011 is in force the nitrate derogation (EC, 2011) for which eligible farmers who want to obtain its benefit have to respect some requirements about manure and land management.

This territory in which the nitrate vulnerable zones represent 62% of utilised agricultural area is characterised by an intensively managed agriculture with high livestock density accounting for a big part of the Italian livestock, in particular more than 27% of cattle and 51% of pigs. Recent studies confirmed the potential impacts of the agricultural and livestock activities. Fumagalli et al. (2011, 2012) highlighted the high use of production factors such as N, fossil energy and plant protection products to sustain animal and crop productions. Perego et al. (2012) reported how the intensive maize-based cropping systems based on the use of organic and inorganic fertilisers could determine high risk of nitrate pollution as well as Carozzi et al. (2012, 2013, 2013a) showed how alternative low-ammonia emission techniques have to be prescribed during manure distribution on fields. Provolo (2005) showed the negative environmental impact of some manure management systems by mapping some indicator results such as the livestock manure production, the ratio between nutrients brought to the land and the uptake of the crop and the amount of N applied per hectare.

The awareness of the environmental concerns related to livestock activities with whole-farm perspective led to the development of a DSS able to provide the stakeholders, such as policy makers, farmers and their consultants, with an assessment tool to evaluate the introduction of different livestock manure management systems. The design and evaluation of different scenarios could allow the identification of the best management which could be characterised by available techniques and technologies.

An integrated decision support system is here presented to be used in the Lombardy region to address all the major components of manure management (production, storage, treatment and land application) for a variety of livestock types. It was developed on the basis of the previous experience carried out by Provolo (2005) who evaluated different livestock manure managements. The DSS allows an integrated assessment at farm and territorial scale using two different tools aimed at two different stakeholders.

The objective of this work is to present the DSS ValorE, which helps stakeholders (i) to find the best option for minimising the risk of environmental pollution (mainly N), (ii) improving the value of manure from different livestock in environmental, technical, agronomic and economic terms, (iii) planning manure treatment plants, and (iv) evaluating the effects of new technologies on farm management as well as checking, *ante factum*, possible impacts of new policies.

ValorE: a DSS to enhance livestock manure management

ValorE (Valorisation of Effluents) is a user-friendly software developed to cope with different livestock (i.e., cattle, swine, poultry, sheep, goats and horses) and to suggest and analyse alternative manure management options at farm and territorial scale. Such DSS consists of three main components: data management subsystem, model management subsystem and user-interface. A simple representation of the DSS structure is reported in Fig. 1. Several external databases are directly linked and periodically interrogated in order to supply the DSS database management system with the relevant input, while a software tool developed in the .NET environment and implemented using object oriented programming (OOP – C# language), provides the logic to manage the scenario simulation linking agronomic and environmental farm-scale models. The two interfaces allow managing the simulation at farm and territorial

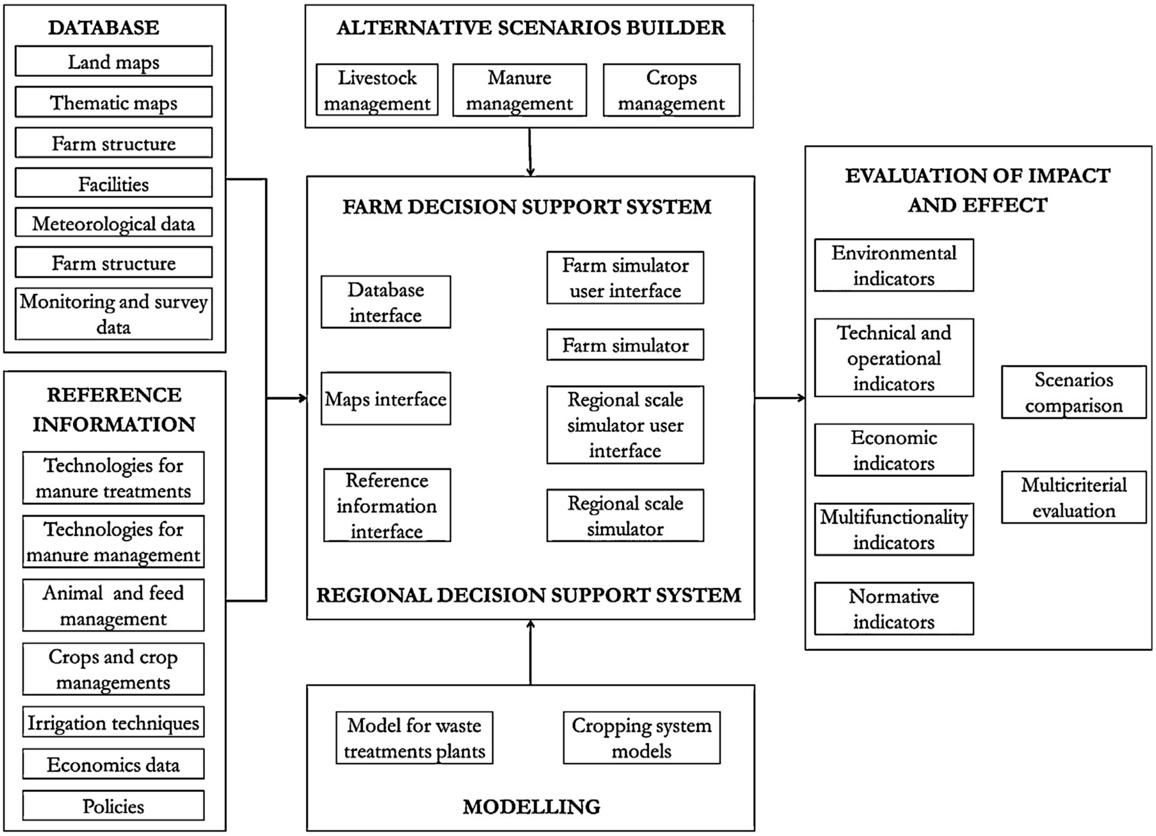


Fig. 1. Schema showing the general structure of the ValorE DSS.

scale respectively. The territorial interface is a web portal connected to a WebGIS (geographical information system) handling the spatially distributed inputs and outputs of the DSS. All the maps and tables produced by the software are in Italian language since an English version has not yet been released.

Databases and reference information

All information needed to run the system are stored on databases provided by the Lombardy Regional Government. Such data include (i) farm structure, (ii) meteorological data at daily time step, and (iii) pedological characterization of the whole region.

Another database created by the team group contains several tables of default data called there after “reference tables”.

Farm structure

The database of the Agricultural Informative System of Lombardia Region (SIARL) contains data related to the farm structure for the whole region. All information are periodically updated by farmers. In particular, farmers have to provide details about the regulatory compliance on the matter of N management (Provolo, 2005). This database collects information of 87% of farms surveyed by the Italian institute of statistics during the 6th Agricultural census launched in 2010. The database includes information on distribution of the herd according to animal age categories, animals housing, manure and slurry storage and treatment. Moreover, land use data of every cadastral plot are stored for each farm providing information on the area allocated to the different crops over the years.

Meteorological database

The Lombardia Region has made available twenty-year time series of daily meteorological data such as maximum and minimum temperature (°C) and precipitation (mm) in 14 stations representative of the regional climate zones.

Soil data

A vectorial soil map at scale 1:50,000 is available, where 1038 soilscapes are defined and characterised by at least one soil profile. Soil physical and chemical properties, such as texture, structure, organic matter, pH, soil cation exchange capacity, derived from field and laboratory analysis are available for each horizon of the soil profile down to 2 m depth. The soils are classified according to the WRB classification (FAO, 1998).

Technological and agronomic management data

Only a part of the information needed to run the DSS is directly available from the SIARL database (Regione Lombardia, 2010), therefore another database containing five reference tables of default data was produced. Default data derived from existing literature, experts knowledge and farmers’ interviews are:

- the technique, functional and economic features of available technologies used for the manure treatment;
- the animals ration for various livestock categories in terms of protein and phosphorous content;
- the main crops grown in the regional arable land and the related agronomic management, such as sowing and harvesting time, organic and mineral N supply;
- the irrigation techniques, the frequency and the water volumes typical of the different areas of the region;
- the current regulation on the matter of (i) Nitrate Vulnerable Zones definition, (ii) allowed timing of manure application, (iii) restriction on manure fertilisation in particular areas such as riparian zones and protected areas, (iv) guidance for manure incorporation (Regione Lombardia, 2007).

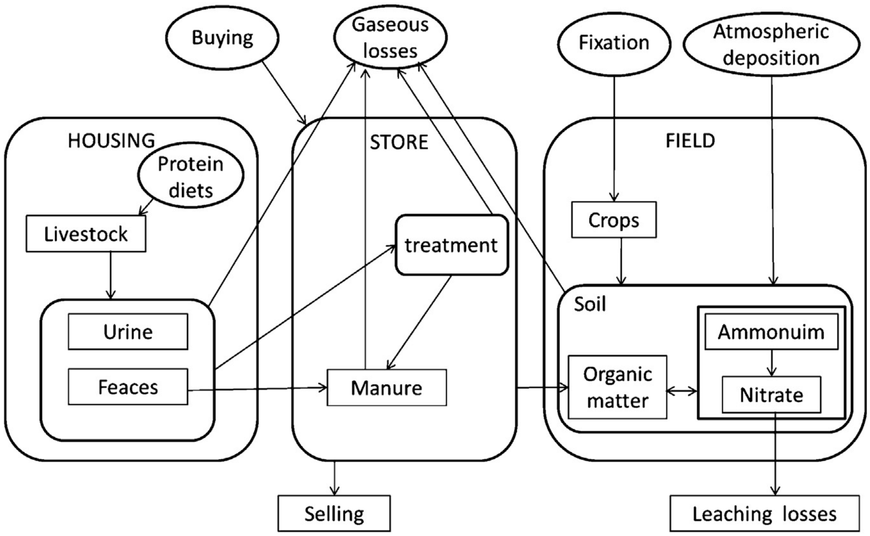


Fig. 2. Schema showing the simulated nitrogen flows at farm level (modified from Berntsen et al. (2003)).

DSS development

The DSS has to meet a series of requirements to be useful for different kind of stakeholders (e.g., farmers and their consultants, Public Authorities, producers organisations, scientists, etc.) and for an easy updating and maintenance. The territorial part of the DSS is a web portal, whereas the farm simulator can be installed and run on any computer running windows XP OS or later versions without specific hardware requirement. Moreover, the development of an easy way of operating was a main objective (no more than 5 clicks to get to a complete analysis following the suggestion of the "three click rule" for user friendly and more impactful web design) with report simulation results either in maps and tabular form.

The intended purpose of the software is to simulate at farm scale each stage of livestock excreta cycle from production by the herd to the crop N uptake as well as the N cycle and losses occurring via leaching, and gaseous emission (volatilisation and denitrification). Fig. 2 shows the simulated N flows at farm level. The software consists of different modular components relating a specific stage of the manure production process. Each component allows for selection of strategies to simulate a specific process and each module results represent the input data for the subsequent one (Fig. 3).

Excretion module

In order to evaluate the impact of the different livestock rations on urine and faeces produced by cattle and swine, the excretion of N and P content is simulated as a function of feed intake and animal performance. In this analysis, dairy cattle, beef and pigs farms are considered as the main source of production of slurry in Lombardy.

With regard to cattle, the model allows estimating separately for urine and faeces, the amount of N and P excreted by quantifying the amount of manure. Instead, the amount of K excreted is estimated as a fixed percentage of live weight, as recommended by existing legislation. For dairy cattle, the excretion is computed by a sub-model from the following input variables: (i) the body weight of lactating dairy cows, dry cows, heifers and calves (ii) the milk production level, (iii) the milk fat and protein content, (iv) the dry matter intake, (v) and the protein content of feed. In particular, the dry matter intake is calculated by using the equation proposed by the National Research Council of USA (2001). The model produces the following output data: (i) the excreted products as fresh matter (kg FM d^{-1}), calculated according to Nennich et al. (2005), (ii) urine and its N content (kg d^{-1}), calculated according to Fox et al. (2004), (iii) the amount of faeces, calculated as difference between the total excreted products and urine (kg d^{-1}), (iv) the N faeces content and, (v) the milk N content (kg d^{-1}).

The model developed for pigs estimate the excreted amount of N, P and K according to several studies (Pomar et al., 1991a,b,c; Le Bellego et al., 2001; van Milgen and Noblet, 2003). In particular, the estimate is carried out for physiological stages of growth and production of the animal. The model quantifies the feed intake based on the animal growth (kg d^{-1}) and feed conversion efficiency for the considered growing phases and for number of farrows and litters size for the sow. The nitrogen, P and K intakes (kg d^{-1}) are estimated based on feed intake (kg d^{-1}) and diet contents, while excretions are determined from diet and protein digestibility and mineral absorption (%) for the considered physiological stages. The model allows to calculate the manure production (i.e., dry matter and volume) and the N, P and K excretion in faeces and urine. For other animal species such as poultry, sheep, goats and horses,

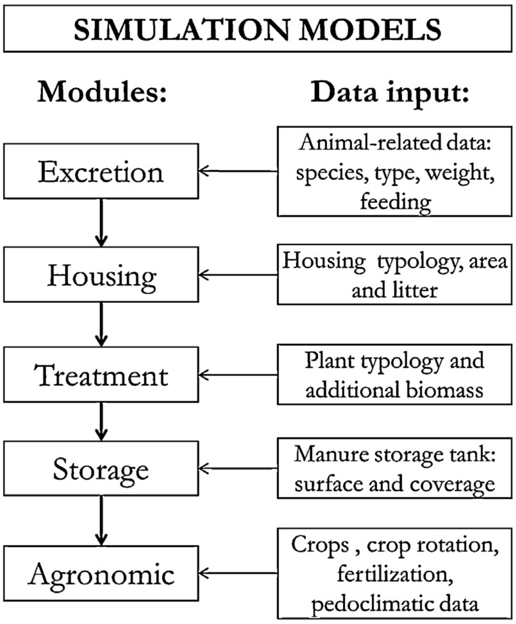


Fig. 3. Modular component of the DSS relating to each specific stage of the manure production processes. Each module implements its specific simulation model.

the excretion is estimated as a fixed percentage of live weight, as recommended by existing legislation (Regione Lombardia, 2007).

Housing, treatment and storage modules

Slurry is subjected to chemical and physical modifications with relative gaseous losses to the atmosphere. For each stage of the storage and treatment process the module simulates the amount of slurry mass and its N, P and K content together with the investment and operating net costs of any joint production (energy, compost, fertilisers, etc.).Moreover, it allows the assessment of the feasibility and suitability of alternative techniques in plant management.

The input data of the slurry storage and treatment module are: (i) the chemical and physical composition of the excreted products expressed as kg of dry matter, kg FM, faeces TKN (Total Kjeldhal nitrogen) content, urine TKN and P_2O_5 content in faeces and urine), (ii) the litter fraction of the manure, and (iii) the rainfall. The effect of the typology of livestock housing and the effect of different types of slurry storage are simulated according to IPCC (2006) and EEA (2009), considering also the experience of Amon et al. (2006) and Webb and Misselbrook (2004). A wide range of treatments is considered in the module: solid–liquid separation (Dinuccio et al., 2008; Fangueiro et al., 2008; Cocolo et al., 2012), anaerobic digestion with biogas and energy production (Amon et al., 2007; Biswas et al., 2007), ammonia stripping (Bonmatì and Flotats, 2003), nitrification and denitrification (Rousseau et al., 2008), aerobic stabilisation (Loyon et al., 2006; Beline et al., 2007) and composting (Paillat et al., 2005; Szanto et al., 2007).

The slurry module calculates: (i) the final volume of the stored slurry, (ii) the final chemical and physical composition, (iii) the solid and liquid fraction, (iv) the gaseous losses to the atmosphere, and (v) the possible production of biogas for the anaerobic digestion plants and other joint products of treatments.

Economic aspects are involved in the estimation of the weight of manure management options on farm income, since it has been recognised the importance of cross compliance on the economy of agricultural sector (Bezlepkina et al., 2008; De Roest et al., 2011). For each phase of managing slurry and manure (housing type, treatments, storage, distribution), the module calculates investment and operating costs (Berglund and Börjesson, 2006; Gourmelen and Rieu, 2006). For the housing systems, while the investment cost is related to the cost of construction (e.g., raw material, facilities) the operating cost depends on bedding materials, energy consumption and cost of facilities maintenance and labour. In the case of manure storage and its cover and of plant for manure treatment the investment cost is mainly calculated as a function of specific technical parameters, namely the treated volume and the power required. For all treatment modules, the operating cost is related to energy consumption, raw materials, facilities maintenance and labour cost. The cost of manure distribution is a function of transported volumes and distance from farm to field. Operating costs are broken down into monetary costs and non cash charges, so that it is possible to draw cash flow and analyse the investment in term of net present value and internal interest rate. The annual manure management cost considers the operating cost and amortisation cost related to the economic life of facilities and structures (6, 8, 10 and 15 years).

Agronomic module

The agronomic module is based on the crop simulation model, ARMOSA (Perego et al., 2013a,b), but they do not exactly coincide because the efficacy of process-based models at large scale is questionable due to the long computational times and the parameterisation constrains required. Therefore, a meta-model was developed, providing comparable results as the original model but a lower computational effort (Forsman et al., 2003), to ensure the quality of estimation while increasing the simulation speed.

The cropping system model ARMOSA. ARMOSA model simulates crop growth, water and N dynamics in arable land, under different climatic conditions, crops and management practices. It is a simulation model specifically developed on the basis of field data and it implements approaches largely validated in the scientific literature and used for practical applications. Crop growth model development is based on SUCROS–WOFOST (Supit et al., 1994; Van Ittersum et al., 2003). Water dynamics are simulated using the cascading approach, or the Richards' equation, solved as in the SWAP model (Van Dam et al., 2008); that model was previously calibrated under maize-based systems in Lombardy plain (Bonfante et al., 2010; Perego et al., 2012). Nitrogen dynamics is simulated according to the SOILN approach (Johnsson et al., 1987; Eckersten et al., 1996), but with some improvements. In SOILN only three pools of organic and mineral N are simulated: humus, litter, manure, while in ARMOSA each type of organic matter has been differentiated with reference to mineralisation rates, respiration losses and C/N ratio, allowing for separate calculations for the different types of organic fertilisers or crop residuals incorporated into the soil. Depth of incorporation is also taken in account and NH_4 and NO_3 pools are considered. NH_4 pool can be up taken by plants, oxidised to NO_3, fixed by the clay component of the soil, and immobilised in the organic matter; losses due to ammonia volatilisation are also simulated. NO_3 pool is subject to plant uptake, leaching and denitrification. Several options to use for medium-long time simulation are included: it is possible to define sowing and harvest date, crop rotation, automatic irrigation, set of fertilisation. The crop uptake is calculated on the basis of minimum, critical and maximum N dilution curves. Soil temperature is simulated considering the approach of Campbell (1985). ARMOSA model was calibrated and validated using a large dataset consisting of 3500 SWC daily data of soil profile (0.8–1.3 m depth), soil solution N concentrations, N leaching, N uptake and crop growth data (Perego et al., 2012).

The agronomic meta-model. The need to operate on a territorial scale involves the use of the meta-model, developed on the basis of the ARMOSA model. Such procedure represents an easy approach, quick in generating results of N losses and crop yields under different cropping systems, management and pedo-climatic conditions. The meta-model was developed on the basis of the examples provided by the literature (Forsman et al., 2003; Galelli et al., 2010). It was set up starting from the results of 70,000 simulation under different scenarios of cropping systems in the Lombardy. In particular, the agricultural management was defined as a function of the farm type and the pedo-climatic conditions of the region. Such different pedo-climatic conditions were identified using a cluster analysis as a function of median soil particles diameter, stone and organic carbon content along soil profile of 2 m depth. The meta-model development involved the sensitivity analysis (Morris, 1991; Saltelli et al., 2005) of the input variables on the ARMOSA output in order to finally reduce the input data. The output of the meta-model, which resulted by ARMOSA outputs, are: crop yield ($t\,ha^{-1}$), N leaching ($kg\,ha^{-1}\,year^{-1}$), crop N uptake and removal ($kg\,ha^{-1}\,year^{-1}$), water percolation ($mm\,year^{-1}$), N mineralisation ($kg\,ha^{-1}\,year^{-1}$), ammonia N volatilisation ($kg\,ha^{-1}\,year^{-1}$), denitrification ($kg\,ha^{-1}\,year^{-1}$), soil N fixation ($kg\,ha^{-1}\,year^{-1}$). For different crops, such assilage maize and grain maize (*Zeamayze* L.), winter wheat (*Triticumaestivum* L.), alfalfa (*Medicagosativa* L.), permanent meadow, foxtail millet (*Setariaitalica* L.), and Italian ryegrass (*Loliummultiflorum* L.), a multiple linear regression was calculated applying the stepwise method in order to identify the significant factors in determining the model outputs with average R^2 of 0.82. In Fig. 4 the development of the agronomic meta-model

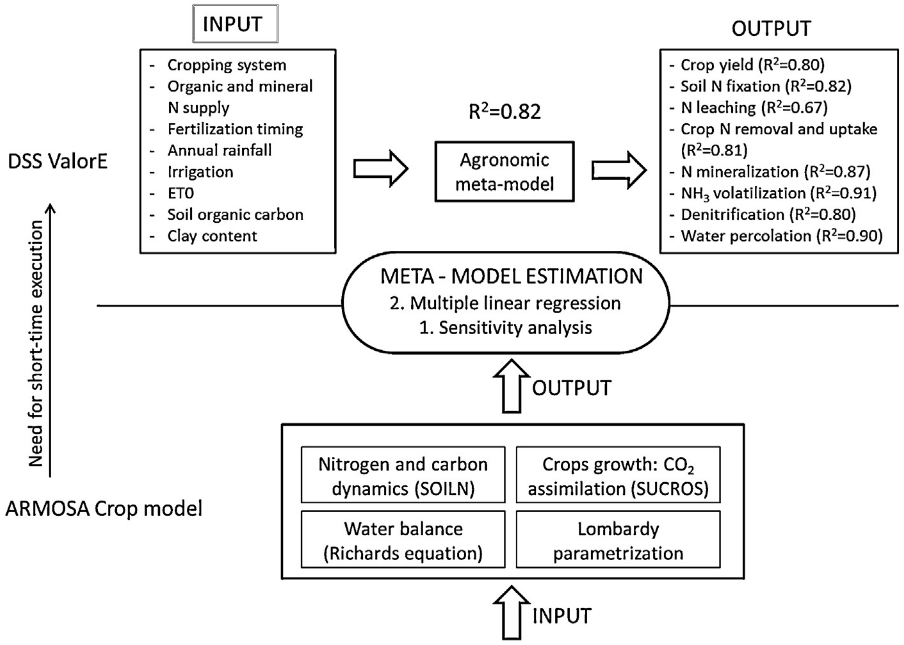


Fig. 4. Schema showing the development of the agronomic meta-model from the biophysical model ARMOSA.

is displayed and the R^2 of the multiple linear regression for each variable are reported.

Farm and territorial simulations

The above model structure was implemented in a software module that manages the inputs provided by the external databases and by the user and consequently activates each model in cascade. It works at farm level so outputs can be used in the farm simulator or aggregated at different scale in the territorial simulator.

The farm simulator is aimed at farmers and their consultants and it allows to analyse in detail the management and technological alternatives available for the specific farm from the manure production as a function of animal diet, to its final distribution on field. The more sustainable farm management strategies are suggested to reduce environmental impact (mainly N feature) and to better use the livestock manure. The software is downloadable from the website of the Lombardy Region, which collects the data of the structure and management of farms in the regional database.

The territorial scale application of ValorE can be included on the domain of the Spatial Decision Support Systems (SDSSs), defined by Malczewski (1999) as interactive computer-based systems designed to support a user or a group of users in achieving a higher effectiveness of decision-making while solving a semi-structured spatial decision problem. Moreover, in a earlier definition, Densham (1991) introduced the SDSSs as systems explicitly designed to provide the user with a decision-making environment that enables the analysis of geographical information to be carried out in a flexible manner. In the ValorE software the integration of GIS and DSS tools highlights the distinguishing capabilities and peculiar functions of a SDSS. ValorE is able to handle complex spatial data structures (e.g., crops, soils, and meteorological stations), to conduct analyses within the domain of spatial analysis by selecting the geographic area of interest, and to provide spatially-explicit outputs through GIS maps, allowing to describe phenomena in which location plays an important role (e.g., N leaching). The linking of DSS to a GIS tool is a common strategy to deal with spatial decision problems, environmental planning and land allocation (Geneletti, 2004; Peeters et al., 2012; Bottero et al., 2013).

In detail the territorial scale application of the ValorE System supports the users decision in two ways:

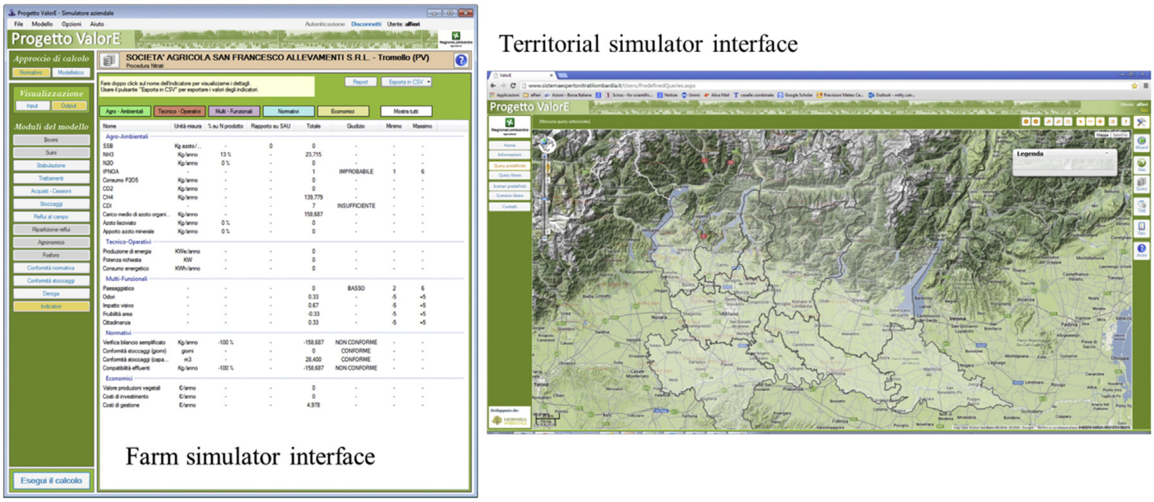
- it gives the possibility to investigate the current situation of the farm management practices in the whole Lombardy region by means of a set of default or custom queries on the actual information of the geo database and
- it provides a scenario generator and the simulator, to analyse the effects of hypothetical implementation of alternative management practices, of new technologies, or future scenarios of meteorological data as well as the impact of several regulatory measure and/or incentives.

In the latter case, the analysis follows a step-by-step procedure which starts by defining the geographical area in which the scenario would be applied and continues selecting the main topics (crops, technologies, agricultural practices and so on) of interest. For each topic selected, the scenario can be characterised by a large set of options which one could modify the actual situation in the farms of the selected area. Each scenario is evaluated by the modelling system at farm level and results are aggregated at spatial level in several indicators that take into account environmental, economic, technical, multifunctional and normative aspects. The territorial simulator, available to regional and public authorities at request, works at a larger spatial scale (virtually the whole region) and it is completely resident on web.

To improve the usability of the software, particular effort was devoted to enhance data retrieving performance from the databases and model calculation speed. Moreover, both interfaces were developed to be intuitive, requiring a short training time for learning main commands and sequences of actions (Fig. 5).

Tasks of the DSS ValorE

In order to carry out comparative analysis, the software offers the possibility to analyze the current perspective in terms of manure management system at farm or territorial scale by interrogating the available databases. Then, it is possible to modify the farm management by generating different alternative scenarios



SOCIETA' AGRICOLA SAN FRANCESCO ALLEVAMENTI S.R.L. - Tromello (PV)
Procedura Nitrati

Fare doppo click sul nome dell'indicatore per visualizzarne i dettagli.
Usare il pulsante "Esporta in CSV" per esportare i valori degli indicatori.

Nome	Unità misura	% su N prodotto	Rapporto su SAU	Totale	Giudizio	Minimo	Massimo
Agro-Ambientali							
SSB	Kg azoto/...	-	0	0	-	-	-
NH3	Kg/anno	13 %	-	23,715	-	-	-
N2O	Kg/anno	0 %	-	0	-	-	-
IPNOA	-	-	-	1	IMPROBABILE	1	6
Consumo P2O5	Kg/anno	-	-	0	-	-	-
CO2	Kg/anno	-	-	0	-	-	-
CH4	Kg/anno	-	-	139,779	-	-	-
CDI	-	-	-	7	INSUFFICIENTE	-	-
Carico medio di azoto organi...	Kg/anno	-	-	158,687	-	-	-
Azoto lisciviato	Kg/anno	0 %	-	0	-	-	-
Apporto azoto minerale	Kg/anno	0 %	-	0	-	-	-
Tecnico-Operativi							
Produzione di energia	KWe/anno	-	-	0	-	-	-
Potenza richiesta	KW	-	-	0	-	-	-
Consumo energetico	KWh/anno	-	-	0	-	-	-
Multi-Funzionali							
Paesaggistico	-	-	-	0	BASSO	2	6
Odori	-	-	-	0.33	-	-5	+5
Impatto visivo	-	-	-	0.67	-	-5	+5
Frubilità area	-	-	-	-0.33	-	-5	+5
Cittadinanza	-	-	-	0.33	-	-5	+5
Normativi							
Verfica bilancio semplificato	Kg/anno	-100 %	-	-158,687	NON CONFORME	-	-
Conformità stoccaggi (giorni)	giorni	-	-	0	CONFORME	-	-
Conformità stoccaggi (capa...	m3	-	-	28,400	CONFORME	-	-
Compatibilità effluenti	Kg/anno	-100 %	-	-158,687	NON CONFORME	-	-
Economici							
Valore produzioni vegetali	€/anno	-	-	0	-	-	-
Costi di investimento	€/anno	-	-	0	-	-	-
Costi di gestione	€/anno	-	-	4,978	-	-	-

Fig. 5. User interfaces at farm and territorial scale in ValorE software.

both at farm and territorial scale thanks to an extensive choice of options. Changes can be focused on manure management system and on cropping system features. Current and alternative scenarios sustainability can be evaluated and compared through indicators. More over a specific tool of the DSS allows the investigation of effects due to policy measures.

Query task

The territorial scale software can be used as a tool for easy interrogation of regional databases. Default and custom queries can be executed and the results are available in form of maps and exportable reports (Excel or PDF format).

The query system is based on a WebGis interface, to help users to obtain aggregated information for specific geographic areas (e.g., whole region, provinces, municipalities, farms, etc.). The query procedure involves at first, the selection of the aggregation level (e.g., farm, municipality and province) and, secondly, the selection of the geographic area of interest (e.g., one or more municipalities). Default and custom queries are related to several domains: animals herd, animal housing, manure storage, manure treatments, cropping systems, economical and mechanisation aspects, policies aspects (e.g., normative compliance of slurry storages) and pedo-climatic characteristics. An example of a custom query procedure is reported in Fig. 6. The default query option provides a set of about 40 queries previously selected as relevant by a group of experts and stakeholders. Users can however change the parameterisation of the query itself (e.g., selection criteria of several queries could be the utilisable agricultural area (UAA) of the farm, the number of the livestock units, the typology of housing, the soil type, etc.).

Alternative scenarios generator

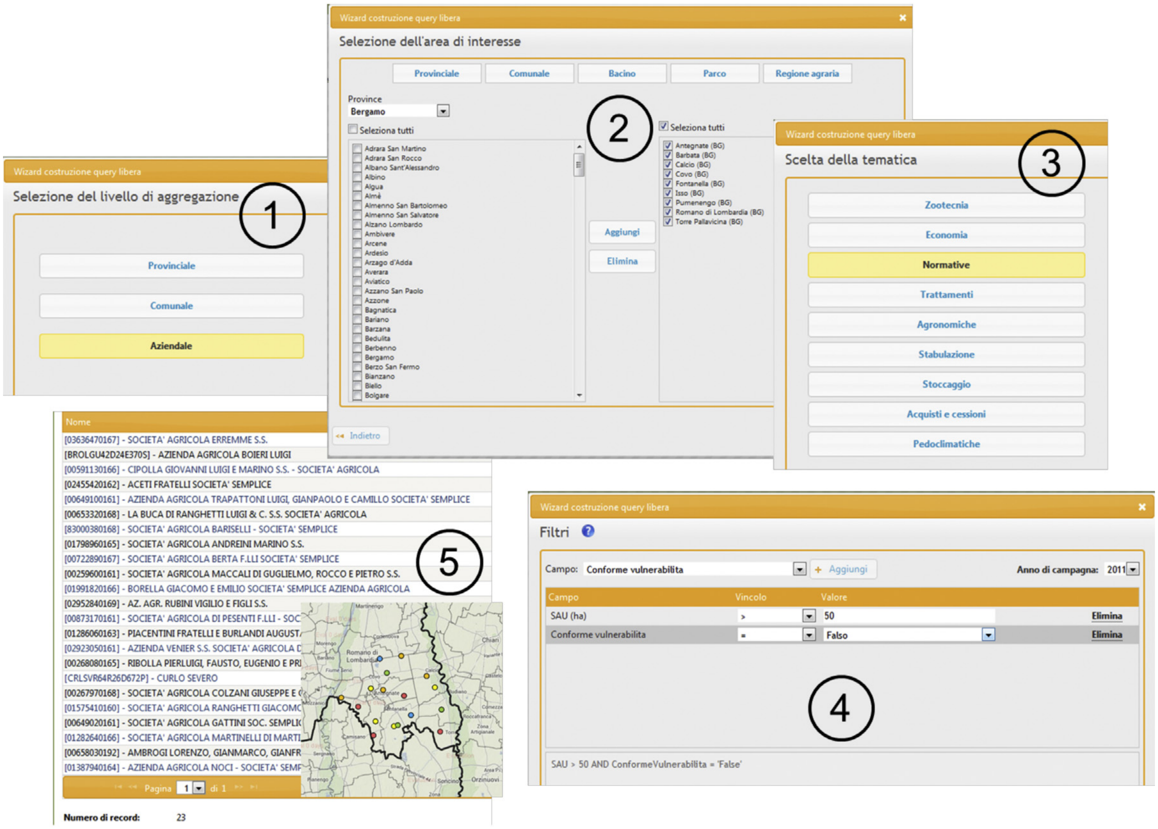
The user can also quickly generate many different alternative scenarios by choosing options related to animal housing systems, storage facilities, manure treatment and land application methods and by modifying crop rotations.

The farm simulator allows creating management options at farm scale by modifying several inputs, such as (i) number of LSU (Livestock Standard Units), protein content in animal ration and daily weight gain (kg d^{-1}), (ii) livestock housing (e.g., straw based or slurry based tying stalls), (iii) slurry treatment (solid–liquid separation, anaerobic digestion with biogas and energy production, ammonia stripping, nitro-denitro process, aerobic stabilisation and composting), (iv) manure storage features (i.e., storage and covering types), (v) type and timing of manure application, (vi) cropping systems (e.g., changes in the crops rotation by introducing new crops and cover crops) and (vii) fertiliser management on the basis of calculated fertilisation plan. To assist the choice of the users all the manure treatment options are detailed through predefined flowcharts.

New scenarios at territorial scale can be generated with the WebGIS interface (Fig. 5) by introducing alternative agricultural management for a sample of farms into a selected area. The territorial simulator allows defining alternative management only relative to four domains such as animal housing, manure treatment, storage facilities and cropping systems. In the case of cropping system and manure treatment domains users can select the management options such as, the method of manure distribution, the introduction of a cover crop and several manure treatments (e.g., solid–liquid separation, biogas production, etc.). To simplify the stakeholders analysis, in the case of animal housing and manure storage domains, users can firstly choose the aim (i.e., the reduction of the manure amount or the ammonia emission) getting from the DSS different management options proposal. Scenarios evaluation at selected scale is obtained by aggregation of farms sample results. The ways in which users can operate about the different components of the manure management and the cropping systems at farm and regional scales, are summarised in Table 1. The software control ensures that adopted management is in agreement with current regulation and farm characteristics. For example, a particular type of treatment requires a minimum volume of manure to be considered functional or the crude protein content of the diet has to be included in a default range of values.

Indicators

The evaluation of current and alternative scenarios and their comparison are computed through different indicators. They can be considered as a synthetic representation of the consequences on technical, agronomic, environmental, energetic, social and economic aspects brought by the adoption of a particular management. The major part of these indicators is quantitative, however, some of them, are expressed in a qualitative scale as bad, fair,



Province: Bergamo

☐ Seleziona tutti

☐ Adrara San Martino
☐ Adrara San Rocco
☐ Albano Sant'Alessandro
☐ Albino
☐ Algua
☐ Almè
☐ Almenno San Bartolomeo
☐ Almenno San Salvatore
☐ Alzano Lombardo
☐ Ambivere
☐ Arcene
☐ Ardesio
☐ Arzago d'Adda
☐ Averara
☐ Aviatico
☐ Azzano San Paolo
☐ Azzone
☐ Bagnatica
☐ Bariano
☐ Barzana
☐ Bedulita
☐ Berbenno
☐ Bergamo
☐ Berzo San Fermo
☐ Bianzano
☐ Biello
☐ Bolgare

☑ Seleziona tutti

☑ Antegnate (BG)
☑ Barbata (BG)
☑ Calcio (BG)
☑ Covo (BG)
☑ Fontanella (BG)
☑ Isso (BG)
☑ Pumenengo (BG)
☑ Romano di Lombardia (BG)
☑ Torre Pallavicina (BG)

Campo: Conforme vulnerabilita

Anno di campagna: 2011

Campo	Vincolo	Valore
SAU (ha)	>	50
Conforme vulnerabilita	=	Falso

SAU > 50 AND ConformeVulnerabilita = 'False'

Nome
[03636470167] - SOCIETA' AGRICOLA ERREMME S.S.
[BROLGU42D24E370S] - AZIENDA AGRICOLA BOIERI LUIGI
[00591130166] - CIPOLLA GIOVANNI LUIGI E MARINO S.S. - SOCIETA' AGRICOLA
[02455420162] - ACETI FRATELLI SOCIETA' SEMPLICE
[00649100161] - AZIENDA AGRICOLA TRAPATTONI LUIGI, GIANPAOLO E CAMILLO SOCIETA' SEMPLICE
[00653320168] - LA BUCA DI RANGHETTI LUIGI & C. S.S. SOCIETA' AGRICOLA
[83000380168] - SOCIETA' AGRICOLA BARISELLI - SOCIETA' SEMPLICE
[01798960165] - SOCIETA' AGRICOLA ANDREINI MARINO S.S.
[00722890167] - SOCIETA' AGRICOLA BERTA F.LLI SOCIETA' SEMPLICE
[00259600161] - SOCIETA' AGRICOLA MACCALI DI GUGLIELMO, ROCCO E PIETRO S.S.
[01991820166] - BORELLA GIACOMO E EMILIO SOCIETA' SEMPLICE AZIENDA AGRICOLA
[02952840169] - AZ. AGR. RUBINI VIGILIO E FIGLI S.S.
[00873170161] - SOCIETA' AGRICOLA DI PESENTI F.LLI - SOC
[01286060163] - PIACENTINI FRATELLI E BURLANDI AUGUST
[02923050161] - AZIENDA VENIER S.S. SOCIETA' AGRICOLA D
[00268080165] - RIBOLLA PIERLUIGI, FAUSTO, EUGENIO E PRI
[CRLSVR64R26D672P] - CURLO SEVERO
[00267970168] - SOCIETA' AGRICOLA COLZANI GIUSEPPE E
[01575410160] - SOCIETA' AGRICOLA RANGHETTI GIACOMO
[00649020161] - SOCIETA' AGRICOLA GATTINI SOC. SEMPLIC
[01282640166] - SOCIETA' AGRICOLA MARTINELLI DI MARTI
[00658030192] - AMBROGI LORENZO, GIANMARCO, GIANFR
[01387940164] - AZIENDA AGRICOLA NOCI - SOCIETA' SEMP

Numero di record: 23

Fig. 6. Example of custom query operated on regional database using the ValorE software to extract the sample for the case study: (1) selection of the aggregation level: farm, (2) selection of the geographic area of interest: nine municipalities, (3) selection of the domain: normative aspect, (4) filtering criteria: farm UAA higher than 50 ha and no compliance with reccomended organic N limits, and (5) list of the farms and their localisation on map.

good, excellent. The complete list of indicators is reported in Table 2.

Several indicators are related to agro-environmental aspects such as (i) CO_2, CH_4, NH_3, N_2O gaseous emissions to the atmosphere, (ii) crop prevalence at farm or regional scale (Crop Diversity Indicator, CDI, Bockstaller and Girardin, 2000), which estimates cropping systems impact on biodiversity and landscape in terms of crops allocation and field size, (iii) soil surface N balance (Oenema et al., 2003), that compares the difference between in-going and out-going N fluxes through the soil surface, and (iv) agricultural nitrate hazard index (IPNOA, Capri et al., 2009) which summarises the results of N supply, soil nitrogen content, meteorological condition, agricultural practices and irrigation adopted.

Table 1
Summary of how the users could generate alternative scenarios.

Manure management component	Farm simulator	Regional simulator
	User opportunity	
Livestock excretion	Change of the LSU, change of the protein content of the animal ration, change of the milk or meat yield and change of the live weight daily increase	
Livestock housing	Choice of the bedding and stable types for each animal age category	Choice of the aim: to reduce manure amount or ammonia emission
Treatment	Choice of the predefined alternative as a composition of manure treatments with a specific objective or design of the new alternative	Choice of the predefined alternative as a composition of manure treatments with a specific objective
Storage	Add new storage, choice of the covering type, choice to buy or sell manure	Choice of the aim: to reduce manure amount or ammonia emission
Land application	Change of the type and timing of application	Change of the type of application
Cropping system	Introduction of a new crop or cover crop and adoption of NMP	Introduction of a cover crop

LSU: livestock standard units; NMP: nitrogen management plan.

Each manure management plant is described by technical indicators, such as power required and energetic consumption and by economic indicators, which describe the operating costs. For new plants the investment costs and, in case of biogas production, the economic revenues are also estimated. The economic performance of the farm at cropping system level is defined via the variable costs sustained for the crop production and the relative value of production.

Regulatory indicators assess the compliance of a farm and/or a sample of farms to mandatory standards related to N and manure management to prevent the risk of N pollution.

To complete the assessment of the scenarios, multi-functional indicators are used to estimate the value of the human perception related to the impact of the manure management techniques on the area outside the farms. In addition, possible changes in crop rotation can influence the value of the indicator that qualitatively classifies the landscape based on crop types cultivated.

All indicators describing the current scenario (at farm scale) are already calculated for the entire regional area and stored in a database to reduce the computational time in what-if analysis.

Table 2
Indicators calculated and used for the evaluation of sustainability of the manure management options.

Agro-ecological indicators	Units	References
NH_3-N volatilisation	kg N year^{-1}	EEA (2009)
N_2O-N emission	kg N year^{-1}	EEA (2009)
CO_2 emission	kg N year^{-1}	EEA (2009)
CH_4 emission	kg N year^{-1}	EEA (2009)
NO_3-Nleaching	kg N year^{-1}	EEC (1991)
P_2O_5 erosion	kg P year^{-1}	Renard et al. (1997)
Soil surface N balance	kg N year^{-1}	Oenema et al. (2003)
IPNOA	Score from 1 (low risk) to 6 (high risk)	Capri et al. (2009)
Crop diversity indicator	Score from 0 (worst case) to 10 (best case)	Bockstaller and Girardin (2000)
Technical indicators		
Power installed	kW	EEA, Renewable gross final energy consumption (ENER 028) – Assessment published January 2011
Energy requirement	kWh year^{-1}	
Multi-functional indicators		
Landscape quality		Tempesta and Thiene (2006)
Odour emission	Score from -5 (worst case) to +5 (best case)	ERM (1998)
Visual impact		
Territorial accessibility		
Citizenship feedback		
Regulatory indicators		
Compliance of slurry storage	kg N year^{-1}	Regione Lombardia (2007)
Compliance of N-manure applied	kg N year^{-1}	EEC (1991)
Calculated N balance	kg N year^{-1}	Regione Lombardia (2007)
Economic indicators		
Variable costs	€	Fumagalli et al. (2012)
Value of production	€	Fumagalli et al. (2012)
Investment costs	€	Berglund and Börjesson (2006)
Operating costs	€ year^{-1}	Gourmelen and Rieu (2006)
Revenues from biogas	€ year^{-1}	De Roest et al. (2011)

Multi-criteria analysis

To identify the optimal or compromise solutions, which have to take into account the farming system characteristics, the agronomical, social, environmental and economic objectives as well as the expectations of the stakeholders involved, a subsequent multi-criteria analysis has to be performed. An on-going work is the implementation of a multi-criteria analysis module based on the MEACROS software (Mazzetto and Bonera, 2003). This software performs concordance analysis providing preference rankings for the alternatives and allowing sensitivity analysis of weighted values as well as displaying the results in a graphic form. Following the general rules of multi-criteria analysis, indicators and their weights are set in a configuration file on the base of a work of a panel of experts. Indicators and weights can be easily modified keeping the software up to date. In detail, the indicators (criteria) describing the current and alternative scenarios (impact matrix) are successively clustered into homogeneous groups referring to technical, economic and environmental aspects for which different decision makers can attribute a priority (weight). Alternatively, users can set both the relative importance of groups and the relative weights of criteria within each group. Then the model performs comparative analysis providing preference ranking for the alternatives based on the type of aspect that tend to prevail after experts judgement (output appraisal matrix).

A case study using the DSS ValorE

The DSS was applied to a selected area with the main objective to evaluate options for reducing the reactive N losses through air and water. The simulation was done using input data from the regional databases updated at 2011 and from reference information derived from literature and regional regulations. As reported in Fig. 6, the data sample for the case study were obtained through a custom query. The studied area is represented by nine neighbouring municipalities localised in the south part of the province of Bergamo. Such area was chosen because is a nitrates vulnerable zone with high organic N load. Within the area, only livestock farms with over 50 ha of UAA and that do not respect the limit of 170 kg per year/hectare of N from organic fertilisers, were selected. The final sample was composed by 23 farms (20 dairy farms, one swine farm and two farms with both animals) where maize was the main crop cultivated covering, on average, the 70% of the farms UAA. The UAA of the selected farms represented on average the 32% of that of the own municipality. None of the farms had a manure treatment plant and covered manure storages. The actual configuration was labelled as “actual scenario” (ACT) while the two hypothetical configurations were labelled as “alternative scenarios” (ALT1) and (ALT2). For ACT, the farms organic N load aggregated at municipality level was very high and ranged from 249 to 929 kg ha^{-1} of farms UAA. The first alternative scenario (ALT1) hypothesised involved the implementation on farms of the nitro-denitro treatment plant with removal of nitrogen while the second option considered the construction of a rigid cover for all of the stores available on farm (ALT2). The two scenarios were generated through the regional simulator following the instructions summarised in Table 1. For ALT1, from the list of the liquid manure treatments available, was first selected the predefined nitro-denitro treatment aiming at the nitrogen removal to be further implemented in 100% of the farms. The predefined treatment involves that the liquid manure is first separated in a liquid and solid fraction. The liquid fraction enters in the nitro-denitro plant and successively stored in a tank for the final agronomic use. The remaining part is moved to a belt press and stored in covered facility together with the solid fraction obtained from the first separation. This final product could be applied on fields or sold outside farm. For ALT2, the software defined the covering of all of the liquid manure storages available on farm having previously selected as final aim the reduction of N volatilisation in 100% of the farms.

The first positive effect of ALT1 was the strong reduction of the organic N available to be distributed on fields (Fig. 7). As reported in Table 3 the reduction ranged from 26% to 61% demonstrating that the nitro-denitro process would be a reliable solution to get compliancy with nitrate directive under derogation limits of 250 kg N ha^{-1} (EC, 2011). Moreover, relevant advantages from the environmental point of view can be obtained: N lost through leaching and volatilisation were reduced from 38% to 75% and from 24% to 34%, respectively (Table 3 and Fig. 7). Emissions of CH_4 were strongly reduced as well as the liquid manure volume available to be distributed: this implies lower demands for manure storage capacity, a better control and management of the application of manure as fertiliser and lower odour emissions. Because of the 50% of N is lost as N_2 to the atmosphere, the fertilisation value of manure was halved thus implying to review the N fertilisation plans for more better N use efficiency. From an economic point of view the expected costs simulated by the software were increased considerably: the investment costs were remarkable varying from 200,000 to 1,600,000 Euro and the operating costs have grown by almost three times mainly due to the energy requirement by the plant (Table 3). Overall, the adoption of ALT1 could require a higher organisation as it grows the complexity of farm management.

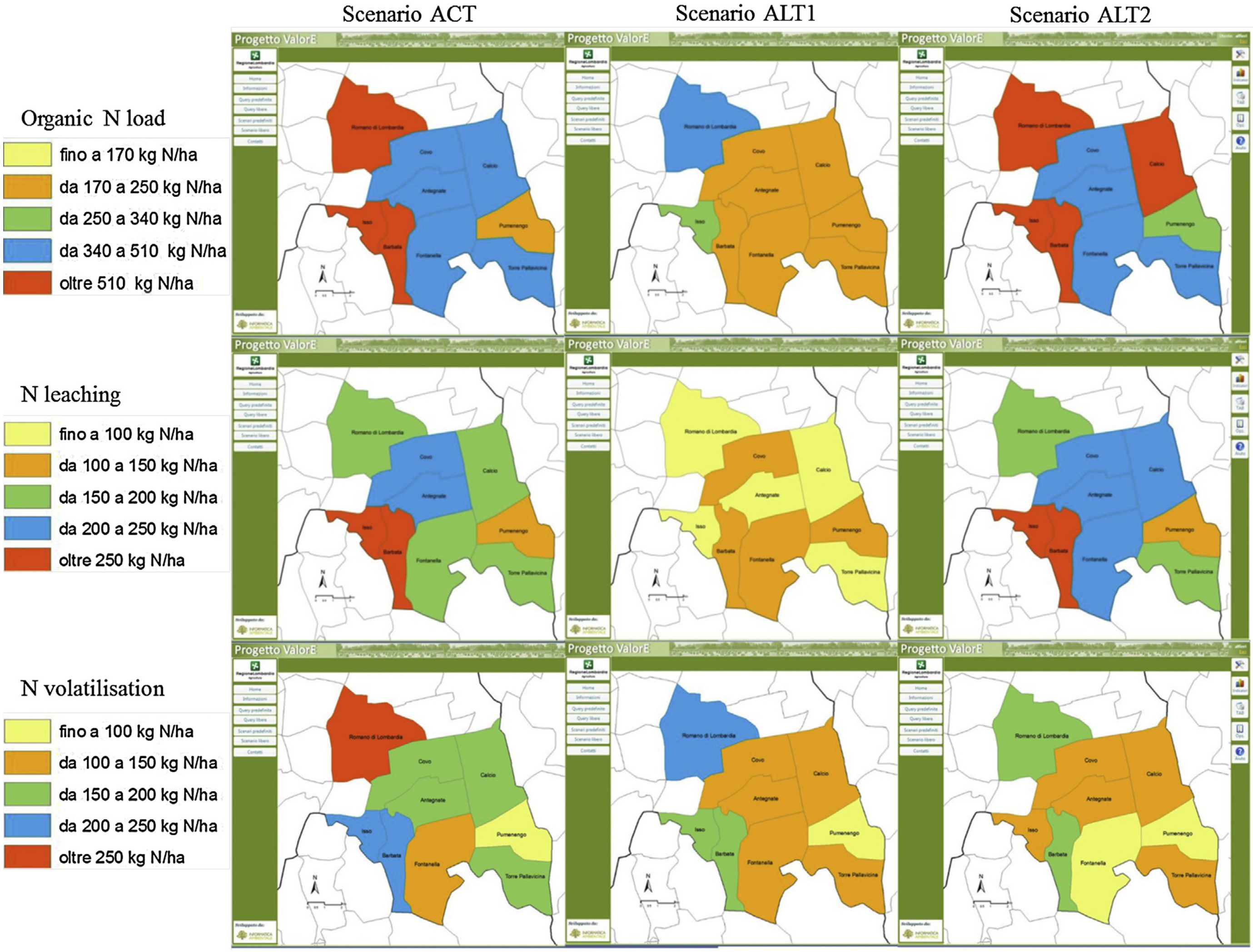


Fig. 7. Mean organic N load, N leaching and N volatilisation (kg ha^{-1}) aggregated at municipality level under the current scenario (ACT) and after the implementation of nitro-denitro plants (ALT1) and the covering of all manure storages (ALT2). (in the legend: fino = up to; da = from; a = to; oltre = more than).

The effectiveness of covering of the manure stores was highlighted by the reduction of N lost through volatilisation process (from – 18% to −36%) and of methane emission. At the same time a mean reduction of the total liquid manure volume by 7% (Table 3) occurred due to the exclusion of rainfall water from the system. However, since ALT2 involved a mean increase of available N to be applied on field by 9%, compared to ACT, a more accurate nitrogen management at field scale to contain volatilisation and N leaching is needed. In fact, the N leaching was expected to increase by 10%. As reported, the necessary investment were lower compared to ALT1 and ranged from 36,000 to 227,000 Euro while operating costs were similar to ACT.

Outcomes obtained from this application suggest that both alternatives could be a viable solution to reduce environmental impacts caused by manure management (e.g., N losses), even though investment and operating costs were significant. However, the aids provided by the measure 121 of the current RDP applied in the Lombardia region, could offset the economic investment by 35–40%. The application of the DSS on an area intensively managed, demonstrated how an intervention planned at territorial level could be a useful solution for the manure management issue, even thought his requires a strong collaboration between farmers and industry, with the monitoring and coordination of the institutions which should provide regulations and economic helps.

Model validation, updating procedures and stakeholders interaction

The model validation step is an on-going procedure carried out by a group of potential users such as agronomists and Italian farmers organisations. Twenty farms have been identified as representative of the entire regional area by applying selection criteria (e.g., farm belonging to the nitrate vulnerable area, minimum agricultural area equal to 40 ha, number of animals over 150 and 2000 for cattle and swine, respectively) to get real data through farmer's interviews. This lets us to estimate the reliability of the model, to detect weaknesses of the system and to do a general improvement of the applicative usability.

Databases are updated to acquire the latest reference data available. The SIARL database is annually updated with the new information provided by the farmers and at the same time meteorological and soil databases could be refreshed if new information is available. The knowledge base could be modified with changes in regulations and/or new scientific achievements (e.g., parameters for crop modelling). Variations of the raw materials price such as energy, fertilisers and crop products are also taken into account.

Following the indications provided by the literature that reports the importance of the participatory processes on DSS' success (Van Meensel et al., 2012) we are currently involving stakeholders that

Table 3
Average value of some indicators calculated by ValorE and aggregated at municipality scale under the current scenario (ACT) and after the implementation of nitro-denitro plants (ALT1) and the covering of all manure storages (ALT2).

Municipality	Scenario	Organic N load	SSB	N leaching	N-NH_3 volatilisation	N-N_2O emission	CH_4 emission	CO_2 emission	Phosporous losses	Liquid manure volume	Operating costs	Investment costs	Power requirement
		kg ha^{-1}								m^3	€		Kwh ha^{-1}
Antegnate	ACT	439	299	203	156	2	133	0	45	8734	153,099	–	–
	ALT1	203	117	94	120	4	11	14	41	5951	471,696	759,446	982
	ALT2	484	345	227	113	2	47	0	45	8191	148,876	87,585	–
Barbata	ACT	521	549	280	214	2	231	0	80	20,131	255,633	–	–
	ALT1	227	368	138	163	4	13	20	71	16,053	926,997	1,640,131	1387
	ALT2	576	649	312	158	2	113	0	80	18,863	244,816	163,248	–
Calcio	ACT	483	370	189	184	1	204	0	72	29,640	274,434	–	–
	ALT1	189	112	80	140	3	9	19	69	18,615	1,161,216	2,410,975	1432
	ALT2	542	416	213	124	1	68	0	73	28,527	266,082	227,035	–
Covo	ACT	412	270	218	152	2	122	0	53	7442	134,746	–	–
	ALT1	216	129	107	114	3	7	13	49	5066	426,545	753,842	1096
	ALT2	452	304	243	110	2	43	0	54	7015	131,377	80,773	–
Fontanella	ACT	376	411	199	131	3	98	0	125	10,157	200,380	–	–
	ALT1	205	232	124	112	5	11	11	120	6068	573,648	837,556	1212
	ALT2	409	443	215	95	3	36	0	125	10,080	198,861	91,532	–
Isso	ACT	602	379	269	202	4	179	0	65	10,272	180,912	–	–
	ALT1	315	259	83	152	7	16	19	68	7169	571,016	915,431	2456
	ALT2	658	573	315	148	4	64	0	63	9748	176,509	106,807	–
Pumenengo	ACT	249	226	139	66	3	28	0	100	1652	54,618	–	–
	ALT1	186	173	137	60	4	8	5	100	1385	138,709	226,260	265
	ALT2	261	247	139	54	3	14	0	100	1446	52,890	28,189	–

Table 3 (*Continued*)

Municipality	Scenario	Organic N load	SSB	N leaching	N-NH_3 volatilisation	N-N_2O emission	CH_4 emission	CO_2 emission	Phosporous losses	Liquid manure volume	Operating costs	Investment costs	Power requirement
		kg ha^{-1}								m^3	€		Kwh ha^{-1}
Romano di Lombardia	ACT	929	775	173	268	4	282	0	53	7485	104,253	–	–
	ALT1	408	275	78	210	8	23	26	53	4143	311,326	400,624	4048
	ALT2	1027	857	193	172	4	99	0	55	7171	101,756	36,240	–
Torre Pallavicina	ACT	423	863	179	151	3	9	0	82	5592	87,603	–	–
	ALT1	220	778	98	116	5	3	16	75	3824	292,674	435,596	483
	ALT2	463	980	197	112	3	5	0	83	4610	79,355	50,425	–

actively collaborate to test it on real cases, to debug and propose new software features and improvement.

Conclusions

The DSS developed in the ValorE Project, funded by Regione Lombardia for 1,100,000 € (about 1,500,000 USD) is an attempt to create an instrument for environmental protection in a very intensive agricultural area with one of the highest livestock density in the World. Through the ValorE software a detailed analysis can be carried out for all farms in the region, and alternative management scenarios and hypothesis of policies can be tested. The spatial and integrated approach grants the possibility to deal with conflicting objectives, interests and expectation of stakeholders involved and offers to decision-makers a comprehensive tool for improving strategy and decision making. The advantage of the DSS ValorE over other similar systems is that it was designed to manage different livestock manure and types and not to be site-specific bound, being coupled to a GIS.

From the software structure point of view, several benefits can be highlighted. The OOP targeting at modularity and reusability allows a more intuitive and stronger separation among data, models and interfaces. The architecture of the software and the OOP offer an easy and automatic updating of the application and of the model algorithms as well as the possibility to maximise the ease of maintenance. The software is adaptable to work with different databases, provided that they contain the same information. This feature could offer a possibility to further share and synchronise different databases of the other Regions of northern Italy, such as Emilia Romagna, Piemonte and Veneto to get an unique evaluation and decision making tool for similar agricultural areas. This opportunity is emphasised by the fact that the four Regions for which it was granted the nitrate derogation (EC, 2011), account for more than 70% of livestock in Italy: in particular, 67.1% of dairy cattle, 60.6% of other cattle, 81% of pigs and 79.4% of poultry.

The first prototype of ValorE was appreciated by public bodies, producers organizations and farmer's consultants. Since it was first released the number of users has reached more than 200 and the 60% of them are agronomists, entailing about 4000 farms.

Based on the results of this study, we deem that further research should focus on the following objectives:

a. continuous interaction with stakeholders in the debug activities;
b. improvement of the software to satisfy the further request of the users;
c. implementation of the software in order to simulate the rules, constraints and limits of the nitrate derogation;
d. to make the software able to assists farmers in the preparation and submission of the Agronomic Utilisation Plans for livestock manure to obtain the authorisation by the regional government for spreading manure.

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References

Acutis, M., Perego, A., Bernardoni, E., Rinaldi, M., 2010. AQUATER: software as a DSS for irrigation management in semi-arid Mediterranean areas. Ital J. Agron. 5 (2), 205–216.

Amon, B., Kryvoruchko, V., Amon, T., Zechmeister-Boltenstern, S., 2006. Methane, nitrous oxide and ammonia emissions during storage and after application of dairy cattle slurry and influence of slurry treatment. Agric. Ecosyst. Environ. 112, 153–162.

Amon, T., Amon, B., Kryvoruchko, V., Zollitsch, W., Mayer, W., Gruber, L., 2007. Biogas production from maize and dairy cattle manure–Influence of biomass composition on the methane yield. Agric. Ecosyst. Environ. 118, 173–182.

Beline, F., Boursier, H., Daumer, M.L., Guiziou, F., Paul, E., 2007. Modelling of biological processes during aerobic treatment of piggery wastewater aiming at process optimization. Bioresour. Technol. 98, 3298–3308.

Berglund, M., Börjesson, P., 2006. Assessment of energy performance in the life-cycle of biogas Production. Biomass Bioenergy 30, 254–266.

Berntsen, J., Petersen, B.M., Jacobsen, B.H., Olesen, J.E., Hutchings, N.J., 2003. Evaluating nitrogen taxation scenarios using the dynamic whole farm simulation model FASSET. Agric. Syst. 76, 817–839.

Bezlepkina, I., Jongeneel, R., Brouwer, F., Dillen, K., Meister, A., Winsten, J., De Roest, K., Demont, M., 2008. Costs of compliance with EU regulations and competitiveness of the EU dairy sector. In: EAAE International Congress, August 26–29, 2008, Ghent.

Biswas, J., Chowdhury, R., Bhattacharya, P., 2007. Mathematical modeling for the prediction of biogas generation characteristics of an anaerobic digester based on food/vegetable residues. Biomass Bioenergy 31, 80–86.

Bockstaller, C., Girardin, P., 2000. Mode de calcul des indicateurs agro-ecologiques. INRA, France (Unpublished internal technical report).

Bonfante, A., Basile, A., Acutis, M., De Mascellis, R., Manna, R., Perego, A., Terribile, F., 2010. Swap, CropSyst and Macro comparison in two contrasting soils cropped with maize in northern Italy. Agric. Water Manage. 97, 1051–1062.

Bonmatì, A., Flotats, X., 2003. Air stripping of ammonia from pig slurry: characterization and feasibility as a pre- or post treatment to mesophilic anaerobic digestion. Waste Manage. 23, 261–272.

Bottero, M., Comino, E., Duriavig, M., Ferretti, V., Pomarico, S., 2013. The application of a Multi Criteria Spatial Decision Support System (MCSDSS) for the assessment of biodiversity conservation in the Province of Varese (Italy). Land Use Policy 30, 730–738.

Campbell, G.S., 1985. Soil Physics with Basic. Elsevier, Amsterdam.

Capri, E., Civita, M., Corniello, A., Cusimano, G., De Maio, M., Ducci, D., Fait, G., Fiorucci, A., Hauser, S., Pisciotta, A., Pranzini, G., Trevisan, M., DelgadoHuertas, A., Ferrari, F., Frullini, R., Nisi, B., Offi, M., Vaselli, O., Vassallo, M., 2009. Assessment of nitrate contamination risk: the Italian experience. J. Geochem. Explor. 102, 71–86.

Carozzi, M., Ferrara, R.M., Fumagalli, M., Sanna, M., Chiodini, M., Perego, A., Chierichetti, A., Brenna, S., Rana, G., Acutis, M., 2012. Field-scale ammonia emissions from surface spreading of dairy slurry in Po Valley. Ital. J. Agrometerol. 3, 15–24.

Carozzi, M., Ferrara, R.M., Rana, G., Acutis, M., 2013a. Evaluation of mitigation strategies to reduce ammonia losses from slurry fertilisation on arable lands. Sci. Total Environ. 449, 126–133.

Carozzi, M., Loubet, B., Acutis, M., Rana, G., Ferrara, R.M., 2013. Inverse dispersion modelling highlights the efficiency of slurry injection to reduce ammonia losses by agriculture in the Po Valley (Italy). Agric. For. Meteorol. 171–172, 306–318.

Calliera, M., Berta, F., Galassi, T., Mazzini, F., Rossi, R., Bassi, R., Meriggi, P., Bernard, A., Marchis, A., Di Guardo, A., Capri, E., 2013. Enhance knowledge on sustainable use of plant protection products within the framework of the Sustainable Use Directive. Pest Manage. Sci. 69, 883–888.

Cocolo, G., Curnis, S., Hjorth, M., Provolo, G., 2012. Effect of different technologies and animal manures on solid–liquid separation efficiencies. J. Agric. Eng. 43 (2), e9.

De, S., Bezuglov, A., 2006. Data model for a decision support in comprehensive nutrient management in the United States. Environ. Model. Softw. 21, 852–867.

De, S., Kloot, R.W., Covington, E., Bezuglov, A., Taduri, H., 2004. AFOPro: a nutrient management decision support system for the United States. Comput. Electron. Agric. 43, 69–76.

Densham, P.J., 1991. Spatial decision support systems. In: Maguire, D.J., Goodchild, M.F., Rhind, D.W. (Eds.), Geographical Information Systems: Principles and Applications. John Wiley and Sons, New York, pp. 403–412.

De Roest, K., Jongeneel, R., Dillen, K., Winsten, J., 2011. Cross compliance and competitiveness of the european beef and pig sector. In: Sorrentino, A., Henke, R., Severini, S. (Eds.), The Common Agricultural Policy after the Fischler Reform. Ashgate.

Djodjic, F., Montas, H., Shirmohammadi, A., Bergström, L., Ulén, B., 2002. A decision support system for phosphorus management at a watershed scale. J. Environ. Qual. 31, 937–945.

Dinuccio, E., Berg, W., Balsari, P., 2008. Gaseous emissions from the storage of untreated slurries and the fractions obtained after mechanical separation. Atmos. Environ. 42, 2448–2459.

Eckersten, H., Jansson, P.-E., Johnsson, H., 1996. SOILN model. User' s manual. Version 9.1. Division of agricultural hydro-technics, Communications, 96:l Department of soil sciences. Swedish University of Agricultural Science, Uppsala.

EC, 2000. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000. Establishing a Framework for Community Action in the Field of Water Policy. Official Journal of the European Communities, L 327/1.

EC, 2011. Commission Implementing Decision [C (2011) 77770] of 3 November 2011 on Granting a Derogation Requested by Italy with Regard to the Regions of Emilia Romagna, Lombardia, Piemonte and Veneto Pursuant to Council Directive 91/676/EEC Concerning the Protection of Waters Against Pollution Caused by Nitrates from Agricultural Sources. Official Journal of the European Union, L 287/236.

EEC, 1991. Council Directive 91/676/EEC of December 12, 1991 Concerning the Protection of Waters Against Pollution Caused by Nitrates from Agricultural Sources. Official Journal, L 375, pp. 1–8.

EEA, 2009. EMEP/EEA Air Pollutant Emission Inventory Guidebook 2009. EEA Technical Report no. 9. EEA, Cophenagen.

ERM, 1998. A Handbook on Environmental Assessment of Regional Development Plans and EU Structural Funds, Programmes. European Commission, Bruxelles.

Fangueiro, D., Senbayran, M., Trindade, H., Chadwick, D., 2008. Cattle slurry treatment by screw press separation and chemically enhanced settling: effect on greenhouse gas emissions after land spreading and grass yield. Bioresour. Technol. 99, 7132–7142.

FAO, 1998. World Reference Base For Soil Resources, Food and Agriculture Organization of the United Nations International Society of Soil Science. International Soil Reference and Information Centre World Soil Resources Reports.

Forsman, A., Grimvall, A., Scholtes, J., Wittgren, H.B., 2003. Generic structures of decision support systems for evaluation of policy measures to reduce catchment-scale nitrogen fluxes. Phys. Chem. Earth 28, 589–598.

Fassio, A., Giupponi, C., Hiederer, R., Simot, C., 2005. A decision support tool for simulating the effects of alternative policies affecting water resources: an application at the European scale. J. Hydrol. 304, 462–476.

Fox, D.G., Tedeschi, L.O., Tylutki, T.P., Russell, J.B., Van Amburgh, M.E., Chase, L.E., Pell, A.N., Overton, T.R., 2004. The Cornell net carbohydrate and protein system model for evaluating herd nutrition and nutrient excretion. Anim. Feed Sci. Technol. 112, 29–78.

Fumagalli, M., Acutis, M., Mazzetto, F., Vidotto, F., Sali, G., Bechini, L., 2011. An analysis of agricultural sustainability of cropping systems in arable and dairy farms in an intensively cultivated plain. Eur. J. Agron. 34, 71–82.

Fumagalli, M., Acutis, M., Mazzetto, F., Vidotto, F., Sali, G., Bechini, L., 2012. A methodology for designing and evaluating alternative cropping systems: application on dairy and arable farms. Ecol. Indic. 23, 189–201.

Galelli, S., Gandolfi, C., Soncini-Sessa, R., Agostani, D., 2010. Building a metamodel of an irrigation district distributed-parameter model. Agric. Water Manage. 97, 187–200.

Geneletti, D., 2004. A GIS-based decision support system to identify nature conservation priorities in an alpine valley. Land Use Policy 21, 149–160.

Giupponi, C., 2007. Decision support systems for implementing the European Water Framework Directive: the MULINO approach. Environ. Model. Softw. 22, 248e258.

Gourmelen, C., Rieu, M., 2006. Evaluation du coût de la gestion des effluents dans différents types d'exploitations porcines. Journées de la Recherche Porcine 38, 263–270.

IPCC, 2006. In: Eggleston, H.S., Buendia, L., Miwa, K., Ngara, T., Tanabe, K. (Eds.), IPCC Guidelines for National Greenhouse Gas Inventories. Prepared by the National Greenhouse Gas Inventories Programme. Published: IGES, Japan.

Johnsson, H., Bergstrom, L., Jansson, P.-E., 1987. Simulated nitrogen dynamics and losses in a layered agricultural soil. Agric. Ecosys. Environ. 18, 333–356.

Karmakar, S., NKetia, M., Laguë, C., Agnew, J., 2010. Development of expert system modeling based decision support system for swine manure management. Comput. Electron. Agric. 71, 88–95.

Karmakar, S., Laguë, C., Agnew,J., Landry, D., 2007. Integrated decision support system (DSS) for manure management: a review and perspective. Comput. Electron. Agric. 57, 190–201.

Le Bellego, L., van Milgen, J., Dubois, S., Noblet, J., 2001. Energy utilization of low-protein diets in growing pigs. J. Anim. Sci. 79, 1259–1271.

Loyon, L., Guiziou, F., Béline, F., Peu, P., 2006. Gaseous emissions (NH_4^+, N_2O, CH_4, CO_2) during pig slurry biological aerobic treatment and treatment by-products storages. Int. Congr. Ser. 1293, 299–302.

Malczewski, J., 1999. GIS and Multicriteria Decision Analysis. John Wiley and Sons, New York, pp. 392.

Mazzetto, F., Bonera, R., 2003. MEACROS: a tool for multi-criteria evaluation of alternative cropping systems. Eur. J. Agron. 18, 379–387.

Mazzocchi, C., Sali, G., Corsi, S., 2013. Land use conversion in metropolitan areas and the permanence of agriculture: Sensitivity Index of Agricultural Land (SIAL), a tool for territorial analysis. Land Use Policy 35, 155–162.

Morris, M.D., 1991. Factorial sampling plans for preliminary computational experiments. Technometrics 33 (2), 161–174.

National Research Council, 2001. Nutrient Requirements of Dairy Cattle, 7th rev. ed. National Academy of Sciences, Washington, DC, USA.

Nennich, T., Harrison, J.H., VanWieringen, L.M., Meyer, D., Heinrichs, A.J., Weiss, W.P., St-Pierre, N.R., Kincaid, R.L., Davidson, D.L., Wright, P.E., 2005. Prediction of manure and nutrient excretion from dairy cattle. J. Dairy Sci. 88, 3721–3733.

Oenema, O., 2006. Nitrogen budgets and losses in livestock systems. Int. Congr. Ser. 1293, 262–271.

Oenema, O., Kros, H., de Vries, W., 2003. Approaches and uncertainties in nutrient budgets: implications for nutrient management and environmental policies. Eur. J. Agron. 20, 3–16.

Ogilvie, J.R., Barry, D.A., Goss, M.J., Stonehouse, D.P., 2000. Balancing environmental and economic concerns in manure management by use of on-farm computerized decision support program, MCLONE4. In: Moore, J.A. (Ed.), Animal, Agricultural and Food Processing Wastes, Proceedings of the eighth International Symposium. Des Moines, IA, 9–11 October. ASAE, St. Joseph, MI.

Paillat, J.M., Robin, P., Hassouna, M., Leterme, P., 2005. Predicting ammonia and carbon dioxide emissions from carbon and nitrogen biodegradability during animal waste composting. Atmos. Environ. 39, 6833–6842.

Pallottino, S., Sechi, G.M., Zuddas, P., 2003. DSS for water resources management under uncertainty by scenario analysis. Environ. Model. Softw. 20, 1031–1042.

Peeters, A., Ben-Gal, A., Hetzroni, A., Zude, M., 2012. Developing a GIS-based Spatial Decision Support System for Automated Tree Crop Management to Optimize Irrigation Inputs. In: Seppelt, R., Voinov, A.A., Lange, S., Bankamp, D. (Eds.), International Environmental Modelling and Software Society (iEMSs) 2012 International Congress on Environmental Modelling and Software. Managing Resources of a Limited Planet: Pathways and Visions under Uncertainty, Sixth Biennial Meeting. Leipzig, Germany.

Perego, A., Basile, A., Bonfante, A., De Mascellis, R., Terribile, F., Brenna, S., Acutis, M., 2012. Nitrate leaching under maize cropping systems in Po Valley (Italy). Agric. Ecosyst. Environ. 147, 57–65.

Perego, A., Giussani, A., Fumagalli, M., Sanna, M., Chiodini, M., Carozzi, M., Alfieri, L., Brenna, S., Acutis, M., 2013a. Crop rotation, fertiliser types and application timing affecting nitrate leaching in Nitrate Vulnerable Zones in Po valley. Ital. J. Agromet. 2, 39–50.

Perego, A., Giussani, A., Sanna, M., Fumagalli, M., Carozzi, M., Alfieri, L., Brenna, S., Acutis, M., 2013b. The ARMOSA simulation crop model: overall features, calibration and validation results. Ital. J. Agromet. 3, 23–38.

Perini, A., Susi, A., 2004. Developing a decision support system for integrated production in agriculture. Environ. Model. Softw. 19, 821–829.

Petersen, S.O., Sommer, S.G., Bèline, F., Burton, C., Dach, J., Dourmand, J.Y., Leip, A., Misselbrook, T., Nicholson, F., Poulsen, H.D., Provolo, G., Sørensen, P., Vinnerås, B., Weiske, A., Bernal, M.-P., Böhm, R., Juhász, C., Mihelic, R., 2007. Recycling of livestock manure in a whole-farm perspective. Livest. Sci. 112, 180–191.

Pomar, C., Harris, D.L., Savoie, P., Minvielle, F., 1991a. Computer simulation model of swine production systems. 3. A dynamic herd simulation model including reproduction. J. Anim. Sci. 69, 2822–2836.

Pomar, C., Harris, L., Minvielle, F., 1991b. Computer simulation model of swine production systems. I. Modeling the growth of young pigs. J. Anim. Sci. 69, 1468–1488.

Pomar, C., Harris, L., Minvielle, F., 1991c. Computer simulation model of swine production systems. 2. Modeling body composition and weight of female pigs, fetal development, milk production, and growth of suckling pigs. J. Anim. Sci. 69, 1489–1502.

Power, D.J., 1997. What is a DSS? Online Exec. J. Data Intensive Decis. Support 1 (3), http://www.taborcommunications.com/dsstar/971021/100015.html (accessed 15.10.12).

Provolo, G., 2005. Manure management practices in Lombardy (Italy). Bioresour. Technol. 96, 145–152.

Regione Lombardia, 2007. Deliberazione della Giunta regionale no. 8/5868 del 21 novembre 2007, Integrazione con modifica al programma d'azione per la tutela e risanamento delle acque dall'inquinamento causato da nitrati di origine agricola per le aziende localizzate in zona vulnerabile (d.lgs. no. 152/2006, art 92 e d.m. 7 aprile 2006) e adeguamento dei relativi criteri e norme tecniche generali di cui alla Dgr no. VI/17149/1996, approvati con deliberazione di Giunta no. VIII/5215 del 2 agosto 2007.

Regione Lombardia, 2010. SIARL Sistema Informativo Agricolo Regione Lombardia, https://www.siarl.regione.lombardia.it/index.htm (accessed 30.09.13).

Renard, K.G., Foster, G.R., Weesies, G.A., McCool, D.K., Yoder, D.C., 1997. Predicting Soil Erosion by Water: A Guide to Conservation Planning with the Revised Universal Soil Loss Equation (RUSLE). Agriculture Handbook No. 703. U.S. Department of Agriculture, Agricultural Research Service, Washington, DC.

Riparbelli, C., Di Guardo, A., Serrano, A., Capri, E., Brenna, S., 2008. In: Sànchez-Marrè, M., Béjar, J., Comas, J., Rizzoli, A., Guariso, G. (Eds.), Sustainable Use of Pesticides: an Innovative Experience in Lombardy Region, Italy. 4th Biennial Meeting of iEMSs. International Environmental Modelling and Software Society (iEMSs).

Rousseau, P., Béline, F., Steyer, J.P., Volcke, E.I.P., Bernet, N., 2008. Combined anaerobic digestion and biological nitrogen removal for piggery wastewater treatment: a modeling approach. Water Sci. Technol. 58, 133–141.

Saltelli, A., Ratto, M., Tarantola, S., Campolongo, F., 2005. Sensitivity analysis for chemical models. Chem. Rev. 105, 2811–2827.

Sørensen, C.G., Jacobsen, B.H., Sommer, S.G., 2003. An assessment tool applied to manure management systems using innovative technologies. Biosyst. Eng. 86, 315.

Steinfeld, H., Gerber, P., Wassenaar, T., Castel, V., Rosales, M., de Haan, C., 2006. Livestock's Long Shadow: Environmental Issues and Options. Food and Agriculture Organization of the United Nations, Rome.

Supit, I., Hooijer, A.A., Diepen van, C.A., 1994. System Description of the WOFOST 6.0 Crop Simulation Model Implemented in CGMS. Publication EUR 15956 EN of the Office for Official Publications of the EU, Luxembourg.

Szanto, G.L., Hamelers, H.V.M., Rulkens, W.H., Veeken, A.H.M., 2007. NH_4^+,N_2O and CH_4 emissions during passively aerated composting of straw–rich pig manure. Bioresour. Technol. 98, 2659–2670.

Tempesta, T., Thiene, M., 2006. In: Angeli, F. (Ed.), Percezione e valore del paesaggio, Milano.

Van Dam, J.C., Groenendijk, P., Hendriks, R.F.A., 2008. Advances of modeling water flow in variably saturated soils with SWAP. Vadose Zone J. 7, 640–653.

Van Ittersum, M.K., Leffelaar, P.A., Van Keulen, H., Kropff, M.J., Bastiaans, L., Goudriaan, J., 2003. On approaches and applications of the Wageningen crop models. Eur. J. Agron. 18, 201–234.

Van Meensel, J., Lauwers, L., Kempen, I., Dessein, J., Van Huylenbroeck, G., 2012. Effect of a participatory approach on the successful development of agricultural decision support systems: the case of Pigs2win. Decis. Support Syst. 54, 164–172.

van Milgen, J., Noblet, J., 2003. Partitioning of energy intake to heat, protein, and fat in growing pigs. J. Anim. Sci. 81, E86–E93.

Webb, J., Misselbrook, T.H., 2004. A mass-flow model of ammonia emissions from UK livestock production. Atmos. Environ. 38, 2163–2176.

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A client–server software for the identification of groundwater vulnerability to pesticides at regional level

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HIGHLIGHTS

- Groundwater vulnerability to pesticides can be identified by applying spatial modelling.
- A software system is proposed to evaluate potential groundwater vulnerability to pesticides.
- Environmental and pesticide data are pre-loaded into the system.
- Results can be used to evaluate limitations in use of pesticides or further investigations.

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ABSTRACT

The groundwater VULnerability to PESticide software system (VULPES) is a user-friendly, GIS-based and client–server software developed to identify vulnerable areas to pesticides at regional level making use of pesticide fate models. It is a Decision Support System aimed to assist the public policy makers to investigate areas sensitive to specific substances and to propose limitations of use or mitigation measures. VULPES identify the so-called Uniform Geographical Unit (UGU) which are areas characterised by the same agro-environmental conditions. In each UGU it applies the PELMO model obtaining the 80th percentile of the substance concentration at 1 metre depth; then VULPES creates a vulnerability map in shapefile format which classifies the outputs comparing them with the lower threshold set to the legal limit concentration in groundwater (0.1 μg/l).

This paper describes the software structure in details and a case study with the application of the terbuthylazine herbicide on the Lombardy region territory. Three zones with different degrees of vulnerabilities has been identified and described.

1. Introduction

Contamination of groundwater is an important side-effect of Plant Protection Products (PPPs) use, as their residues are commonly found in groundwater (Leistra and Boesten, 1989; Vighi and Funari, 2005; Arias-Estévez et al., 2008; Bozzo et al., 2013). It is generally accepted that leaching losses within agricultural fields should be minimised (Tiktak, 2000), as the presence of PPPs in groundwater can seriously limit drinking water availability, since such type of contamination could persist for long periods and the process of water purification is highly expensive. This is of particular concern since for example 65% of the whole drinking water in Europe comes from groundwater stocks (Bouraoui, 2007). To prevent the risks of groundwater contamination, the European Commission issued several Directives which directly and indirectly regulate the use of PPPs in EU. For instance, the Council Directive 80/778/EEC (Council of the European Union, 1980), amended by Directive 98/83/EC (Council of the European Union, 1998) has set to 0.1 μg/l and 0.5 μg/l the maximum allowable concentrations in drinking water for each individual pesticide and for their total sum, respectively. In addition, Council Directive 91/414/EEC (Council of the European Union, 1991), repealed and replaced by Regulation (EC) No 1107/2009 on 21 October 2009 (European Commission, 2009a), laid down the authorisation procedures of PPPs to be marketed within the European Union. The estimation of the risk of groundwater contamination is part of the registration, which is granted if the chemical and each of its relevant metabolites after leaching have a calculated concentration in groundwater of less than 0.1 μg/l. The assessment is done through a tiered approach, which was developed by the FOCUS (i.e., Forum for the Coordination of Pesticide Fate Models and their Use) group (FOCUS, 2000). At the first tier, nine realistic worst-case environmental

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scenarios (a combination of soil, climate and crop parameters), which should collectively represent agriculture in the EU, are used in combination with a set of pesticide leaching models, namely PEARL (Tiktak et al., 2000), PRZM (Suarez, 2005), PELMO (Klein, 2000), and MACRO (Jarvis, 1994). The models all report concentrations at 1 m depth for comparative purposes, under the assumption that groundwater is unlikely to be affected by pesticides at concentrations exceeding 0.1 μg/l if those concentrations are not encountered at a shallow depth. However, even if this approach can be useful for the authorisation purposes, this does not necessarily represent concentrations reached by PPPs in groundwater. In fact, it has been pointed out that simulations undertaken for a few standard scenarios (such as those utilised in the authorisation procedures) may result in large errors in the estimation of the groundwater contamination in specific regions (Van Alphen and Stoorvogel, 2002; Centofanti et al., 2008).

More recently, the Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009, commonly referred to as “the Sustainable Use of Pesticides Directive” (European Commission, 2009b), established a framework for Community action to achieve the sustainable use of PPPs. Among the requirements of the Directive, it obliges Member States to adopt a National Action Plan (NAP). The plan should define a national strategy to set down objectives, quantifiable measures and timeframes to reduce the risks associated with the use of pesticides. This Directive asks Member State to pay particular attention to groundwater by taking appropriate measures to avoid PPPs contamination. Use of PPPs in areas for the abstraction of drinking water, or in sensitive areas (or vulnerable areas) should be reduced as far as possible (using appropriate risk mitigation measures), or eliminated, if appropriate. Consequently, for groundwater, the correct implementation of this Directive requires Member States to develop tools based on a very detailed knowledge of local environmental conditions and scenario refinements, in order to identify vulnerable situations or ‘risk areas’ and to enable more targeted model simulations for specific crops.

The vulnerability concept may or may not include an assessment of whether or not contaminants are discharged in the area of interest. According to Dixon (2005), vulnerability assessment which focuses only on a description of natural factors that may favour or not transport processes of chemicals to groundwater is often referred as aquifer sensitivity (also named natural vulnerability or intrinsic vulnerability). Vulnerability assessment that takes into consideration also the characteristics of the contaminant and human activities is generally referred to as “specific vulnerability” or “integrated vulnerability”. In other words, aquifer sensitivity is referred to intrinsic properties of the studied area, such as the hydrogeological setting (depth to groundwater, presence or absence of confining layers or clay caps), the recharge of groundwater, soil hydraulic conductivity, soil retardation and attenuation factors (U.S. Environmental Protection Agency, 1993; Palmer and Lewis, 1998; Lowe and Butler, 2003). On the contrary, specific vulnerability combines the aquifer sensitivity with the pollutant properties, as different contaminants behave differently, depending on their physical–chemical properties and resistance to degradation. In addition, it also considers human activities that could enhance the movement of the contaminants to groundwater (for instance agricultural practices such us irrigation, land use) (Aller et al., 1987; Connell and Daele, 2003; Bozzo et al., 2013). In recent years, many approaches have been developed to evaluate both the intrinsic and specific aquifer vulnerability and comprehensive reviews of groundwater vulnerability assessment methods are present in literature (Zhang et al., 1996; Worrall and Besien, 2005; Pavlis et al., 2010).

The advent of GIS (Geographic Information Systems) has facilitated the assessment of groundwater vulnerability through mapping since its first appearance. In fact, GIS provide a means of extracting information relevant to pesticide fate from databases containing georeferenced information. In this, coupling of GIS and predictive leaching models of PPPs can be very effective in addressing the problem of spatial and temporal variability of the different parameters involved in leaching processes and in producing specific vulnerable groundwater cartography (Worrall et al., 2002). Consequently, it has the potential to facilitate the analysis of groundwater vulnerability in a spatial context such as regional scale, which exactly matches with previously described policy objectives. In recent years, a number of studies reported different methodologies in which the groundwater vulnerability is evaluated by coupling GIS and predictive models (Wilson et al., 1993; Tiktak et al., 2002; Holman et al., 2004; Ares et al., 2006; Balderacchi et al., 2008; Ayman, 2009).

In the present work a new GIS-based and client–server software is developed to identify areas vulnerable to PPPs at regional level making use of pesticide fate models. The area investigated is divided in polygons with homogeneous environmental characteristics and the transport of pesticide is modelled with the PELMO model, in each polygon. The software system is actually used by the Lombardy and Veneto regions of Italy for PPPs risk management purposes.

VULPES has been designed and implemented to transfer the actual scientific knowledge in terms of environmental risk assessment of pesticide to the risk assessors. It allows applying consolidated models and methodologies used in standardised scenarios for regulatory purposes to real data (pedology, weather and agronomic management) following the recent trend hoped by EFSA for the next generation of pesticide evaluations. Other model systems (GEO PEARL, GEO PELMO, FITOMARCHE) has been developed to evaluate groundwater leaching of pesticide at territorial scale, but they use simplified data and/or they are metamodels.

The present paper represents the first step of a wider research project and it is aimed at a description of the developed methodology. An example of application using the herbicide terbuthylazine in the Lombardy Region (northern Italy) is given to illustrate the functionalities of VULPES. Further steps are under analysis, including the application of the system to several active ingredients for a better calibration of the process and the environmental validation of the exposure predictions.

2. Materials and methods

2.1. General considerations on the proposed tool

VULPES is a regional exposure assessment tool for evaluating the groundwater impact of the use of pesticide at regional level (currently it works at NUTS 2 level).

As reported in the Introduction section, the PPPs registration process at European level foresees the calculation of the groundwater leaching potential applying four pesticide fate models to a set of nine standard groundwater scenarios as a combination of weather, soil and cropping data, which collectively represent agriculture in the EU. The recent Directive 2009/128/EC on “Sustainable Use of Pesticides” obliges Member States to identify sensitive areas to PPPs, making use of the same pesticide fate models of the registration procedure, but applying them to real-world data. In the same way, the Italian Legislative Decree No. 152/2006 (Italian Parliament, 2006) requires the Italian Regions to evaluate vulnerable areas to PPPs in order to eventually adopt limitations of PPPs use or mitigation measures.

VULPES responds to this specific need, providing a simple tool which couples environmental models to GIS representation of the territory in order to identify areas vulnerable to PPPs. VULPES applies the same pesticide fate models of the FOCUS group to real environmental data (pedology, weather, irrigations, crops) thus likely approaching to the real impact on the area.

As illustrated in Fig. 1, VULPES stores a set of alphanumeric data linked to cartographic layers, i.e., influence areas of relevant weather stations, the pedology map and areas where irrigation is allowed. The extent of the three layers refers to the same geographical area and the inside elements have different geometries. In order to obtain a unique

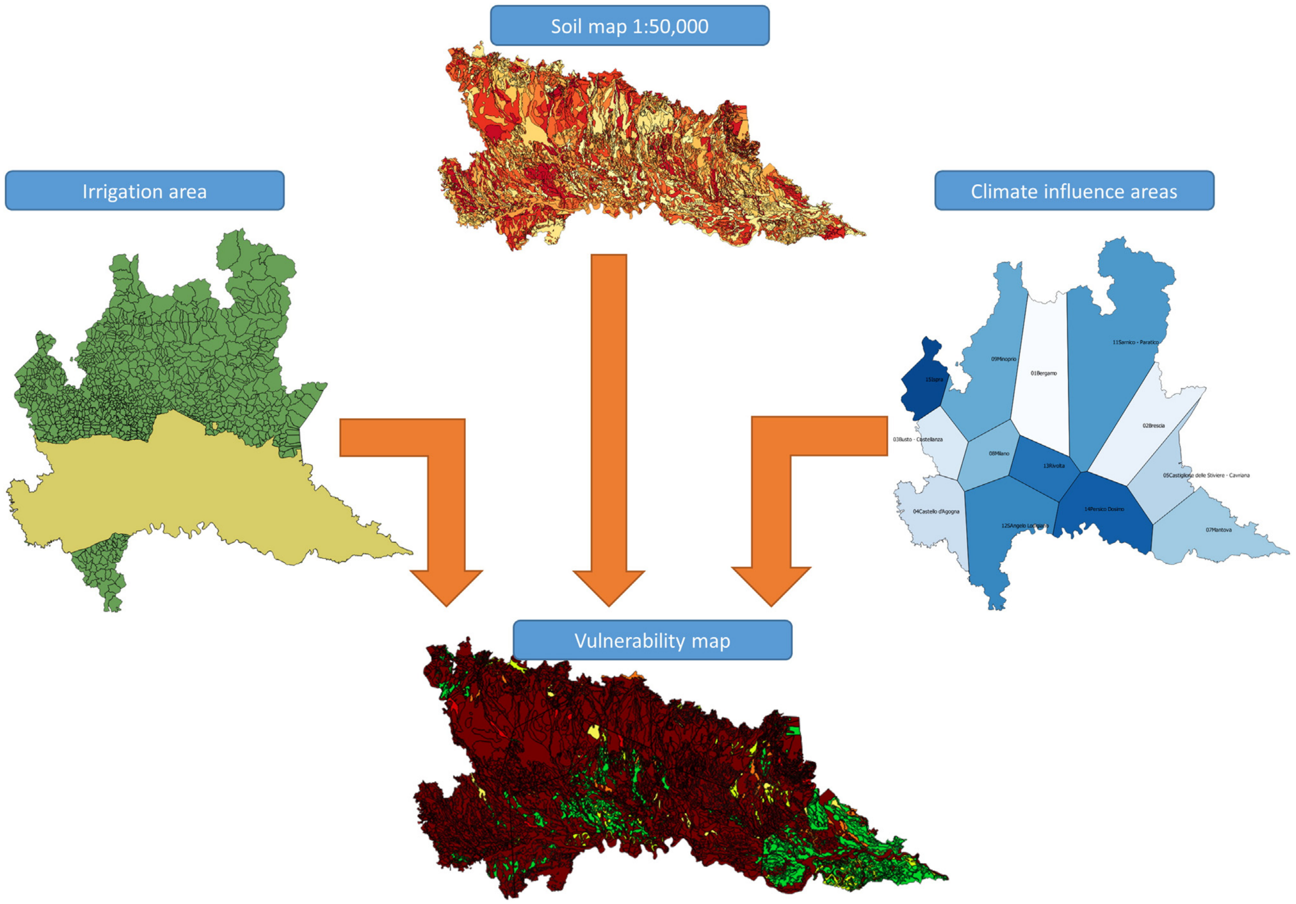


Fig. 1. Maps used in the system. The vulnerability map is calculated making use of spatial data from soil, weather, irrigation and administrative unit maps.

map in which every polygon element is characterised by a unique triplet of weather, pedology and irrigation amount, VULPES intersects the pedology map, the weather influence map and the irrigation area map. Polygon elements of the new map (called UGU — Uniform Geographical Unit) are the minimum element on which the chromatographic model PELMO can run. As an example, Lombardy region in Italy provided a pedology map with about 4000 polygons, a meteorological influence map with 13 polygons and an irrigation area map with two polygons; the intersected map has a total number of 5701 polygons with a unique set of soil, weather and irrigation data.

Other databases in VULPES contain crop parameters and data on plant protection products (PPP) (in particular physical–chemical properties for each active ingredient), which complete the set of data needed by pesticide fate models.

Users of the VULPES system interact with a simple client application whose purpose is to acquire input data such as crop and PPP to start a simulation on the area of interest.

VULPES then sends the input to the server tier and starts a simulation with the one-dimensional model PELMO in each UGU polygon for the entire duration of the historical weather series. PELMO calculates the concentration at 1 m soil depth of each active ingredient of the selected PPP and expresses the final output value as 80th percentile of the cumulated values of pesticide concentration of the several years simulated. At the end of simulations of all UGU polygons, the system generates a new vulnerability map of the area, classifying each UGU polygon into six classes according to the potential risk, with the clear characterisation of the worst case (concentration values > 0.1 μg/l, corresponding to the regulatory limit for drinking water) in red colour.

The flowchart of software operations is depicted in Fig. 2.

2.2. The software system

A schematic overview of the software system is presented in Fig. 3. VULPES is a client–server software system realised by a modular environment in the server side and a thin application client for the user.

The server side implements three main objects:

A. the database, logically divided into 2 sections: a) the environmental and spatial data such as soil profiles, weather data, irrigations, crops and their parameters; b) available commercial formulation of PPP (commercial labels) including the active ingredients, rates of application, physical–chemical properties and degradation in soil (DegT50) data;
B. the GIS engine which elaborates the spatial data identifying the homogeneous polygons for each simulation and builds the visual representation of results as a vector layer;
C. the simulation engine which receives the user input provided by the means of the client software and runs PELMO simulations for all the UGU polygons identified.

The client software is a simple Windows desktop application, which can be installed via a setup package by the final user. It communicates via http (HyperText Transfer) protocol with the server side tier and its purpose is to collect user choices in terms of PPP use and crop selection, leaving the agri-environmental and territorial description of the region on the server side. In Fig. 4 a picture of the client interface and the requested input data is reported.

Users should identify the crop of interest and the phenological stage (already filtered for the crop selected) at which the application occurs,

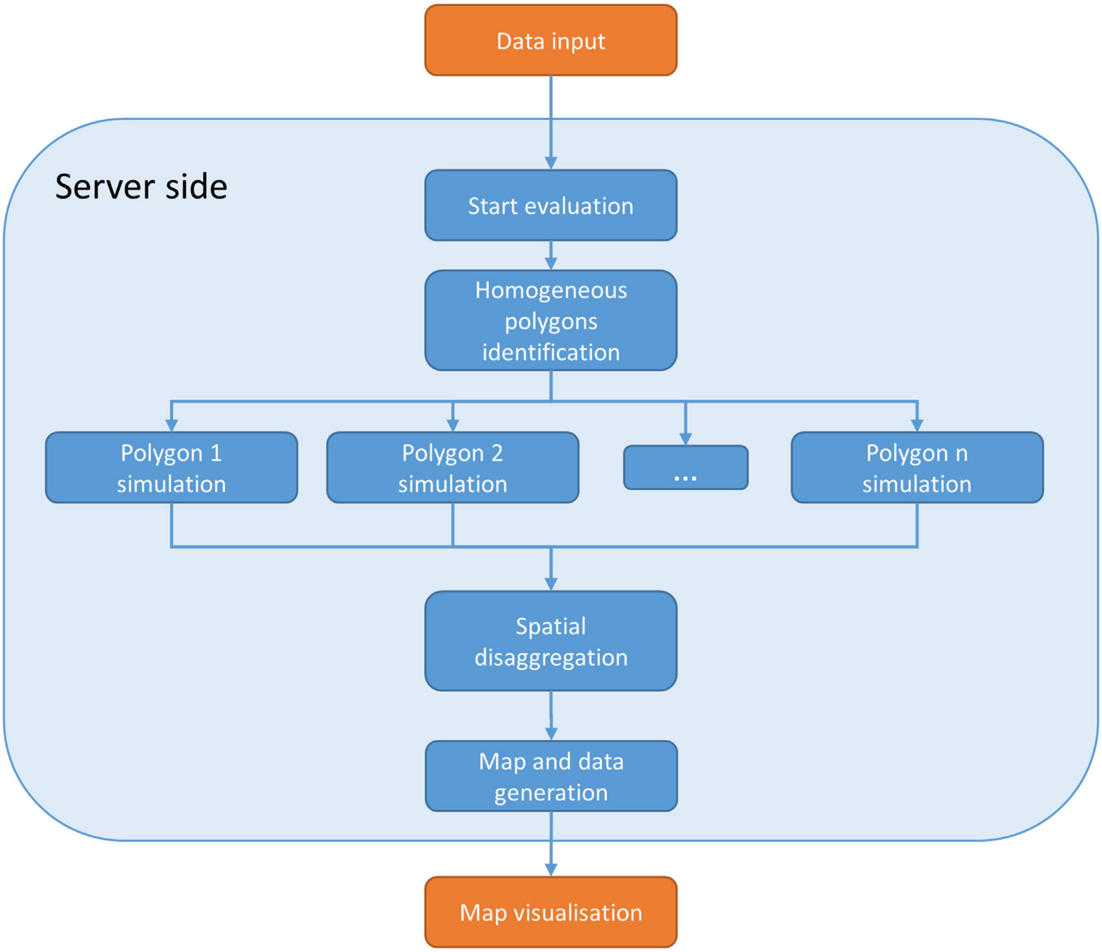


Fig. 2. Flowchart of the VULPES operations. Client-side operation are reported in orange while server-side ones are reported in blue. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the PPP as the commercial formulation name (the software also provides its composition in terms of active ingredients), the date of the first application (a label advises on the correct range of dates on the basis of the phenological stage applied), the rate and the unit of measure at which the PPP is used.

2.2.1. A. The database

As previously reported, the database is divided in two distinct sections: a sub-database contains the agro-environmental parameters that characterise the area under evaluation, such as soil profiles properties, weather data, irrigation practices and crop related parameters, and another sub-database contains information on PPPs properties. The database structure has been designed to be populated by external databases publicly available, such as regional soil maps or standard weather stations output. Spatial data have been included into a geodatabase (Microsoft SQL Server 2008) in order to hasten retrieval operations and GIS calculations.

2.2.1.1. Soils. The soil sub-database can receive data at 1:250,000 or 1:50,000 detail; in particular, the latter is considered the best scale suited to obtain useful indications at regional (NUTS 2) or province (NUTS 3) levels.

Its data content derives from a soil map of the region, formed by several areas (Cartographic Units — CU) each containing one or more (up to three) different soils, named Soil Units (SU). In turn, each Soil Unit presents a collection of soil profiles, which gives information about the physical and chemical properties of the soil itself. Each CU is characterised by the percentage of each contained SU. The system allows the user to select three different ways to take into account the SU variability within the CU. It can simulate a) the predominant SU, i.e., the SU with the highest percentage in the U, b) simulate all the SU and provide the weighted mean of the output variable, c) simulate all the SU and provide the worst case of the output variable.

Soils are identified at the same level of the “series” of the Soil Taxonomy classification by the U.S. department of Agriculture (Soil Survey Division Staff, 2010). Soil series consist of pedons that are grouped together because of their similar pedogenesis, soil chemistry, and physical properties. The profiles assigned to the same series have horizons similar in composition, thickness and arrangement but may differ in a number of properties, not discriminating between different series, which involve differences in the use or application in the management of the soil and are used to distinguish phases within the series.

2.2.1.2. Weather. Daily weather data is stored in a sub-database linked to a web service. Web services are software systems designed to support interoperable machine to machine interaction over a network. It has an interface described in a machine-processable format (specifically WSDL — Web Service Description Language). Other systems interact with the Web service in a manner prescribed by its description using SOAP (Simple Object Access Protocol) messages, typically conveyed using HTTP with an XML serialisation in conjunction with other Web-related standards (W3C, 2004; Benslimane et al., 2008).

The Weather web service contains the historical series of the meteorological stations distributed in the area under evaluation and representative of the different climate conditions. Each historical series is 20 years long at least.

Evaluation data

Evaluation identifier

Fill in input data (all data is mandatory):

Crop

Irrigation? ☐

Operation ○ Weeding ○ Pest control ○ Both

Formulato :

Composition (Label)

Phenological period

Date of first application 22/05 *Date should be between - and -

Number of applications 0

Interval between applications 0 (days)

Unit of measure

Rate 0,00 (kg/ha)

Water volume per Hectare 0,00 (l/ha)

Soil data selection

● Predominant soil

○ Weighted mean

○ worst case

Simulate only the soil (SU) with the main percentage in the CU

Output data

Output folder

Shapefile name .shp

Fig. 3. Component diagram of the software system — There is a client application, which communicates with a server tier realised by a database, a model engine and a GIS engine.

The Weather web service provides functionalities to add, remove and retrieve meteorological data stored in it. VULPES queries the Weather web service in order to check the availability of stations, parameters or time periods into the series. Weather parameters are daily rainfall, potential evapotranspiration, relative humidity, air temperature (both minimum and maximum).

2.2.1.3. Crops. A crop database contains the parameter set needed to describe the behaviour of some agricultural crops. Currently, the user may choose between oats, wheat, three varieties of maize (first period grain, second period silage, third period silage), barley, rye, pear on bare soil, pear on grassy soil, grapevine on bare soil, grapevine on grassy soil, spring lettuce, summer lettuce, autumn lettuce, melon, potato, tomato, sugar beet, and two varieties of soy (first and second periods).

Parameters refers to the maximum interception storage of the crop (cm), the maximum rooting depth of the crop (cm), the maximum areal coverage of the canopy (%), the surface condition of the crop after harvest (fallow, cropping, residue) and the detailed phenological phases, expressed in terms of the extended BBCH codes (scale used to identify the phenological development stages of a plant) (Hack et al., 1992). Moreover, a simple tool on the client desktop application allows the user to make available new crops or modify existing ones providing the above-mentioned parameters.

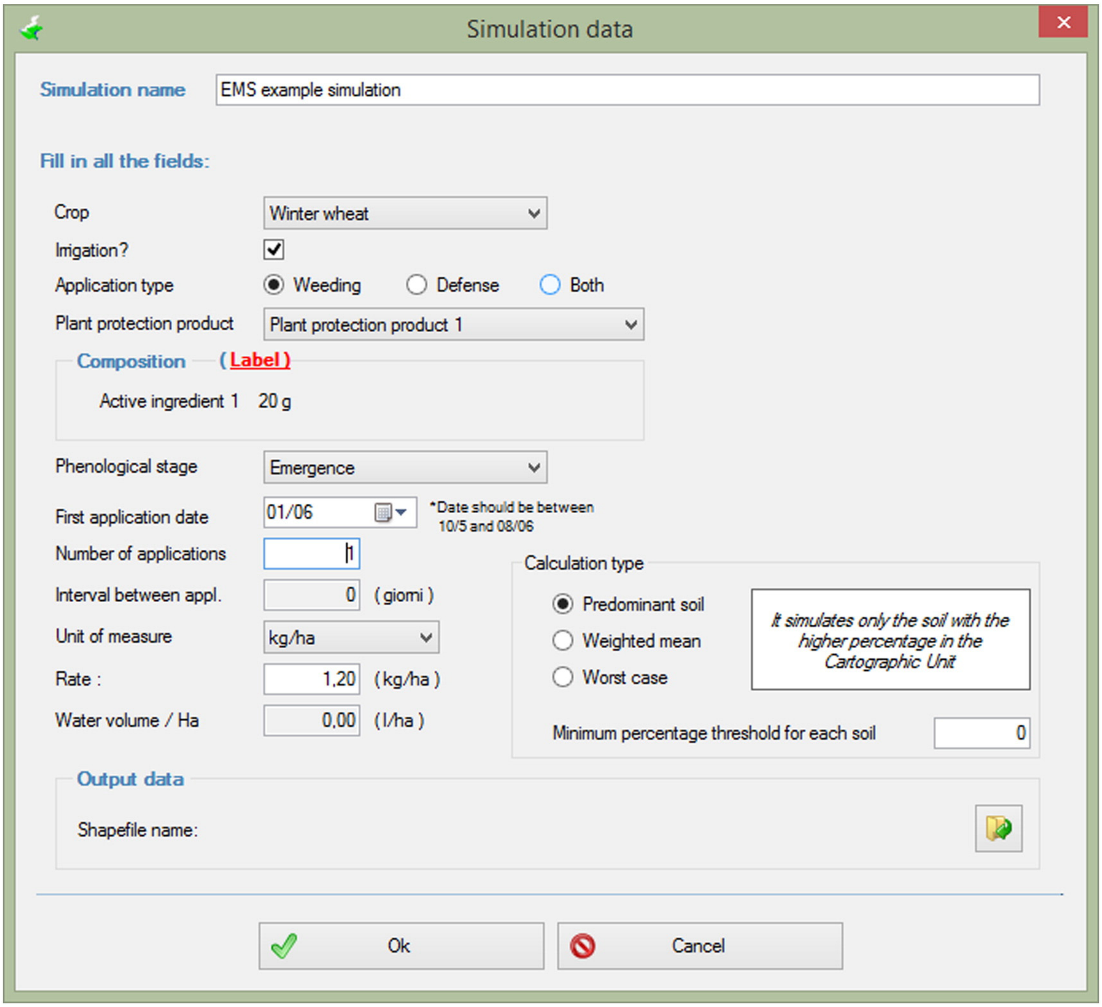
2.2.1.4. Plant protection products. Physical–chemical properties and degradation data of active ingredients contained within commercial formulations of PPPs are needed as input to run environmental fate models. On the other hand, the tool here described is intended to be used by a public administrator who needs to study the leaching behaviour of a commercial formulation without knowing its exact composition. To facilitate these two needs, two external databases feed continuously the inner pesticide sub-database. In particular, the software collects the information of the currently commercial formulations as they are constantly updated by an automated procedure of data download by an external documentation service named Pestidoc (Vellere et al., 2006), maintained by ICPS (International Centre for Pesticides and Health Risk Prevention, Milan). Each pesticide is characterised by its trade name, the regulatory label in which the user can notice the authorised doses, crops and application rules. Moreover, the Pestidoc database describes the composition of each PPP in terms of active ingredients with the relative percentage, the registration and expiration date and the date of withdrawal, the distributors and producers. Currently, the database contains about 11,400 commercial formulations, considering those commercially available, those revoked and those expired.

On the other side, physical–chemical properties and any other relevant information ruling the environmental fate of PPPs are imported from the PPBD database maintained by the University of Hertfordshire, UK (Pesticide Properties DataBase, Lewis et al., 2007). The PPDB currently holds approximately 1200 active ingredients data records and a further 600 records for associated metabolites; data stored covers general information (i.e., chemical names, chemical group, formula), physical–chemical properties (water solubility, vapour pressure, n-octanol–water partition coefficient, Henry's law constant dissociation constants), environmental fate data (degradation rates in soil, sediments and water, the organic-carbon sorption coefficient and the Freundlich coefficient).

2.2.2. B. Spatial data

'Spatial data' refers to environmental variables treated as objects in a geometric space. Indeed, it means the allocation of soils, weather, irrigations and pesticide use in the region under study.

Soils are generally provided by agricultural or pedological services of the public administration by the means of soil map at 1:250,000 and 1:50,000 scales. Generally soil maps are realised in a vector format, as a collection of polygons named Cartographic Units and are linked to a database of soil profiles, grouped into Soil Unit (Dobos et al., 2006). The VULPES system actually stores the soil maps of Lombardy and Veneto regions of Italy at a 1:50,000 scale. Soil map of other areas could be easily added by the means of a systematic user-friendly graphical user interface.



Simulation name EMS example simulation

Crop: Winter wheat

Irrigation? ☑

Application type: ● Weeding ○ Defense ○ Both

Plant protection product: Plant protection product 1

Composition (**Label**)

Active ingredient 1 20 g

Phenological stage: Emergence

First application date: 01/06 *Date should be between 10/5 and 08/06

Number of applications: 1

Interval between appl. 0 (giorni)

Unit of measure: kg/ha

Rate : 1,20 (kg/ha)

Water volume / Ha 0,00 (l/ha)

Calculation type: ● Predominant soil ○ Weighted mean ○ Worst case

It simulates only the soil with the higher percentage in the Cartographic Unit

Minimum percentage threshold for each soil 0

Output data

Shapefile name:

Fig. 4. The client application. Here is visible the input data required by the user to build a regional scenario evaluation.

Spatialisation of weather data is provided by dynamically creating an influence area map (in vector format) of the weather stations used by the means of Voronoi diagrams. Voronoi diagrams are a way of dividing space into a number of regions. A set of points (called seeds, sites, or generators) is specified beforehand and for each seed there will be a corresponding region consisting of all points closer to that seed than to any other. The regions are called Voronoi cells (Okabe et al., 2000). In climatology, Voronoi diagrams are used to calculate the rainfall of an area or generally the influence of weather parameters of a meteorological station (intended as “seed”). In this usage, they are generally referred to as Thiessen polygons. When the territory has a complex pattern (for example an alternating of hills and plains) Voronoi cells should be calculated using a higher number of meteorological stations in order to represent such a variability even in term of weather parameters.

Irrigation occurrences are identified by introducing an irrigation areas map in the VULPES system. This map identifies areas in which irrigation is mostly practiced and it permits to link data between irrigation areas, crops and irrigation amounts, stored into the database server. Irrigation amounts for each crop have been calculated by runs of a crop growth model, CropSyst (Stöckle et al., 2003) for each year of weather data.

Simulations with VULPES system work on a unique map, which is the overlay of soil, weather influence area and irrigation area (Fig. 1). The resulting map identifies polygons of the region with a unique set of weather, pedological and irrigation data (UGU: Uniform Geographic Units). They can be considered as the environmental scenarios that can be processed by the one-dimensional model PELMO.

2.2.3. C. The pesticide fate model

PELMO is a one-dimension model, which simulates water and chemical transport in the unsaturated zone within and below the plant root zone (Klein et al., 1997). The PELMO model has been tested to predict the environmental concentration of pesticides by both the model developers (Klein, 1997; Klein et al., 1997, 2000) as well as third parties (Boesten, 2004; Dubus et al., 2003; Ferrari et al., 2003).

Soil hydrology is simulated with a “tipping bucket approach” (Carsel et al., 1984) where water moves to the layer below only if water in the layer exceeds the field capacity while solute transport is based on convection–dispersion process (Klein et al., 1997; FOCUS, 2000). Within each layer, soil properties and concentration of pesticide are considered homogeneous and different behaviours are taken into account in the surface layer, root zone layers and compartments below the root zone.

The main processes depicted by the model include water movement, chemical transport, substance degradation, sorption, volatilisation, run off, soil erosion, soil temperature, plant uptake and substance application (FOCUS, 2009). Klein et al. (2000) and Dubus et al. (2003) evaluated the wide range of inputs (including soil, climate and pesticide parameters) and their importance in PELMO. In particular, sorption of pesticides is estimated according to the Freundlich equation, which considers some physicochemical parameters of the active ingredient: the sorption constant (k_f, (mg/g)/(mg/ml)), the pesticide in soil water

(c_{sol}, mg/ml), the Freundlich exponent (1/n, dimensionless), and the sorption constant (k_d, (mg/g)/(mg/ml)). When active ingredient physical–chemical properties do not cover the Freundlich exponent and/or the sorption constant k_f VULPES infers the calculation of the sorption constant k_d by using a Freundlich exponent of 1 and then it uses K_{oc} instead of the K_f. Since most of the substances has a Freundlich exponent less than 1, according to Freundlich isotherm, this choice is equivalent to lower the adsorption and then it can be considered conservative.

PELMO calculates the water and pesticide movement for each day of weather data provided: if the weather series is sufficiently large, it can take into account extreme events such as a long period of dryness or high precipitation rates concentrated in short periods. Depending on the type of data aggregations, output could be provided in daily, monthly and yearly summaries.

2.3. Output

The PELMO model, applied to each UGU polygon resulting from the combination of weather, soil and irrigation areas, calculates the concentration at 1 m soil depth of each active ingredient of the selected PPP and expresses the final output value as 80th percentile of the annual average of cumulated values of pesticide concentration. When water-table depth is above 1 m, the concentration at the interface soil–water table is used. Results are then collected on a vectorial GIS map, where the value of substance concentration of each polygon is aggregated into six classes according to the potential risk, with the clear characterisation of the worst case (concentration values > 0.1 μg/l, corresponding to the regulatory limit for drinking water) in red colour. The user can change the classification of the output adapting it to the needs.

The resulting map can be considered as a basis for the evaluation of the groundwater specific vulnerability, intended as the combination of groundwater sensitivity maps with the chemodynamic properties of the active ingredient and land use practices such as spatial distribution of crops and real use of that substance into the territory (Aller et al., 1987; Connell and Daele, 2003; Bozzo et al., 2013). In fact, at this step, the obtained map provides information about the intrinsic vulnerability of the territory combined with the chemodynamic characteristics of the modelled active ingredient. In order to evaluate more in details the areas potentially vulnerable by a specific pesticide in a specific year, the groundwater vulnerability map can be intersected with a land use map in which is highlighted the presence of the simulated crop on the area.

As accompanying measures to the groundwater vulnerability map, the software produces the tabular values for each polygon of the hydrological and pesticide fate output, as reported in Table 1. These variables are calculated as the mean of the correspondent yearly output values produced by the model and they are visible on the map for comparison purposes.

2.4. Example simulation

This section presents a case study of the application of VULPES to the Lombardy region (Northern Italy) cropped with maize and treated with a commercial formulation containing the herbicide terbuthylazine, which can be used in both pre- and post-emergence treatments.

Maize is the main crop of the area: according to the Expert System ValorE (Acutis et al., 2014) which elaborates data from the Agricultural Information System of the Lombardy Region (Regione Lombardia, 2008), maize occupies the 29% of the arable lands and it is widespread in all the region. Terbuthylazine is an herbicide that belongs to the chloro-triazine family. In plants, it acts as a powerful inhibitor of photosynthesis and it is widely used on maize in the area. Table 2 reports the main physical–chemical properties of terbuthylazine used for the simulation (Lewis et al., 2007).

The software system uses soil data from the regional Map of Soil (ERSAF, 2014) at 1:50,000 scale, which describes in details the foothill zones (south of the Alps range and north of the Apennines range) and the PO Valley plain.

Climate data are derived from the Environmental protection agency of the Region (ARPA), which counts about 280 meteorological stations scattered throughout the plain part of the region; we selected 13 stations (Fig. 5) homogeneously distributed in the area under evaluation, each of them with 24 years of daily meteorological data (rainfall, potential evapotranspiration, mean, maximum and minimum temperature, relative humidity and global solar radiation). Starting from their locations, the VULPES system builds a new vectorial map of station influence areas using the Thiessen polygon algorithm. The intersection of the influence area of meteorological stations, soil map and irrigation area map produces the simulation map, where any UGU polygon has a unique set of pedological, meteorological and irrigation properties.

The pesticide application has been set using the client software with the following parameters:

- crop: first stage maize for grain;
- application period: pre-emergence;
- application date: 18th of March;
- number of applications: one;
- PPP: a commercial formulation containing terbuthylazine (300 g/l);
- rate: 2.8 l/Ha for the PPP, corresponding to 850 g/Ha of terbuthylazine active ingredient.

VULPES acquires from the database the pedological and weather data associated at each UGU polygon and physical–chemical properties of the active substance; it produces the input files for the PELMO model which runs a simulation for each UGU. Results are then used to build a map of groundwater vulnerability considering the whole territory cropped with maize. The evaluation run of terbuthylazine in Lombardy region produced the map reported in Fig. 6.

The simulation on each UGU polygon identified the 80th percentile of the active ingredient concentration at 1 m soil depth. Subsequently, the software aggregated results into six classes as described in the Output section.

The map reported in Fig. 6 is a combination between the intrinsic vulnerability of the territory and the chemodynamics properties of the active ingredient. It has been subsequently filtered with a raster map of land use (yearly produced by ERSAF — Regional Authority for

Table 1
Output variables.

Pesticide concentrations (kg/Ha)	Water movement (cm)
Total plant uptake	Storage at day 0
Total decay of pesticide	Total precipitation on canopy
Total volatilisation	Total evaporation on canopy
Total erosion	Total throughfall on canopy
Total runoff	Total runoff on surface soil
Pesticide leached below root zone	Total infiltration in surface soil
Pesticide leached below core	Total evapotranspiration from soil profile
	Total recharge below root zone
	Total recharge below core

Table 2
Physicochemical properties of Terbuthylazine active ingredient.

Parameters	Terbuthylazine
Molecular weight (g mol^{-1})	2.30E + 02
Water solubility (mg l^{-1})	6.60E + 00
Henry constant (Pa m^3 mol^{-1})	3.24E-03
Vapour pressure (mPa)	1.20E-01
logKow (−)	3.40E + 00
Freundlich exponent (1 / n) (−)	9.30E-01
Kfoc (−)	2.31E + 02
$DegDT50_{soil}$ (days)	7.51E + 01

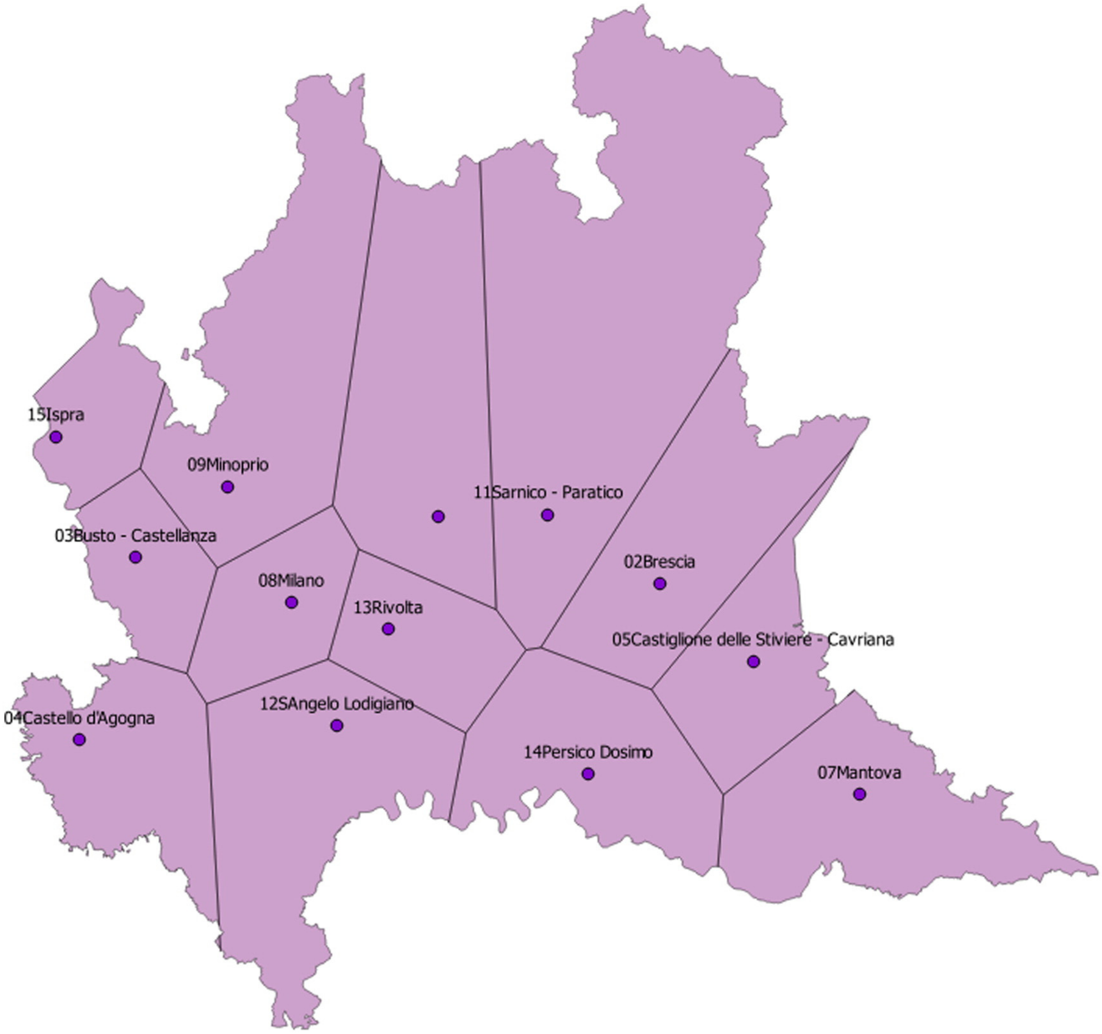


Fig. 5. Weather stations and meteorological influence areas. Polygons are obtained applying the Voronoi algorithm using the weather stations as seeds.

Agricultural and Forestry Services) in Lombardy region in which the presence of maize crop has been highlighted (result in Fig. 7).

The resulting map allowed us to identify areas of the Lombardy region cropped with maize with a high potential risk of terbuthylazine percolation towards groundwater and other areas with less permeable soils to the substance. In Fig. 7 are bordered three different areas that indicate three different behaviours. The area called Lomellina (box A) is characterised by texture of soil relatively clay and by the presence

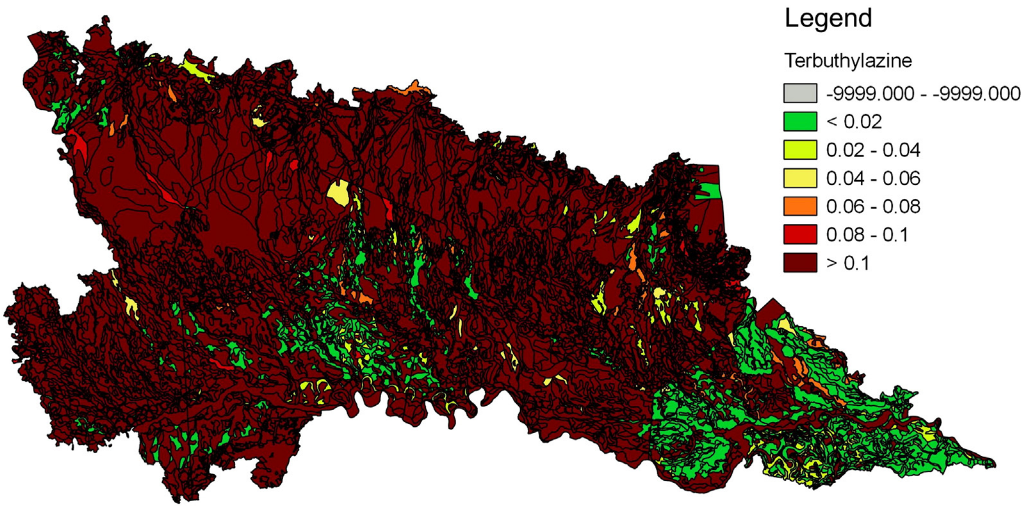


Fig. 6. Map of groundwater vulnerability to the terbuthylazine substance. This map applies to all the soils of the Lombardy region regardless of their use.

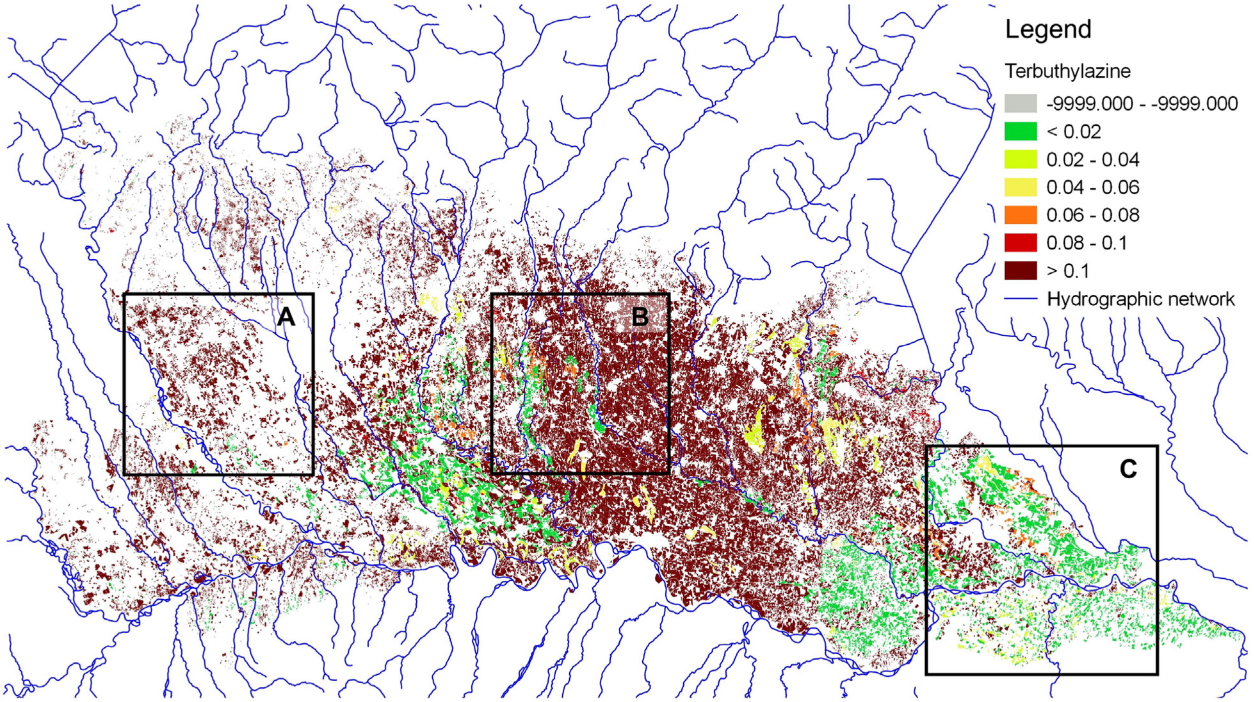


Fig. 7. Vulnerability map of Lombardy region to terbuthylazine substance filtered with maize cropped fields. Boxes A, B and C depict respectively the Lomellina area, the lower Adda-Ticino basin and the East province of Mantua.

of a shallow aquifer and soil usually saturated. In this conditions, terbuthylazine reaches groundwater in a very short time and it can percolate to the next aquifer; however this is an area suited to rice cultivation, so the intersection of the land use map with the vulnerability map in Fig. 6 results in a relatively low presence of vulnerable fields to terbuthylazine on maize. The lower Adda-Ticino basin (box B) is characterised by clay soils partially saturated (as in Lomellina) or sandy–silty, with the presence of a good drainage; here the presence of the maize crop is massive, and then the potentially vulnerable areas are widespread in the basin. The eastern province of Mantua (box C) is characterised by a relatively low level of annual precipitations and by silty–sandy soils with good drainage which keep this area less vulnerable to active ingredient percolation.

3. Conclusions

VULPES is an environmental decision support system that satisfies a specific need in a user-friendly way. It keeps together complex arguments such as environmental modelling, spatial management of environmental variables and a client server architecture using methodologies and expert knowledge with the aim to simplify its usability. In fact, VULPES should prove useful to those charged with the task to identify areas sensitive to specific pesticides, including both regional authorities and the chemical industry. It extends use of pesticide fate modelling from the one-dimension average scenarios of the FOCUS group [8] to the real-world case, adding the spatial variability at the best scale that input data can provide. VULPES could be used as a decision support system dependently to the degree of confidence that users can assume to the outputs. It has been designed to receive environmental data such as soil and weather data made available by the public authorities which operates on the territory: it is an important feature because its functionalities are readily available without the need to make expensive environmental data retrieval.

Moreover, a great effort has been devoted to try to simplify the evaluator work; the database feeding, the simulation process, UGU polygons and the resulting map creation are completely transparent.

Output scale is related to the scale of the inputs. In particular, the soil map which feed the environmental database drives the level of details of the results: the smaller the scale of the pedological map, the greater the detail of the final output. The example reported in this paper has been implemented at the 1:50.000 scale which is the best detail in a NUTS 2 level pedological map currently available at european level.

The PELMO model is one distributed by the FOCUS group, the FOrum for Co-ordination of pesticide fate models and their Use, and successfully tested in several studies. One source of uncertainty or possible error is the adoption of a general-purpose pesticide database such as PPDB the Pesticide Properties DataBase (PPDB). PPDB adopts average values for most of the pH or soil type dependent parameters, such as degT50 or Freundlich parameters.

Nonetheless, PPDB is the most complete and ready-available database of chemodynamics parameters of active substances and at the moment is the best choice to provide the possibility to simulate the commercially available pesticides on the market.

A future development of the software will be the possibility to stock in the database the ranges of validity of each pH and soil type dependent parameter and to use the appropriate available in simulation.

Acknowledgements

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References

Acutis, M., Alfieri, L., Giussani, A., Provolo, G., Di Guardo, A., Colombini, S., Bertoncini, G., Castelnuovo, M., Sali, G., Moschini, M., Sanna, M., Perego, A., Carozzi, M., Chiodini, M.E., Fumagalli, M., 2014. ValorE: an integrated and GIS-based decision support system for livestock manure management in the Lombardy region (northern Italy). Land Use Policy 41, 149–162.

Aller, L., Bennett, T., Lehr, J.H., Petty, R.J., Hackett, G., 1987. DRASTIC: A Standardised System For Evaluating Groundwater Pollution Potential Using Hydrogeologic Settings. US Environmental Protection Agency, Ada, OK (EPA/600/2-87/035).

Ares, J.O., Del Valle, H.F., Olinuck, J.A., 2006. Exploring improved pesticide management in sub-tropical environments with GIS supported fate modeling. Agric. Syst. 91, 189–210.

Arias-Estévez, M., López-Periago, E., Martínez-Carballo, E., Simal-Gándara, J., Mejuto, J., García-Río, L., 2008. The mobility and degradation of pesticides in soils and the pollution of groundwater resources. Agric. Ecosyst. Environ. 123 (4), 247–260.

Ayman, A.A., 2009. Using generic and pesticide DRASTIC GIS-based models for vulnerability assessment of the Quaternary aquifer at Sohag, Egypt. Hydrogeol. J. 17, 1203–1217.

Balderacchi, M., Di Guardo, A., Vischetti, C., Trevisan, M., 2008. The effect of crop rotation on pesticide leaching in a regional pesticide risk assessment. Environ. Sci. Technol. 42, 8000–8006.

Benslimane, D., Dustdar, S., Sheth, A., 2008. Services mashups: the new generation of web applications. IEEE Internet Comput. 10 (5), 13–15. http://dx.doi.org/10.1109/MIC.2008.110.

Boesten, J.J.T.I., 2004. Influence of dispersion length on leaching calculated with PEARL, PELMO and PRZM for FOCUS groundwater scenarios. Pest Manag. Sci. 60, 971–980.

Bouraoui, F., 2007. Testing the PEARL model in The Netherlands and Sweden. Environ. Model Softw. 22, 937–950.

Bozzo, S., Azimonti, G., Villa, S., Di Guardo, A., Finizio, A., 2013. Spatial and temporal trend of groundwater contamination from terbuthylazine and desethyl-terbuthylazine in Lombardy Region (Italy). Environ. Sci. Processes Impacts 15, 366–372.

Carsel, R.f, Smith, C.N., Mulkey, L.A., Dean, J.D., Jowise, P., 1984. User's Manual for the Pesticide Root Zone Model (PRZM) Release 1. EPA — 600/3-84-109. U.S. Environmental Agency, Athens, GA.

Centofanti, T., Hollis, J., Blenkinsop, S., Fowler, H., Truckell, I., Dubus, I., Reichenberger, S., 2008. Development of agro-environmental scenarios to support pesticide risk assessment in Europe. Sci. Total Environ. 407, 574–588.

Connell, L.D., Daele, G.V.D., 2003. A quantitative approach to aquifer vulnerability mapping. J. Hydrol. 276 (71), 88.

Council of the European Union, 1980. Council Directive 80/778/EEC of 15 July 1980 relating to the quality of water intended for human consumption. OJ L 229 pp. 11–29 (30.8.1980).

Council of the European Union, 1991. Council Directive 91/414/EEC of 15 July 1991 concerning the placing of plant protection products on the market. OJ L 230 pp. 1–32 (19.8.1991).

Council of the European Union, 1998. [98/83/EC] Council Directive 98/83/EC of 3 November 1998 on the quality of water intended for human consumption. OJ L 330 pp. 32–54 (5.12.1998).

Dixon, B., 2005. Groundwater vulnerability mapping: a GIS and fuzzy rule based integrated tool. Appl. Geogr. 25 (4), 327–347.

Dobos, E., Carré, F., Hengl, T., Reuter, H.I., Tóth, G. (Eds.), 2006. Digital Soil Mapping as a Support to Production of Functional Maps. Office for Official Publications of the European Communities, Luxemburg.

Dubus, I.G., Brown, C.D., Beulke, S., 2003. Sensitivity analyses for four pesticide leaching models. Pest Manag. Sci. 59, 962–982.

ERSAF — Ente Regionale per i Servizi all'Agricoltura ed alle Foreste, 2014. Cartografia dei suoli. http://www.ersaf.lombardia.it/servizi/Menu/dinamica.aspx?idArea=16915&idCat=16922&ID=16922&TipoElemento=categoria (last accessed 2014-07-21).

European Commission, 2009a. Commission Regulation (EC) No 1107/2009 of 21 October 2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC. OJ L 309 pp. 1–50 (24.11.2009).

European Commission, 2009b. Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009 establishing a framework for Community action to achieve the sustainable use of pesticides. OJ L 309 pp. 71–86 (24.11.2009).

Ferrari, F., Trevisan, M., Capri, E., 2003. Predicting and measuring environmental concentration of pesticides in air after soil application. J. Environ. Qual. 32, 1623–1633.

FOCUS Groundwater Scenarios Workgroup, 2000. FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup 2000. EC Document Reference Sanco/321/2000 rev.2, pp. 1–202.

FOCUS Groundwater Workgroup, 2009. Assessing potential for movement of active substances and their metabolites to ground water in the EU. Report of the FOCUS Ground Water Work Group. EC Document Reference Sanco/13144/2010 version 1, pp. 1–604.

Hack, H., Bleiholder, H., Buhr, L., Meier, U., Schnock-Fricke, E., Weber, E., Witzenberger, A., 1992. Einheitliche Codierung der phänologischen Entwicklungsstadien mono-und dikotyler Pflanzen–Erweiterte BBCH-Skala, Allgemein. Nachrichtenbl. Dtsch. Pflanzenschutzdienst 44, 265–270.

Holman, I.P., Dubus, I.G., Hollis, J.M., 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 (1–3), 73–88.

Italian Parliament, 2006. Legislative Decree No. 152/2006 "Environment Regulation".

Jarvis, N.J., 1994. The MACRO model (Version 3.1). Technical description and sample simulationsReports and Dissert 19. Dept. Soil Sci., Swedish Univ. Agric. Sci, Uppsala, Sweden.

Klein, M., 1997. Statistical distribution of pesticide concentrations in leachate results of a Monte-Carlo analysis performed with PELMO. Chemosphere 35 (112), 379–389.

Klein, M., 2000. PELMO: Pesticide Leaching Model, User Manual Version 3.0.2. Fraunhofer-Institut für Umweltchemie und Ökotoxikogie.

Klein, M., Müller, M., Dust, M., Görlitz, G., Gottesbüren, B., Hassink, J., Kloskowski, R., Kubiak, R., Resseler, H., Schaefer, H., Steinn, B., Vereecken, H., 1997. Validation of the pesticide leaching model PELMO using lysimeter studies performed for registration. Chemosphere 35 (11), 2563–2587.

Klein, M., Hosang, J., Schäfer, H., Erzgräber, B., Resseler, H., 2000. Comparing and evaluating pesticide leaching models. Results of simulations with PELMO. Agric. Water Manag. 44, 263–281.

Leistra, M., Boesten, J.J.T.I., 1989. Pesticide contamination of groundwater in western Europe. Agric. Ecosyst. Environ. 26, 369–389.

Lewis, K.A., Green, A., Tzilivakis, J., 2007. Development of an Improved Pesticide Properties Database for Risk Assessment Applications. EFITA/WCCA Conference, Glasgow, July 2007.

Lowe, M., Butler, M., 2003. Ground-water sensitivity and vulnerability to pesticides, Heber and Round Vallyes, Wasatch County, Utah. Miscellaneous Publication 03–5. Utah Geological Survey.

Okabe, A., Boots, B., Sugihara, K., Nok Chiu, S., 2000. Spatial Tessellations — Concepts and Applications of Voronoi Diagrams. 2nd ed. John Wiley, Hoboken, New Jersey.

Palmer, R.C., Lewis, M.A., 1998. Assessment of groundwater vulnerability in England and Wales. In: Robins, N.S. (Ed.), Groundwater Pollution, Aquifer Recharge and Vulnerability. Special Publications vol. 130. Geological Society, London, pp. 191–198.

Pavlis, M., Cummins, E., McDonnell, K., 2010. Groundwater vulnerability assessment of plant protection products: a review. Hum. Ecol. Risk. Assess. 16 (3), 621–650.

Regione Lombardia, 2008. SIARL—Sistema Informativo Agricolo Regione Lombardia. http://siarl.regione.lombardia.it/index.htm (last accessed 2014-05-28).

Soil Survey Division Staff, 2010. Keys to Soil Taxonomy. 11th ed. United states Department of Agriculture, NCRS, Washington.

Stöckle, C.O., Donatelli, M., Nelson, R., 2003. CropSyst, a cropping systems simulation model. Eur. J. Agron. 18 (3–4), 289–307.

Suarez, L.A., 2005. PRZM-3, A Model for Predicting Pesticide and Nitrogen Fate in the Crop Root and Unsaturated Soil Zones: Users Manual for Release 3.12.2. U.S. Environmental Protection Agency, Washington, DC (EPA/600/R-05/111 (NTIS PB2006-101105)).

Tiktak, A., 2000. Application of the pesticide leaching models to the Vredepeel dataset. II. Pesticide fate. Agric. Water Manag. 44, 119–134.

Tiktak, A., van den Berg, F., Boesten, J.J.T.I., Leistra, M., van der Linden, A.M.A., van Kraalingen, D., 2000. Pesticide Emission Assessment at Regional and Local Scales: User Manual of FOCUS Pearl Version 1.1.1. RIVM Report 711401008Alterra Report 28. RIVM, Bilthoven (142 pp.).

Tiktak, A., De Nie, D.S., Van der Linden, A.M.A., Kruijne, R., 2002. Modelling the leaching and drainage of pesticides in The Netherlands: the GeoPEARL model. Agronomie 22, 373–387.

US Environmental Production Agency, 1993. A Review of Methods for Assessing Aquifer Sensitivity and Ground Water Vulnerability to Pesticide Contamination. USEPA, Office of Water, Washington, DC.

Van Alphen, B.J., Stoorvogel, J.J., 2002. Effects of soil variability and weather conditions on pesticide leaching — a farm-level evaluation. J. Environ. Qual. 31, 797–805.

Vellere, F., Mammone, T., Blasa, R., Colosio, C., 2006. A quick and easy retrieval of information on pesticide toxicity to humans and environment: Pestidoc, chemical as intentional and accidental global threats. NATO Security Through Science Series.

Vighi, M., Funari, E. (Eds.), 2005. Pesticide Risk in Groundwater. CRC Press, Boca Raton.

Wilson, J.P., Inskeep, W.P., Rubright, P.R., Cooksey, D., Jacobsen, J.S., Snyder, R.D., 1993. Coupling geographic information systems and models for weed control and groundwater protection. Weed Technol. 7, 255–264.

World Wide Web Consortium, 2004. Web Services Glossary Retrieved 2014-04-22 at. http://www.w3.org/TR/ws-gloss/.

Worrall, F., Besien, T., 2005. The vulnerability of groundwater to pesticide contamination estimated directly from observations of presence or absence in wells. J. Hydrol. 303, 92–107.

Worrall, F., Besien, T., Kolpin, D.W., 2002. Groundwater vulnerability: interactions of chemical and site properties. Sci. Total Environ. 299, 131–143.

Zhang, R., Hamerlink, J.D., Gloss, S.P., Munn, L., 1996. Determination of non-point source pollution using GIS and numerical models. J. Environ. Qual. 25, 411–418.

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A moni-modelling approach to manage groundwater risk to pesticide leaching at regional scale

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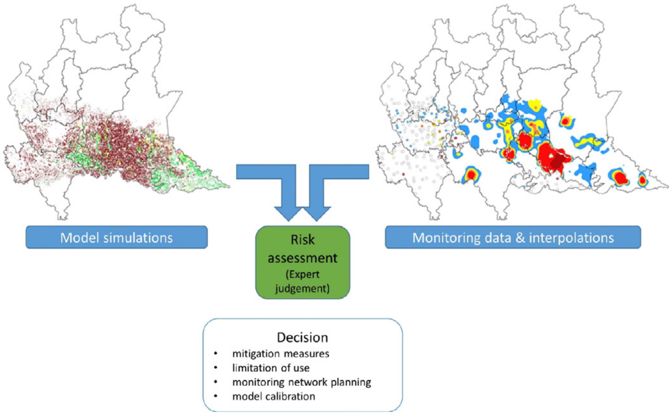
HIGHLIGHTS

- A novel methodology to identify vulnerability areas to pesticides
- Coupling information from fate models and monitoring programmes
- Decision support tool for public risk assessors
- Environmental awareness

GRAPHICAL ABSTRACT



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ABSTRACT

Historically, the approach used to manage risk of chemical contamination of water bodies is based on the use of monitoring programmes, which provide a snapshot of the presence/absence of chemicals in water bodies. Monitoring is required in the current EU regulations, such as the Water Framework Directive (WFD), as a tool to record temporal variation in the chemical status of water bodies. More recently, a number of models have been developed and used to forecast chemical contamination of water bodies. These models combine information of chemical properties, their use, and environmental scenarios. Both approaches are useful for risk assessors in decision processes. However, in our opinion, both show flaws and strengths when taken alone. This paper proposes an integrated approach (moni-modelling approach) where monitoring data and modelling simulations work together in order to provide a common decision framework for the risk assessor. This approach would be very useful, particularly for the risk management of pesticides at a territorial level. It fulfils the requirement of the recent Sustainable Use of Pesticides Directive. In fact, the moni-modelling approach could be used to identify sensible areas where implement mitigation measures or limitation of use of pesticides, but even to effectively re-design future monitoring networks or to better calibrate the pedo-climatic input data for the environmental fate models. A case study is presented, where the moni-modelling approach is applied in Lombardy region (North of Italy) to identify groundwater vulnerable areas to pesticides. The approach has been applied to six active substances with different leaching behaviour, in order to highlight the advantages in using the proposed methodology.

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1. Introduction

Groundwaters are the most sensitive and largest body of freshwater all over the world; very frequently, they are characterized by a very long mean retention time, and thus the consequences of potential pollution have long time scales (Haarstad, 1998). This is obviously of particular concern, since groundwater supplies the vast majority of drinking water. In Europe almost about 65% of water is taken from underground (Bouraoui, 2007), reaching peaks in some countries, such as in Italy, where more than 85% of the drinking water is extracted from aquifers (Onorati et al., 2006). In this context, the European Water Framework Directive (WFD — 2000/60/EC) has represented a first and important framework for developing measures for the conservation, protection and improvement of the quality of water as limited and vulnerable resource (European Commission, 2000). The environmental protection of groundwater is explicitly acknowledged by the Directive 2006/118/EC, also known as the "daughter Directive" to the Framework Directive (European Commission, 2006).

Agricultural activity is the most significant factor and the main cause of chemical pollution in many surface waters and aquifers (i.e. nitrates and Plant Protection Products). For instance, since the early analytical evidences of Plant Protection Products (PPPs) contamination of surface water and aquifers (Leistra and Boesten, 1989; Hallberg, 1989; Funari and Vighi, 1995), there have been increasing evidences of contamination of water resources from pesticides and their metabolites (Guzzella et al., 2006; Hildebrandt et al., 2008; Reemtsma et al., 2013; Bozzo et al., 2013; Stehle and Schulz, 2015). Directive 2006/118/EC has set to 0.1 μg/L and 0.5 μg/L the maximum allowable concentrations in drinking water for each individual pesticide and for their sum, respectively. This value has been also included in the EU Regulation 1107/2009/EC (formerly 91/414/EEC), concerning the placing in the market of PPPs. In Europe, PPPs regulation has been further strengthened by the recent promulgation of the Directive on Sustainable Use of Pesticides (2009/128/EC). According to this directive the EU Member States have to establish National Action Plans (NAPs) to reduce risks of PPPs use and to identify vulnerable areas (or sensible areas), in which a minimization or a prohibition of pesticide use should take place. This Directive represent a major challenge for water quality managers and environmental risk assessors and the availability of supporting information systems and methodologies useful to identify vulnerable areas or to define risk mitigation actions on the territory would be very helpful in their decisions (European Commission, 2009).

At the time being, the approach used by water quality managers to implement risk mitigation measures for PPPs on the territory falls within two categories:

a) monitoring studies, as a mean to disclose the present contamination status and assess the impact of newly implemented measures (Finizio et al., 2011; Bozzo et al., 2013);
b) use of models to predict the environmental distribution and fate of PPPs.

Both approaches show pros and cons. For instance, monitoring campaigns are very useful for regulatory purposes to verify whether the concentration of a chemical (or more) exceeds predetermined trigger values (e.g. 0.1 μg/L in groundwater). On the other hand, the main limitation of the monitoring approach is referred to the informative content of the obtained data. As matter of fact, they represent a snapshot of what is happening (in terms of concentrations) while sampling. In other words, they represent a single point in space and time (static), in a situation in which different dynamic processes act at the same time; consequently, the future state of the environment cannot be forecasted from monitoring data (Suzuki et al., 2004). Furthermore, they do not provide information on the origin of contamination (point and non-point source pollution). Finally, a preliminary set of information are needed to plan monitoring campaigns, both for selecting pesticides to be included in the list of monitored substances (leaching potential, loading rates, availability of analytical techniques) and to define the number and the spatial distribution of sites to be monitored and the sampling frequency (hydrogeology, agronomic practices, climate and soil properties). However, such information is not always easily available. In addition, the high economic costs of monitoring often limit the density of monitoring sites and influence a proper implementation of monitoring plans.

In alternative to monitoring, water quality managers can use predictive approaches. In recent years, many researchers have developed numerous spatially distributed fate and transport models of PPPs. According to Pistocchi (2008), the main advantage of such models is related to their capability of allowing spatially explicit representations (maps) of contaminants from a given spatial distribution of sources (Brown et al., 2002; Suzuky et al., 2004; Bachmann, 2006; Gusev et al., 2005). Advent of GIS has facilitated the development of this approach. For instance, very recently, a new software tool, named VULPES (VUlnerability to PEsticide — Di Guardo and Finizio, 2015) has been suggested as a tool to identify groundwater vulnerable areas in Lombardy and Veneto regions (North of Italy). However, in literature there are a number of papers in which the integration of GIS systems and predictive models have been proposed, both for surface and groundwaters (Wilson et al., 1993; Burkart et al., 1998; Manguerra et al., 1998; Burkart et al., 1999; Tiktak et al., 2002; Verro et al., 2002; Holman et al., 2004).

Undoubtedly, the existing spatially explicit models provide a valuable analytical tool to identify vulnerable areas and to forecast the probable consequences of risk mitigation actions taken from risk managers on a territory. Yet they tend to be rather complex when spatial resolution increases, requiring high computation time. In addition, according to the golden role "garbage in garbage out", if the input data are incorrect or uncertain, the resulting outputs can be wrong or debatable. For instance, the spatial variability of environmental data (i.e. soil properties, climatic conditions, crop distributions, irrigation and management patterns) cannot be easily and finely described at regional scale. In addition, other information such as period of treatments, rate of application, and typologies of pesticides mostly utilized on a particular crop are not always available. This leads to the introduction of biases and uncertainties in the spatial estimation of pesticide transport toward water resources; consequently, this could hamper the correct implementation of risk mitigation actions on the territory, even if the model has been previously validated in other geographical context.

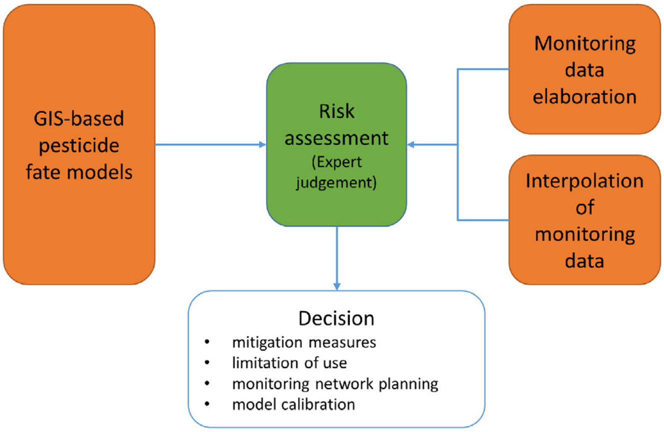

Fig. 1. Flux diagram of the proposed methodology. Colours represent different spatial levels of each action (in orange at regional level, in green at local level). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Main physical–chemical properties of selected active ingredients from PPBD database (Pesticide Properties DataBase, Lewis et al., 2007).

A.I. name	MW [g mol^{-1}]	Water solubility [mg l^{-1}]	Henry's constant [−]	Vapour pressure [mPa]	DegT50 soil [d]	Koc [−]	Freund. exponent [−]	Kfoc [−]	GUS index	Comment on GUS index
Cpyr	350.89	1.05	4.78E−01	1.43E+00	50	8151	–	–	0.15	Not leaching
Gly	169.1	10,500	2.10E−07	1.31E−02	12	1435	9.60E−01	28,700	0.90	Not leaching
s-Met	283.79	480	2.20E−03	3.70E+00	15	226	1.06E+00	226.1	1.93	Moderately Leaching
Pend	281.31	0.33	2.73E−03	1.94E+00	90	17,581	9.69E−01	15,744	−0.47	Not leaching
Tba	229.71	6.6	3.24E−03	1.20E−01	75.1	–	9.30E−01	151	3.41	Leaching
d-Tba	201.68	327.1	8.86E−08	3.50E−01	70.5	–	8.60E−01	78	3.90	Leaching

Recent approaches foresee an integration of modelling techniques with monitoring data in several fields of environmental sciences (Højberg et al., 2007; Hertel et al., 2007; Bertino et al., 2008). For instance, Brandt et al. (2006) suggested the use of a model system in connection with the urban and rural monitoring programmes as a tool to obtain the best available information level concerning the atmospheric pollution in several cities of Denmark. Very surprisingly, in the field of PPPs risk management, the integration of models and monitoring approaches (what we here call moni-modelling approach) has not yet considered. To the best of our knowledge, most of the literature data relates to use monitoring observations as a mean to calibrate or validate predictive models (Bonzini et al., 2006). However, in our opinion, the moni-modelling approach, here presented, could provide invaluable pieces of information for a proper identification of sensible areas to PPPs, where to implement risk mitigation measures. Furthermore, the combined use of monitoring and simulation models could lower the costs of monitoring, as this approach aids risk managers to organize an effective design of future monitoring programmes. Finally, the approach would give valuable help to identify possible shortcomings of models, as field data can be used to improve the quality of simulation models. In this paper, these potential advantages of the moni-modelling approach are discussed by using Lombardy region (Italy) as a case study. Particularly, practical examples will be given by combining the results of the VULPES system (a GIS-based model already used in Lombardy as well as Veneto regions) with measured data of long term monitoring campaigns for 6 different PPPs plus a metabolite characterized by different environmental fate properties.

2. Materials and methods

2.1. Overview of the methodology

The moni-modelling approach, here briefly described (Fig. 1), is based on coupling spatial modelling of environmental fate and long term monitoring data of PPPs occurrence in wells. A methodology of comparison between the results of the two types of information permits to take valuable conclusions on the effective vulnerability of the area.

In the first instance, it foresees the definition of vulnerability maps at regional scale using GIS-coupled models for predicting the potential pesticide concentrations in groundwater at regional scale. In this study, we used the VULPES system (Di Guardo and Finizio, 2015); however, in alternative other available GIS-based models could be utilized (Tiktak et al., 2002; Dixon, 2005; Babiker et al., 2005; Balderacchi et al., 2008).

On the other side, another brick of information for decision making is given by the availability of long term monitoring data of PPPs residues in groundwater. Generally, monitoring points (wells) can be easily georeferenced in a GIS map by using geographical coordinates. Considering the availability of long term data on PPPs residues in groundwater it is possible to create a map of 95th percentile of each PPP monitored observed in each monitoring site. This map can be used as input for a geostatistical analysis (i.e. using an ordinary block kriging interpolation method) to produce a new map highlighting the influence areas of different wells in the territory.

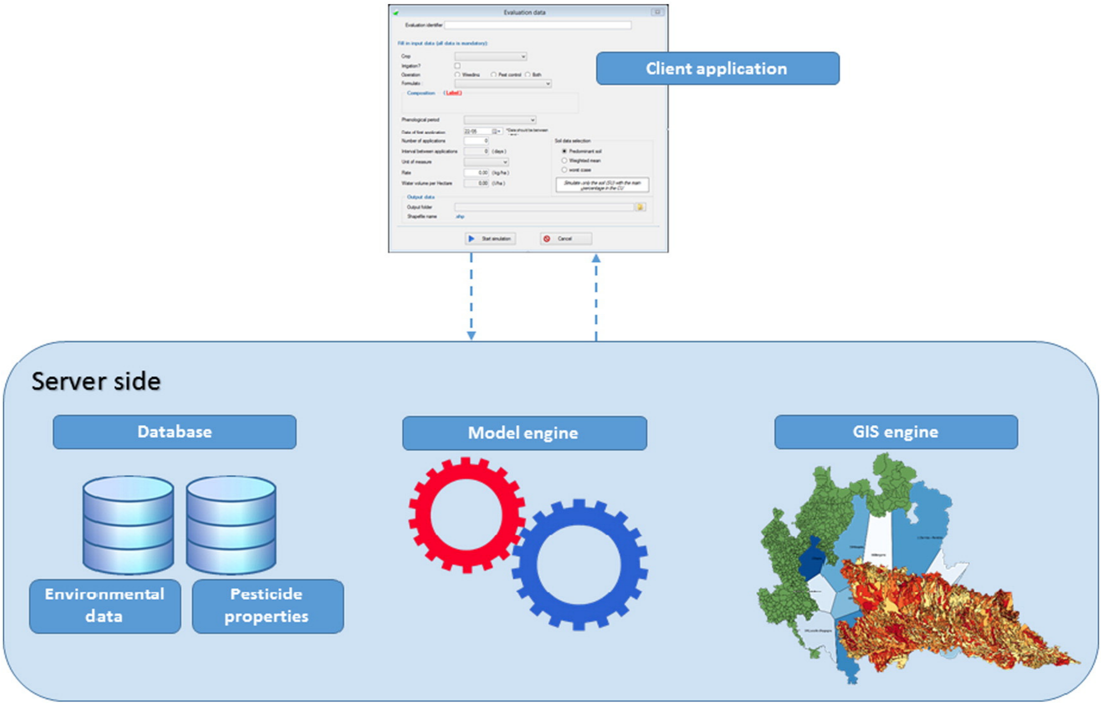

Fig. 2. Flowchart of the VULPES operations divided in client-side and server-side operations.

Table 2
Statistical summary of monitoring data for the six substances.

A.i. name	Total number of monitoring wells	Years of monitoring data	Data above LOD	Data >0.1 μg/L
Cpyr	185	2005–2006	0	0
Gly	289	2005–2009	5	1
Pend	257	2005–2007	1	0
s-Met	333	2005–2009	60	10
Tba	394	2005–2009	217	29
d-Tba	394	2005–2009	349	50

By evaluating both monitoring and modelling results, decision makers will have a powerful tool to identify specific areas at risk where implement risk mitigation measures. In addition, decision maker will have useful information to plan better monitoring networks and/or better calibrations of predictive models.

2.2. Case study: Lombardy region (North Italy)

2.2.1. Description of the area

Lombardy region has an extension of about 23.844 km^2 which almost a half of it is plain (47%) and the rest consists of hills (12%) and mountains (41%). Flat areas extend from West to East, while mountains are located at North (Alps) and in the South-West (Apennine). The last agriculture census (ISTAT, 2010) reports that arable crops are cultivated in the 92.1% of the available crop area of the Lombardy plain, while the remaining part is dedicated to woody crops and grasslands; maize is the main crop of the Lombardy region, where it covers almost a half of the total arable area. The distribution of the maize crop in the Po plain of the Lombardy region (referred to the 2009) is reported in Supporting information (Fig. S1).

2.2.2. Plant Protection Products under evaluation

In order to set up the methodology and to give some examples of how the outcomes could be very useful for risk managers, we considered five PPPs and a metabolite. Particularly, terbuthylazine (Tba), glyphosate (Gly), pendimethalin (Pend) and s-metolachlor (s-Met) herbicides, the insecticide chlorpyriphos (Cpyr) and the terbuthylazine metabolite desethyl-terbuthylazine (d-Tba) were considered. PPPs were chosen because of: a) their high use in maize protection programmes (Table S1 in Supporting information reports the sales data of each active ingredient); b) their inclusion in long term monitoring programmes; c) their different leaching capability. The latter was evaluated by the application of the GUS index (Groundwater Ubiquity Score) proposed by Gustafson (1989). GUS is a simple indicator of the chemical potential for leaching into groundwater and is based on the organic carbon partition coefficient and soil persistence of the considered chemicals. If GUS >2.8 the active ingredient is likely to leach, if GUS <1.8 it is unlikely to leach and if GUS ranges between 1.8 and 2.8 the leaching potential is marginal.

Table 1 reports a summary representation of the main physical–chemical properties and persistence (degradation time in soil: DegT50) of the selected substances; data are from the online PPDB database (Pesticide Properties DataBase, Lewis et al., 2007) maintained by the Agriculture & Environment Research Unit (AERU) at the University of Hertfordshire. In the same table, the GUS index and relative classification are also reported. As could be seen, Cpyr, Pend and Gly are non-leaching molecules, while s-Met, Tba and d-Tba demonstrate different levels of leachability.

2.2.3. The modelling system

VULPES (Di Guardo and Finizio, 2015) is an exposure assessment tool to identify groundwater vulnerable areas to PPPs at regional level. It focuses the attention to the interaction of active ingredients with the agricultural and environmental characteristics of the area.

A schematic overview of the software system is presented in Fig. 2. VULPES is a client–server software system realised by a modular environment in the server side and a thin application client for the user.

Target users are local authority technicians or environmental scientists who are in charge to investigate the impact of active substances in a specific area (currently VULPES works at NUTS 2 level).

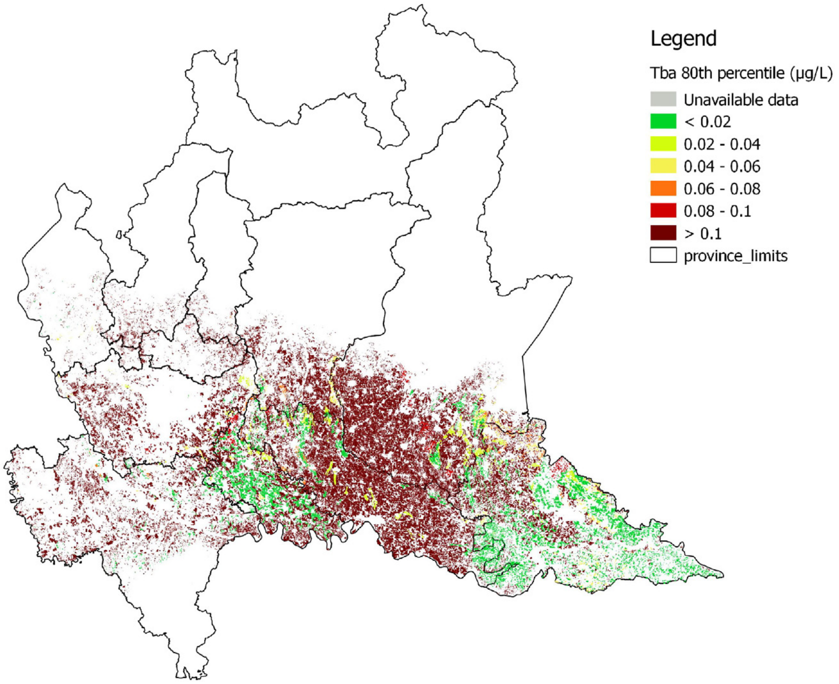

Fig. 3. Vulnerability map for terbuthylazine obtained using VULPES system.

Table 3
Classification of 95th percentile monitoring values of each well for the six active ingredients.

	Observation occurrences in classes (μg L^{-1})						
	<0.02	0.02–0.04	0.04–0.06	0.06–0.08	0.08–0.1	>0.1	Total
Cpyr	127 (69%)	58 (31%)	0	0	0	0	185
Gly	0	0	280 (98%)	0	0	5 (2%)	285
Pend	4 (2%)	194 (76%)	57 (22%)	0	0	0	255
s-Met	115 (36%)	166 (51%)	28 (9%)	5 (1.5%)	1 (0.3%)	7 (2.2%)	322
Tba	278 (59%)	123 (26%)	22 (4.6%)	16 (3.4%)	5 (1%)	29 (6%)	473
d-Tba	228 (48.2%)	137 (29%)	49 (10.4%)	15 (3.2%)	14 (2.9%)	30 (6.3%)	473

VULPES uses the PELMO v.3.2 model to evaluate the pesticide fate in the groundwater. PELMO is a one-dimension model, which simulates water and chemical transport in the unsaturated zone within and below the plant root zone (Klein, 2000).

During a VULPES run, PELMO is applied to each so-called UGU (Uniform Geographical Unit) polygon resulting from the combination of weather, soil and irrigation areas. In each UGU polygon it calculates the concentration at 1 m soil depth of each active ingredient of the selected PPP and expresses the final output value as 80th percentile of the cumulated values of pesticide concentration of the several years simulated. Results are then collected on a vectorial GIS map, where the value of substance concentration of each polygon is aggregated into different classes of vulnerability. A detailed description of VULPES is available in Di Guardo and Finizio (2015).

For s-Met, Pend, Cpyr, Gly simulations were made by considering the maximum allowed application rates for each active ingredient, as reported in the commercial formulation labels. In particular, for consistency with other active ingredients, we analysed a Cpyr formulation that has to be applied only once in crop pre-emergence and incorporated into the soil. Tba dose has been equalled to the maximum allowed dose per hectare reported in the Conclusion on pesticide peer review by EFSA (European Food Safety Agency, EFSA, 2011), which corresponds to 0.85 kg/Ha for Southern Europe. At last, in order to simulate the behaviour of d-Tba, which is a Tba metabolite we applied the maximum allowed dose of Tba multiplied by the formation rate of d-Tba (25% — EFSA, 2011).

Application rates used in VULPES simulations are listed in Supporting information Table S2.

2.2.4. Monitoring data

The presence of the six substances in Lombardy groundwater is actually monitored by ARPA Lombardia (Regione Lombardia, 2003), the environmental protection agency of the Lombardy region. ARPA, among its institutional work, is charged to periodically withdraw and analyse surface and groundwater samples looking for several active substances. We analysed five years data from 2005 to 2009 from 320 monitoring stations evenly distributed in the Po plain part of the Lombardy region (in Fig. S2 of Supporting information there is a map of the monitoring stations). ARPA provided us with two years data for Cpyr (2005 and 2006), three years for Pend (2005–2007) and five years data for the other substances. Moreover, data for s-Met failed to cover the province of Brescia, which is one of the most intensely cropped with maize.

Table 2 reports a brief summary of the main characteristics of the monitoring data provided, putting in evidence for each substance, the total number of monitoring wells and years of monitoring data available. In addition, the number of data above the limit of detection (LOD) and above the trigger value of 0.1 μg/L are also reported. For each well and substance we then calculated the 95th percentile of observed values.

Table S3 in Supporting information reports the number of analysed samples per year.

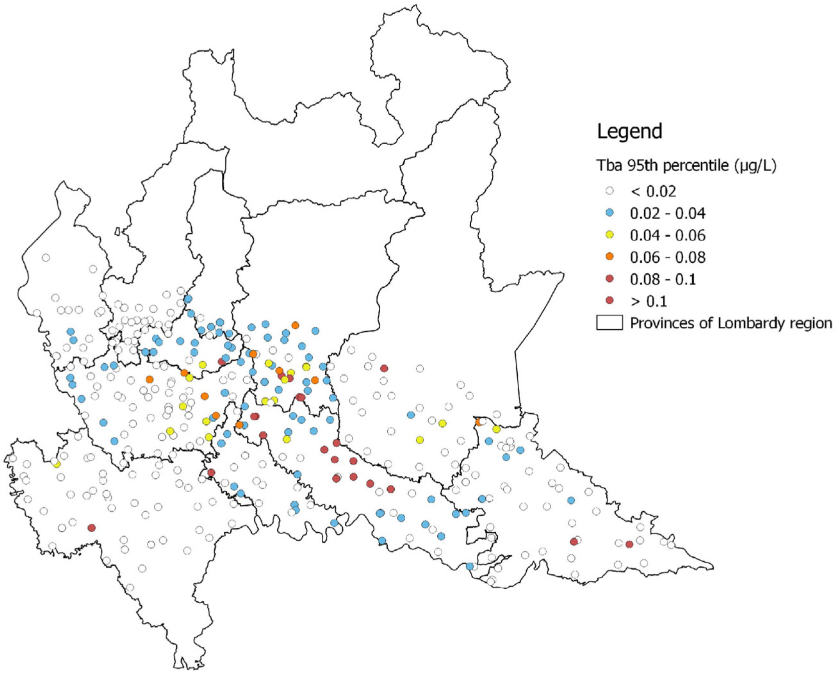

Fig. 4. Spatial distribution and classification of 95th percentile monitoring data for terbuthylazine.

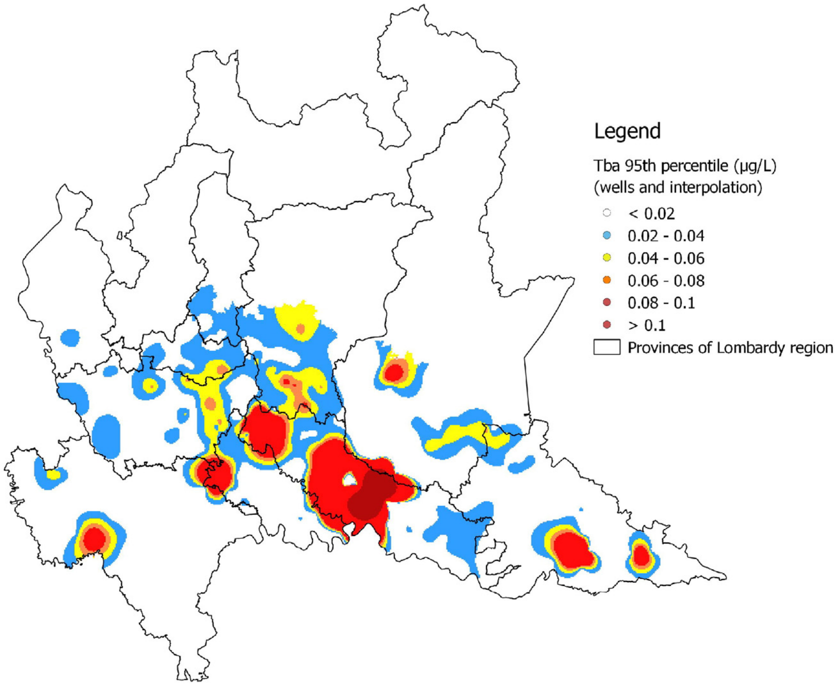

Fig. 5. Map of kriging interpolation of the 95th percentiles of monitoring values for terbuthylazine.

It has to be noted that values below the level of detection (LOD) was taken into account into the next elaborations, assuming an observed value equal to a half of LOD (in agreement with the 2009/90/CE Directive). A critical aspect of the monitoring data provided to us is that the LOD varied in space (among different provinces) and time (among different monitoring years). As an example, LODs of monitoring data of Tba varies from 0.005 µg/L (some observations in Milan, Sondrio, Varese and Monza–Brianza provinces) to 0.05 µg/L (some observations in Como, Cremona, Brescia and Bergamo provinces). Moreover, for the Milan province, LODs varies between 0.01 µg/L to 0.05 µg/L with lower LODs in recent years (2008 and 2009). These differences are mainly due to the different analytical capabilities of the laboratories involved in the analysis of water sample collected during the monitoring programmes.

2.2.5. Geostatistical elaborations

Monitoring data provide information on the local contamination and they are related to a single point in space. In order to compare monitoring data with modelling output expressed as areas of vulnerability, we adopted the ordinary block kriging (Burrough and McDonnel, 1998) as a geostatistical interpolation method to regionalise observed values. Kriging is an optimal interpolation technique based on regression against observed values of surrounding data points, weighted according to spatial covariance values. All interpolation algorithms estimate the value at a given location as a weighted sum of data values at surrounding locations. Almost all assign weights according to functions that give a decreasing weight with increasing separation distance. Kriging assigns weights according to a data-driven weighting function, rather than an arbitrary function.

For each active substance, we elaborated the available monitoring data in order to obtain the 95° percentile for each well and we used the kriging tool implemented in the SAGA-GIS software (Böhner et al., 2006) to elaborate maps of interpolated observation values of substance concentrations in the water table.

3. Results

3.1. Maps of predicted concentration of PPPs residues in groundwater of Lombardy region (vulnerability maps)

VULPES produced six vulnerability maps, which highlight the 80th percentile of the investigated active ingredient concentration at 1 metre below the soil surface taking into account all the years of meteorological data available; results are calculated in each Uniform Geographical Unit, obtained by the intersection of pedological cartographic unit, influence areas of selected meteorological station and irrigation areas. Results are grouped into six categories; hence, values can be directly compared with the legal limit for active ingredient concentration in the groundwater, actually set to 0.1 µg/L.

As an example of the obtained results, we provide here the vulnerability map for terbuthylazine; maps for s-Met and d-Tba are available in Figs. S3 and S4 of Supporting information section. No map has been reported for Cpyr, Gly and Pend because VULPES system did not identify any vulnerability related problem with these substances.

Resulting maps demonstrate two different behaviours. In agreement with GUS index the simulations for Pend, Gly and Cpyr indicated a non-leaching behaviour (each polygon falls into the class below 0.02 µg/L). On the contrary, s-Met demonstrated leachability in some areas (particularly those characterised by highly permeable soils), while Tba (see Fig. 3) and d-Tba are likely to leach in several parts of the region well beyond the trigger value of 0.1 µg/L.

3.2. Maps of measured concentration of PPPs residues in groundwater of Lombardy region

In Table 3, we report a general picture of the 95th percentiles values of monitoring data for each of the considered active ingredient. In order to have a direct comparison with the vulnerability maps produced by VULPES we used the same division in classes. The first three classes

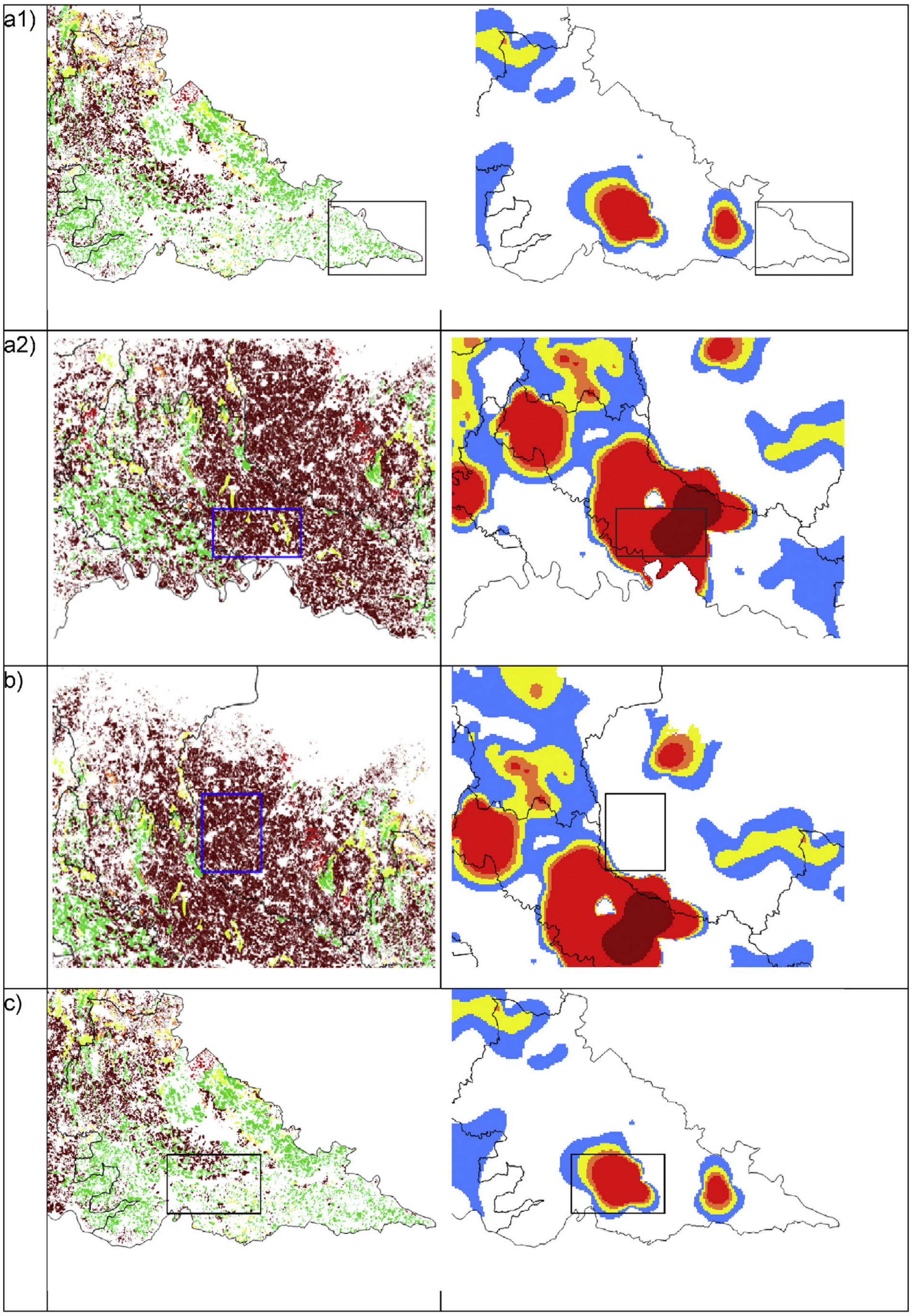

Fig. 6. Different comparison cases between vulnerability and interpolated monitoring data map: a1) consistency between predicted and observed, no risk, a2) consistency between predicted and observed, high level of risk, b) model foresees risks, monitoring data do not provide evidences, c) model does not foresee risks, monitoring data denote a high level of risk.

could be considered safer for groundwater, while the last three have an increasing level of dangerousness.

For non-leaching substances (Cpyr, Gly and Pend) values fall into the first three classes except for a consistent presence of Gly in 5 wells. Browsing raw data, almost all are below the LOD, hence values in the three classes testify the different LOD used in several part of the region. Among leaching substances, the 96% of s-Met data falls into the first three classes, while only the remaining 4% lies within the higher ones. The same general trend applies for Tba and d-Tba (89% and 87% values falls into the first three classes respectively). However, noticeably, 6% of values are above the trigger limit for both substances.

In Fig. 4, the obtained classification for each monitoring site is reported, based on the 95th percentiles of measured values of Tba residues in groundwater of Lombardy region (the classification scheme is analogous to that used in VULPES). Same pictures can be found in Figs. S5 and S6 of Supporting information section for d-Tba and s-Met. For Cpyr, Gly and Pend no maps were produced since monitoring data were almost always below the LOD.

In order to get a spatial distribution of the yearly-observed monitoring data we apply the ordinary block kriging as a geostatistical interpolation method.

As an example, we report in Fig. 5 the map for Tba obtained starting from the concentration data of the monitoring wells. Resulting maps for d-Tba and s-Met can be found in Supporting information section as Figs. S7 and S8. Cpyr, Gly and Pend do not have evidences in wells; hence, no meaningful maps could be obtained by kriging interpolation.

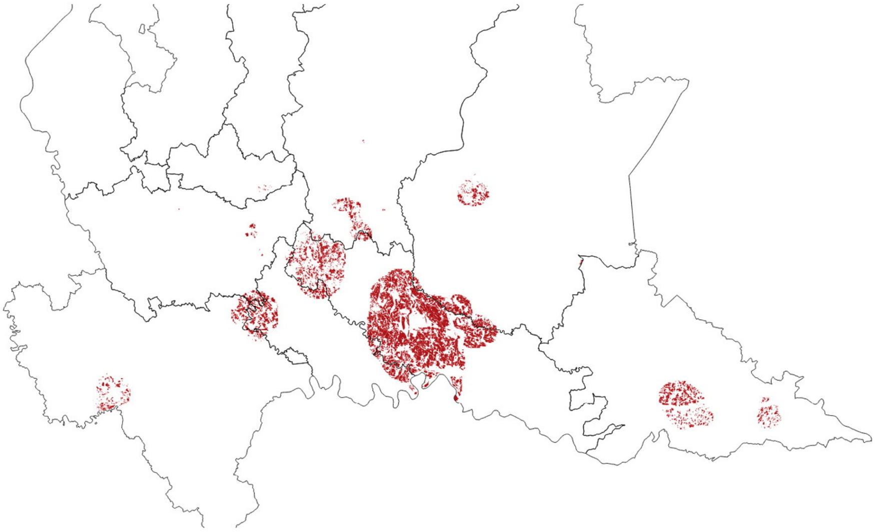

Fig. 7. Map of areas where predicted and observed data agree on groundwater leaching above 0.8 μg/L.

Fig. 5 represents the hypothetical spatial distribution of Tba in the groundwater taking into consideration the 95th percentile of data from 2005 to 2009.

Comparing with Fig. S1 in Supporting information, the presence of Tba in the water table seems follow the area where maize is more intensively cropped. In particular, the central part of the Po plain is almost completely interested, having values well beyond the threshold limit of 0.1 μg/L; the province of Mantua (East) and the province of Pavia (West) show contamination in limited areas.

4. Discussion

VULPES allows identifying potentially vulnerable areas to pesticides on a territorial scale, while monitoring data gives information on single points where contamination occurred. The integration of these two types of data within the same system provides risk assessors with a more reliable set of information in order to take decisions about the limitation of use or the need of further investigations; moreover, it could be the basis to modify or re-design the monitoring network where there is a clear evidence of uncovered areas.

Fig. 8. Distribution of monitoring wells in proximity of towns and in any case outside the cropped areas.

Analysis of map of interpolated monitoring data and vulnerability map could be done at two different spatial levels, following a top-down approach.

At a regional level, in case of not leaching substances (such as Cpyr, Gly and Pend), results provided by the two maps are practically identical and we can assume that the driving factors are physical-chemical properties of substances, regardless of environmental characteristics of the area. In this case, the analysis could be stopped at regional level, since no further investigation should be done.

In case of leaching active ingredients (such as Tba, d-Tba and s-Met), when leachability strongly depends to environmental characteristics of the area, analysis should be focused at a local level. Particularly, both vulnerability map produced by VULPES and map of interpolated monitoring data should be analysed in deep details in order to highlight whether information are concordant or discordant.

At this scale, 3 different situations could occur (Fig. 7): a) predicted and observed data are consistent (no risk or a certain level of potential pollution in the area), b) models forecast a feasible level of vulnerability, but no observations support it, c) observations denote a pollution in the area, but models indicates no vulnerability. All the alternatives will be discussed in the following paragraphs

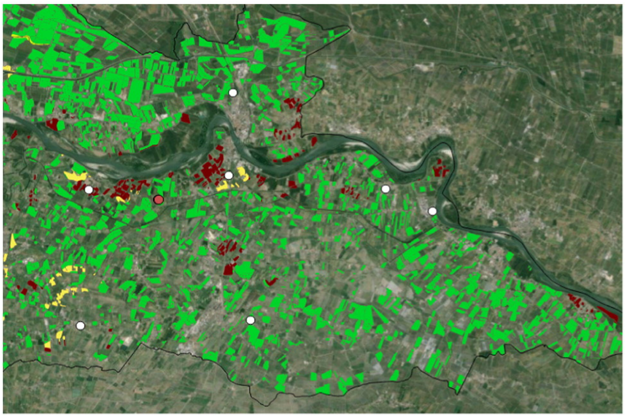

Fig. 9. Example of point source contamination clearly explained by the monitoring data and supported by the vulnerability map.

Case a. Agreement between predicted and observed data.

When there is agreement on the lack of pollution in a particular area (case a1 in Figure 6), then the risk assessor could reasonably judge that no mitigation measures or limitation of use are necessary in that area, even if occasional controls through monitoring should be considered.

On the contrary, when the agreement is on the presence of the substance in the water table (case a2 in Fig. 6), than, depending on the extension of the area or the level of pollution, the risk assessor could be confident on adopting mitigation measures or limitation of use of the active ingredient. In addition, risk assessor could improve the monitoring scheme in the area to better evaluate in time and space the level of pollution. In this case, a simple intersection of the two maps borders the area where the risk assessor could take a decision: as an example, in Fig. 7 we intersected maps of monitoring and predicted data for Tba taking into account, for each map, only values above 0.8 μg/L.

Case b and c. Disagreement between predicted and observed.

4.1. Vulnerability detected by model and no observed values in monitoring data

When there is no agreement between the vulnerability map from leaching models and the map of interpolated monitoring data in specific areas (Case b and c in Fig. 6), than the map of monitoring wells should be introduced in the analysis to provide refined information on possible reasons of discordance.

The first case is when the leaching model forecasts a high vulnerability to the active ingredient, while the surrounding wells does not provide values of it above the LOD, as in case b of Fig. 6. Analysing in details the location of wells, we could distinguish two case. If they belong to non-agricultural areas or to agricultural areas not cultivated at maize (wells in Fig. 8, representing the rectangle of case c of Fig. 6) than probably their position in the area should be improved to evaluate if the vulnerability forecasted by the model could be definitively confirmed or not. The risk assessor could operate in that direction and re-evaluate the area with new data.

If monitoring wells are correctly placed in areas cultivated with the studied crop and assuming the representativeness of the observed data, then there should be some weaknesses on input parameters of model simulations. They could belong to a wrong representation of the soil permeability of the area or to a lesser use of the active ingredient in the area. The risk assessor could evaluate the realisation of an in-depth analysis of the soil characteristics or take in consideration the effective average use of the active ingredient in the area and re-run the model simulation with the real amounts.

4.2. No vulnerability detected by model and positive values in monitoring data

The opposite occurs when the map elaborated by the leaching model does not forecast vulnerability but the monitoring wells provide values of detection near or above the legal limit for groundwater (0.1 μg/L).

Several considerations could be done. In case of just one exceeding in a well while the others in proximity have values below the LOD than the area could be interested by a point source contamination due for example to an unsustainable use of the active ingredient. For example, case c) in Fig. 6 depicts a disagreement between predicted and observed. However, if the vulnerability map with the map of 95th percentiles of the monitoring values (Fig. 9) is overlapped, then is can be observed that in the area there is only one point well beyond the threshold of 0.1 μg/L (exactly 0.199 μg/L), while the others are below the LOD.

In case of several exceeding in nearby wells, probably the input data (such as pedology, meteorology, irrigation amounts) used as input for the model in the area do not represent its environmental characteristics. Input data should be checked with ad hoc measurement campaigns to verify their representativeness. Another important factor to be taken into account is the real pesticide usage in the area: the gap between observed and predicted could be explained if, for some reasons, commercial formulations containing the active ingredient have been used at higher rates than allowed.

5. Conclusions

The moni-modelling approach here presented provides risk assessors with a complete methodology to investigate the groundwater vulnerability to pesticide, raising the knowledge of the active substance presence and movement in the considered territory. It combines vulnerability maps obtained with pesticide fate models and monitoring data analysis in order to identify areas where mitigation measure or limitation of use of the investigated active ingredient should apply. Moreover, it could be useful to verify the appropriateness of the current monitoring network or to suggest its repositioning. At last, it could identify areas where simulation models could not represent the correct substance transport in the groundwater, probably due to an incorrect parameterisation of the pedo-climatic characteristic of the area.

Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.scitotenv.2015.12.056.

References

Babiker, I.S., Mohamed, M.A.A., Hiyama, T., Kato, K., 2005. A GIS-based DRASTIC model for assessing aquifer vulnerability in Kakamigahara Heights, Gifu Prefecture, central Japan. Sci. Total Environ. 345, 127–140.

Bachmann, T., 2006. Hazardous Substances and Human Health: Exposure, Impact and External Cost Assessment at the European Scale. Elsevier, Amsterdam.

Balderacchi, M., Di Guardo, A., Vischetti, C., Trevisan, M., 2008. The effect of crop rotation on pesticide leaching in a regional pesticide risk assessment. Environ. Sci. Technol. 42 (21), 8000–8006.

Bertino, L., Lisæter, K.A., Scient, S., 2008. The TOPAZ monitoring and prediction system for the Atlantic and Arctic Oceans. J. Oper. Oceanogr. 1 (2), 15–18.

Böhner, J., McCloy, K.R., Strobl, J., 2006. SAGA — Analysis and Modelling Applications. Goltze, Göttingen.

Bonzini, S., Verro, R., Otto, S., Lazzaro, L., Finizio, A., Zanin, G., Vighi, M., 2006. Experimental validation of a geographical information systems-based procedure for predicting pesticide exposure in surface water. Environ. Sci. Technol. 40, 7561–7569.

Bouraoui, F., 2007. Testing the PEARL model in the Netherlands and Sweden. Environ. Model. Softw. 22, 937–950.

Bozzo, S., Azimonti, G., Villa, S., Di Guardo, A., Finizio, A., 2013. Spatial and temporal trend of groundwater contamination from terbuthylazine and desethyl-terbuthylazine in the Lombardy Region (Italy). Environ. Sci. Processes Impacts 15, 366.

Brandt, J., Christensen, J.H., Frohn, L.M., Geels, C., Hansen, K.M., Skjøth, C.A., 2006. THOR — an operational and integrated model system for air pollution forecasting, management and assessment from global to local scale. Contribution to the ACCENT/WMO workshop on data assimilation; group 1. Chemical Data Assimilation for the Observation of the Earth's Atmosphere.

Brown, C.D., Bellamy, P.H., Dubus, I.G., 2002. Prediction of pesticide concentrations found in rivers in the UK. Pest Manag. Sci. 58, 363–373.

Burkart, M.F., Gassman, P.W., James, D.E., Kolpin, K.W., 1998. In regional groundwater vulnerability to agrichemicals. National Soil Tilth Laboratory, Ames, pp. 130–185.

Burkart, M.R., Gassman, P.W., Moorman, T.B., Singh, P., 1999. Estimating atrazine leaching in the Midwest. J. Am. Water Resour. Assoc. 35 (5), 1089–1100.

Burrough, P.A., McDonnel, R.A., 1998. Principles of geographical information systems. second ed. Oxford University Press, Oxford.

Di Guardo, A., Finizio, A., 2015. A client–server software for the identification of groundwater vulnerability to pesticides at regional level. Sci. Total Environ. 530–531, 247–256.

Dixon, B., 2005. Groundwater vulnerability mapping: a GIS and fuzzy rule based integrated tool. Appl. Geogr. 25 (4), 327–347.

European Commission, 2000. Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy. OJ L 327, 22.12.2000, 1–73.

European Commission, 2006. Directive 2006/118/EC of the European Parliament and of the Council of 12 December 2006 on the protection of groundwater against pollution and deterioration. OJ L 372, 27.12.2006, 19–31.

European Commission, 2009. Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009 establishing a framework for Community action to achieve the sustainable use of pesticides. OJ L 309 24.11.2009, 71–86.

European Food safety Agency, 2011. Conclusion on the peer review of the pesticide risk assessment of the active substance terbuthylazine. EFSA J. 9 (1), 1969.

Finizio, A., Azimonti, G., Villa, S., 2011. Occurrence of pesticides in surface water bodies: a critical analysis of the Italian national pesticide survey programs. J. Environ. Monit. 2011 (13), 49–57.

Funari, E., Vighi, M., 1995. Pesticide Risk in Groundwater. CRC Press, Boca Raton.

Gusev, A., Mantseva, E., Shatalov, V., Strukov, B., 2005. Regional Multicompartment Model MSCE-POP. EMEP/MSC-E Technical Report. (May. http://www.msceast.org/index.php/msc-pop accessed October 2015).

Gustafson, D.I., 1989. Groundwater Ubiquity Score: a simple method for assessing pesticide leachability. Environ. Toxicol. Chem. 8, 339–357.

Guzzella, L., Pozzoni, F., Giuliano, G., 2006. Herbicide contamination of superficial groundwater in Northern Italy. Environ. Pollut. 142, 344–353.

Haarstad, K., 1998. Groundwater pesticide vulnerability: comparing simple assessment methods. NGU Bull. 434, 45–52.

Hallberg, G.R., 1989. Pesticide pollution of groundwater in the humid United States. Agric. Ecosyst. Environ. 26, 299–367.

Hertel, O., Ellermann, T., Palmgren, F., Berkowicz, R., Løfstrøm, P., Frohn, L.M., Geels, C., Skjøth, C.A., Brandt, J., Christensen, J., Kemp, K., Ketzel, M., 2007. Integrated Air Quality Monitoring — combined use of measurements and models in monitoring programmes. Environ. Chem. 4, 65–74. http://dx.doi.org/10.1071/EN06077.

Hildebrandt, A., Guillamón, M., Lacorte, S., Tauler, R., Barceló, D., 2008. Impact of pesticides used in agriculture and vineyards to surface and groundwater quality (North Spain). Water Res. 42, 3315–3326.

Højberg, A.L., Refsgaard, J.C., van Geer, F., Flindt, J.L., Zsuffa, I., 2007. Use of models to support the monitoring requirements in the water framework directive. Water Resour. Manag. 21, 1649–1672.

Holman, I.P., Dubus, I.G., Hollis, J.M., 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 (1–3), 73–88.

ISTAT, 2010. 6° censimento nazionale dell'agricoltura. Istituto Nazionale di Statistica (http://censimentoagricoltura.istat.it/accessed October 2015).

Klein, M., 2000. PELMO: pesticide leaching model, user manual version 3.0.2 Fraunhofer-Institut für Umweltchemie und Ökotoxikogie.

Leistra, M., Boesten, J.J.T.I., 1989. Pesticide contamination of groundwater in Western Europe. Agric. Ecosyst. Environ. 26, 369–389.

Lewis, K.A., Green, A., Tzilivakis, J., 2007. Development of an Improved Pesticide Properties Database for Risk Assessment Applications. EFITA/WCCA Conference, Glasgow (July).

Regione Lombardia, 2003, Programma di tutela ed uso delle acque, L.R. 12 Dicembre 2003, n. 26, art. 45, comma 3.

Manguerra, H.B., Tate, W., Lahlou, M., 1998. Arc-View-GLEAMS integration for pesticide source loading estimation. Proc. ASAE Annual International Meeting in Orlando, Florida, Paper No. 982227, p. 136.

Onorati, G., di Meo, T., Fabiani, C., Farrace, M.G., Fava, A., Ferronato, A., Mion, F., Marchetti, G., Martinelli, A., Mazzoni, M., 2006. Groundwater quality monitoring in Italy for the implementation of the EU Water Framework Directive. Phys. Chem. Earth 31 (17), 1004–1014.

Pistocchi, A., 2008. A GIS-based approach for modeling the fate and transport of pollutants in Europe. Environ. Sci. Technol. 42, 3640–3647.

Reemtsma, T., Alder, L., Banasiak, U., 2013. Emerging pesticide metabolites in groundwater and surface water as determined by the application of a multimethod for 150 pesticide metabolites. Water Res. 47, 5535–5545.

Stehle, S., Schulz, R., 2015. Agricultural insecticides threaten surface waters at the global scale. Proc. Natl. Acad. Sci. U. S. A. 112 (18), 5750–5755.

Suzuki, N., Murasawa, K., Sakurai, T., Nansai, K., Matsuhashi, K., Moriguchi, Y., Tanabe, K., Nakasugi, O., Morita, M., 2004. Geo-referenced multimedia environmental fate model (G-CIEMS): model formulation and comparison to the generic model and monitoring approaches. Environ. Sci. Technol. 38 (21), 5682–5693.

Tiktak, A., De Nie, D.S., Van der Linden, A.M.A., Kruijne, R., 2002. Modelling the leaching and drainage of pesticides in The Netherlands: the GeoPEARL model. Agronomie 22, 373–387.

Verro, R., Calliera, M., Maffioli, G., Auteri, D., Sala, S., Finizio, A., Vighi, M., 2002. GIS-based system for surface water risk assessment of agricultural chemicals. 1. Methodological approach. Environ. Sci. Technol. 36, 1532–1538.

Wilson, J.P., Inskeep, W.P., Rubright, P.R., Cooksey, D., Jacobsen, J.S., Snyder, R.D., 1993. Coupling geographic information systems and models for weed control and groundwater protection. Weed Technol. 7, 255–264.

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Sustainable use of veterinary pharmaceuticals on the territory (Sust-PHarm): Linking available database of manure management and environmental fate models

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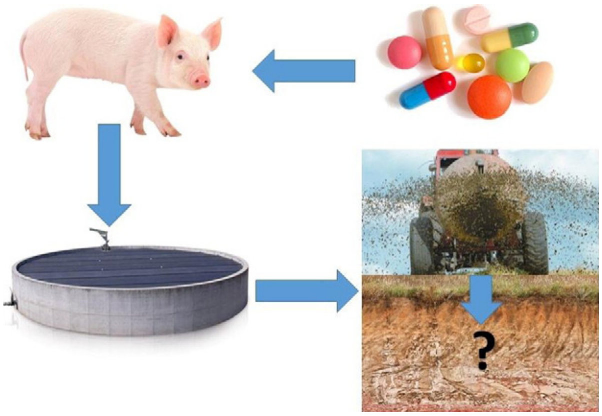
HIGHLIGHTS

- A new methodology to identify groundwater vulnerable areas to veterinary pharmaceuticals
- Coupling information from manure management databases and territorial supporting information tools
- Decision support tool for public risk assessors
- Environmental awareness

GRAPHICAL ABSTRACT



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ABSTRACT

Analogously to the evolution of the EU legislation on pesticides, there is an increasing need of strategies aiming to reach a "sustainable use of veterinary pharmaceuticals". To this end, it is essential to develop tools, such as supporting information systems (SIS), for managing the environmental risks of veterinary pharmaceuticals on a territorial scale. In this context, we propose Sust-PHarm (SUSTainable use of veterinary Pharmaceuticals), a SIS useful to identify groundwater vulnerable areas to veterinary pharmaceuticals at both local and regional scale. As background, Sust-PHarm follows the schemes of SIS for pesticides. The latter are based on the integration of predictive models in GIS. The proposed approach goes a step forward by integrating also data on the typologies of livestock farm, their spatial distribution and manure management techniques. This information allows to identify the potential environmental loads of veterinary pharmaceuticals. In this paper, we discuss the innovative elements characterizing Sust-PHarm through a comparison with the SIS currently used for pesticides. The advantages of Sust-PHarm are discussed using Lombardia Region (Northern Italy) as a case study. Simulations were made on 12 veterinary pharmaceuticals characterized by different physical-chemical properties. Results are compared with the current guidelines for the evaluation of veterinary pharmaceuticals leaching highlighting some substantial differences when realistic data are utilized making our approach more accurate than guidelines one.

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1. Introduction

Veterinary medicinal products (VMPs) are used in livestock production to preserve animal health or to promote growth in certain categories of animal (Boxall et al., 2003). Over time, the quest for 'intensification' in livestock farming has led to an increased use of these compounds, with little regard for the environmental sustainability. In order to provide a point of reference, in 2013, >8122 tons of antibiotics were sold in Europe (ESVAC, 2015). Solely, in Italy, the total sale of antibiotics used in livestock production has been estimated to be about 1328 tons of antibiotics. Moreover, it is not possible to obtain a complete data set not for the used quantities of all other categories of VMPs (parasiticides, hormones, antifungals and so on), nor about the geographic distribution and pattern of use of VMPs in the European territory.

Concerns regarding the fate and effect of VMPs in the environment have been increasing following the detection of their residues in surface waters, groundwater and even drinking water (Farré et al., 2001; Benotti et al., 2009; García-Galán et al., 2010; Huerta-Fontela et al., 2011; Ma et al., 2015; Balzer et al., 2016).

In the last two decades, there have been significant developments in the regulatory requirements for placing in the market new VMPs in consideration of their potential negative environmental impacts. Nowadays, the European Framework Directive 2001/82/EC (European Commission, 2001) regulates the production, placing on the market, labelling, marketing, and use of veterinary pharmaceuticals in the European Union. According to this Directive, the potential impact on the environment of such products must be assessed before granting a marketing authorisation. Currently in EU, the environmental risk assessment (ERA) procedures for VMPs are based on technical guidance documents (CVMP/VICH, 2000; CVMP/VICH, 2005; CVMP, 2008); which are coordinated and continuously updated by the European Medicine Agency (EMA). For groundwater (gw), these guidelines suggest an approach based on the comparison between the calculated concentration in GW (PEC_{gw}: Predicted Environmental Concentration in groundwater) and an arbitrarily set threshold concentration of 0.1 μg/L. The latter is the upper limit of the concentration for Plant Protection Products (PPPs) in drinking water in the EU. If the calculated PEC_{gw} does not exceed the threshold of 0.1 μg/L, then the risk is considered acceptable. To calculate PEC_{gw} it is recommended initially to use simple equations (based on worst case assumptions), reported in the technical guidance documents. If the threshold is exceeded, then it is suggested to use the suite of models developed by the FOCUS (Forum for the Coordination of Pesticide Fate Models and Their Use) to refine the analysis of risk. These models were developed in the frame of the 91/414/EEC Directive concerning the placing PPPs on the market (recently the EU Regulation 1107/2009 has replaced this Directive).

Even if the GW risk assessment procedures for VMPs almost overlap those suggested for PPPs, however, the estimation of the potential loads of VMPs entering the environment is extremely more complicated. In fact, whereas for PPPs the calculation of the environmental loads is quite simple (the application rate expressed as kg/ha), for VMPs there are a number of variables, which can strongly influence the quantities of VMPs entering the environment. For instance, the typology of treated animals, the modes of rearing (pasture, intensive), the route of application (oral or injection), animal metabolism, degradation during the manure storage, disposal of contaminated manure in or into ground (Halling-Sørensen et al., 2001; Boxall et al., 2004; Crane et al., 2008) can be leading factors, which determine the quantities of VMPs available for the subsequent environmental processes such as leaching. Obviously almost all these variables are strongly related to territorial and site specific conditions as well as farming practices that are not easily manageable using predefined scenarios.

For these reasons, analogously to the evolution of the EU legislation on PPPs, where the evaluation of impacts on environmental resources is moving from a scenario approach to a site specific evaluation (as foreseen in the recent Directive on Sustainable Use of Pesticides - European Commission, 2009), also for VMPs there is an increasing need to develop tools for managing the risk of VMPs at a territorial scale. In our view, this will be a fundamental step to move forwards a strategy of "sustainable use of veterinary pharmaceuticals" in livestock production.

In the field of PPPs, a considerable experience has been gained in the last years for managing the risk on a territorial scale. For instance, there a number of studies suggesting different methodologies and tools to evaluate the surface water and groundwater areas at risk to PPPs at both regional and local scale. These tools, which are to all intents supporting information systems, are generally based on the integration of predictive models into GIS (Wilson et al., 1993; Tiktak et al., 2002; Holman et al., 2004; Ares et al., 2006; Balderacchi et al., 2008; Ayman, 2009; Di Guardo and Finizio, 2015). For instance, Di Guardo and Finizio (2015) recently proposed VULPES (VULnerability to PESticide), which is decision support system aimed to assist the public policy makers to identify groundwater areas vulnerable to specific PPPs and to propose limitations of use or mitigation measures.

In this paper, we propose Sust-PHarm as a new tool to evaluate the impact of VMP usage on the groundwater at a territorial scale; it tries to fill the gap of knowledge on the territorial implementation of appropriate risk mitigation measures for VMPs in order to protect groundwater resources quality.

This methodology acquires the finest level of details available of VMPs usage data, livestock consistency and manure management and identifies the algorithms to calculate the VMP loads reaching the soil at field scale. These information, are then coupled to VULPES environment to evaluate the territorial groundwater vulnerability to a specific VMP. In this study, we suggest the use of VULPES, however, it must be underlined that other already available supporting information systems for PPPs could be easily utilized.

Topics of this paper are as follows: (i) description of Sust-PHarm approach highlighting the differences with the traditional supporting information systems already developed for pesticides; (ii) methodology testing: case study results for 12 VMPs intensively used in Lombardia Region (Italy), which shows one of highest livestock manure loads in Europe; (iii) comparison of Sust-PHarm output to the current guidelines for the VMP risk assessment (CVMP, 2008), which uses default data to identify the PEC_{soil} and standard FOCUS models (FOCUS Groundwater Scenarios Workgroup, 2000) to evaluate the PEC_{gw}.

2. Materials and methods

2.1. Sust-PHarm description in comparison with supporting information systems for pesticides

The methodology shares the same overall philosophy and underlying science actually used for modern risk management of pesticides on the territory. Therefore, provides coherent and integrated solutions to VMPs risk assessment and risk reduction for groundwater on a territorial basis. However, there are a number of relevant differences with the approach used for pesticides that gives its own originality to the proposed approach.

Coupling of GIS and predictive pesticide leaching models is very effective in addressing the problem of spatial and temporal variability of the different parameters involved in leaching processes and in producing specific vulnerable groundwater cartography (Worrall et al., 2002). In Fig. 1, the sequential flow of procedures, which is generally required in a support information system for the identification (on the territory) of groundwater vulnerable areas to pesticides, is reported. In the same figure the sequential steps planned for the proposed methodology for VMPs are also reported. Differences in terms of input needed between the two systems are highlighted in green.

The core of both systems are models for predicting the exposure (PEC: predicted environmental concentration) of pesticides or VMPs in groundwater. These models require different information, which

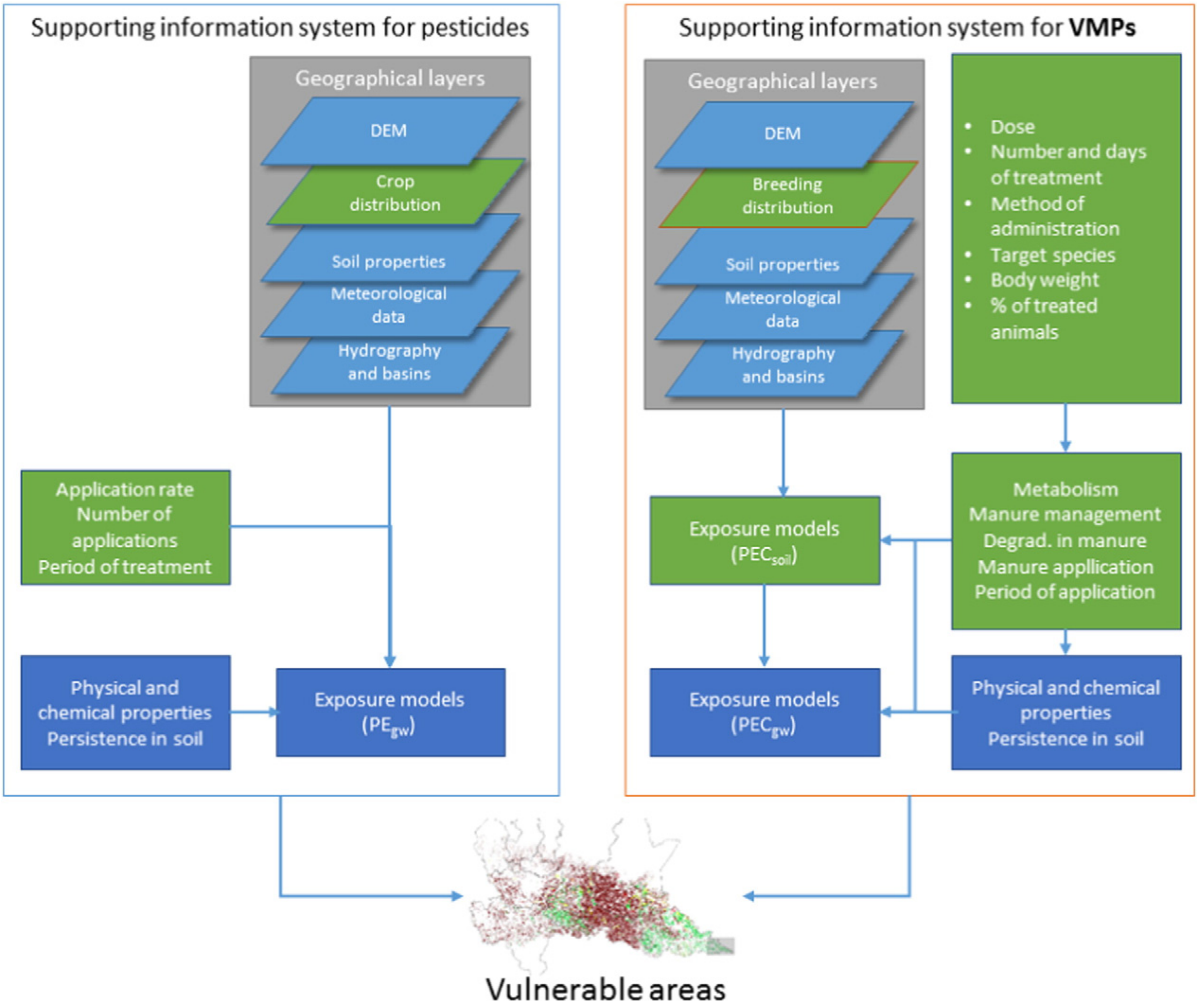

Fig. 1. Flow diagram of input data for support information systems for pesticides and VMPs. Common risk assessment activities are in blue boxes, while differences between the two methodologies are in green boxes.

are referred to: 1) used quantities (environmental load), 2) physical chemical properties and soil degradation of the active ingredient, 3) environmental scenarios. For pesticides, improvements in the models and in the way they are used have clearly gained from the work of FOCUS group (FOCUS Groundwater Workgroup, 2009). Particularly, for groundwater, it has selected PELMO (Klein, 2000), PEARL (Tiktak et al., 2000) and MACRO (Jarvis, 1991) leaching models. In the field of PPPs registration procedures, these models are run using 9 environmental scenarios which were developed by the FOCUS group. These scenarios reflect realistic worst case scenarios in EU. An analogous approach is followed in the registration procedures of new VMPs. In fact, in higher tier risk assessment PELMO and PEARL are suggested as models to predict groundwater concentrations, using the Okehampton scenario (one of the 9 FOCUS scenarios) with an application date two weeks before emergence of winter cereals (CVMP, 2008).

In the last years PELMO and PEARL models have been largely utilized in GIS environment to identify groundwater vulnerable areas to pesticides in a territory. The advantage of this approach is that models run using realistic environmental scenarios, which reflect the specificity of the territory. Characterization of the territory is read from databases containing georeferenced information on land use (e.g. Corine Land Cover 2012 – Copernicus, 2016) and crop distribution, soil properties (e.g. ERSAF, 2016), meteorological data, hydrography. As previously reported, the models require other input data such as physical chemical properties (i.e. water solubility, vapour pressure, soil-water partition coefficient) and persistence (DT_{50}) in soil. Finally, the models require input on the temporal loads on soil of the investigated chemicals; in fact, these models are based on mass balance (the total mass of the chemical into the model must be accounted for in the output from the model). For pesticides, the calculation of the environmental loads is relatively simple and can be obtained by considering the application rates (kg/ha), the number of treatments and the period of application. This information can be easily taken from labels of commercial formulations.

For VMPs the calculation is quite more complex, and this represents the most important and original innovation that differentiates the approach here proposed from the others already available for pesticides. As a matter of fact, the pathway from the treated animals to soil and then to groundwater is completely different from pesticides. After application to animals, a VMP may be absorbed and partially metabolized before being excreted with urine and faeces. In intensive farming, the resulting manure or slurry containing residues of VMPs is collected and stored before being applied to land. During the storage the VMPs can undergo to further degradation. Consequently, to calculate the load of VMPs reaching the soil there is a need to get additional information, which are related to the posology (dose, nr. and days of treatment, method of application), the target species (including their body weight) and the percentage of treated animals. In addition, also the metabolic rate (percentage of active ingredient conversion in metabolites) in animals and degradation in manure as well as its management (application and period of application) should be taken into consideration.

In our study, data about livestock farms, their typologies and geographic distribution along the Lombardia Region were taken from an

Table 1
Physical-chemical and degradation properties of selected active ingredients. MW is the molecular weight, Sol is solubility, K_{ow} is the octanol/water partition coefficient, K_{oc} is the soil organic carbon-water partitioning coefficient, VP is the vapour pressure, pka is the acid dissociation constant, DT_{50} is the half-life (in manure and in soil).

Active ingredient		MW (g/mol)	Sol (mg/L)	Log K_{ow}	K_{oc}	VP (Pa)	pka	DT_{50} manure (d)	DT_{50} soil (d)
Amoxicillin	antibiotic	365.4	3430	0.87	866	6.24E−15	0	4	0.23
Chlortetracycline	antibiotic	478.88	630	−0.62	100,420	2.09E−26	4.5	30	30
Florfenicol	antibiotic	358.21	1320	−0.04	18	1.82E−10	0	10	20
Flumequine	antibiotic	261.25	2190	1.6	180	3.30E−6	6.21	100	150
Lincomycin	antibiotic	406.54	927	0.29	59	2.46E−17	12.9	30	30
Oxytetracycline	antibiotic	460.44	1000	−0.9	52,875	1.29E−22	4.5	43.8	18
Sulfadiazine	antibiotic	250.28	130	−0.09	73.2	5.73E−6	2.49	30	20
Sulphadimethoxine	antibiotic	310.33	343	0.63	38.4	2.11E−07	0	30	20
Sulfamethazine	antibiotic	278.33	1500	0.89	46	1.15E−6	7.59	30	20
Tylosin	antibiotic	916.1	5	1.63	323.7[a]	2.63E−32	13	5	40
Trimethoprim	antibiotic	290.32	400	0.91	2835	1.31E−6	7.12	31.5	110
Ivermectin	antiparasiticide	861.1	4	5.83	4000	1.6E−28	0	45	112

[a] For tylosin, k_{foc} has been used instead of k_{oc}.

expert system called ValorE (valorisation of effluents) that has been recently proposed by Acutis et al. (2014). ValorE is a user-friendly software developed to cope with different livestock categories and to suggest and analyse alternative manure management options at farm and territorial scale. ValorE is currently used in Lombardia Region to improve the manure management for reducing the Nitrogen load at the field and therefore its environmental impact. From ValorE it is possible to get information about the manure management practices at farm scale (quantities, storage times, treatments and spreading at the field). ValorE works in a GIS environment; consequently, it is possible to extrapolate precise information about manure spreading at field scale. Information about manure management practices at farm level were extrapolated from ValorE and linked to VULPES (Di Guardo and Finizio, 2015). As previously reported, the latter is an already available supporting information system useful to identify groundwater vulnerable areas to pesticides and other chemicals.

2.2. Methodology testing

2.2.1. Active ingredients

The developed procedure was tested with VMPs (11 antimicrobials and 1 antiparasiticide), which are largely used in livestock production in Italy. Particularly, the selection was made by taking into consideration the availability of physical chemical properties and usage data. The selection was made also taking into consideration the need to have a wide range of physical chemical properties. They have been collected from different sources, in particular the Veterinary Substance DataBase (Lewis et al., 2011), TOXNET with the toxicological database Hazardous Substances Data Bank (Wexler, 2001), Chemspider (Pence and Williams, 2010) and Drugbank (Wishart et al., 2008). In Table 1, physical chemical properties and degradation parameters are reported for each active ingredient.

Table 2
Route of application and dosage in Italy for the selected VMPs. These mean values could be applied to the Lombardia region test case.

Active ingredient	Route of application	Cattle dose (mg/kg)	Pigs dose (mg/kg)	Days of treatment	Fraction of a.i. excreted
Amoxicillin	oral	30	30	5	0.5
Chlortetracycline	oral	50	50	5	0.8
Florfenicol	Injectable/	20		2	0.8
	oral		10	5	
Flumequine	injectable	6	15	3	0.8
Lincomycin	injectable	5	5	5	0.5
Oxytetracycline	oral	40	50	5	0.8
Sulfadiazine	oral	12	12	7	0.3
Sulphadimethoxine	oral	50	60	5	0.3
Sulfamethazine	injectable	200	200	3	0.3
Tylosin	oral	50	12	5	0.8
Trimethoprim	oral	3	3	7	0.3
Ivermectin	injectable	0.2	0.3	1	1

Usage data have been primarily obtained by the Handbook for Veterinary Medicines from the Italian Ministry of Health (Ministero della Salute, 2016), where treatment doses, duration and route of application are reported for each commercial formulation, together with composition and relative percentages. As a worst case scenario, we selected active ingredients with higher treatment doses within the same therapy. In Table 2 are reported the route of application, the posology for cows and pigs, the duration of treatment and the fraction of a.i. (active ingredient) excreted; the latter has been taken from Boxall et al. (2006), where authors evaluated the influence of animal metabolism for different VMP classes.

2.3. Generic model

In the frame of the authorization procedures for VMPs, the Committee for Medicinal Products for Veterinary Use (CVMP) has published several guidelines (CVMP/VICH, 2000; CVMP/VICH, 2005; CVMP, 2008), which are used to assess the potential environmental impact of VMPs. These guidelines provide an approach to evaluate the predicted environmental concentration on soil (PEC_{soil}) and in groundwater (PEC_{gw}), using a two-tiered assessment for each one of them. The first tier provides algorithms and exclusion criteria to assess the potential extent of exposure in soil and groundwater following a total residue approach (100% release to the environment), meanwhile the second tier provides a more detailed evaluation of exposure of the environment to the a.i. of the VMP.

2.4. PEC_{soil} calculation

CVMP guidelines provide a two-step approach to the calculation of PEC_{soil} for intensively reared animals (which are the ones we consider in this paper): in Phase II (Tier A) a $PEC_{soilinitial}$ is calculated with a so-called total residue approach, i.e. considering the 100% of the active ingredient dose administered in excreted manure (see Eq. (S1) in Supporting information). CVMP provides default values for almost all the parameter of the $PEC_{soilinitial}$ equation (see Table T1 in Supporting

Table 3
Vulnerability classes used to compare generic case and case study leaching to the groundwater.

Vulnerability classes	Ranges of PEC_{gw} (μg/L)	Judges
1	$PEC_{gw} < 0.001$	No contamination
2	$0.001 \leq PEC_{gw} < 0.01$	Light contamination
3	$0.01 < PEC_{gw} < 0.1$	Moderate contamination
4	$0.1 < PEC_{gw} < 0.5$	Contamination
5	$0.5 < PEC_{gw} < 1$	Serious contamination
6	$PEC_{gw} > 1$	Extremely contaminated

Table 4
Figures about farms and livestock extracted from ValorE for the five selected municipalities.

Municipality	Territorial vulnerability to nitrates?	Total number of selected farms	Cattle livestock	Pigs livestock
Bellinzago Lombardo	No	10	15	10
Moscazzano	Yes	10	12	10
Ossago Lodigiano	No	9	13	9
Pieve Fissiraga	No	13	18	13
Tavazzano con Villavesco	No	7	9	7

information), except for the active ingredient dose and the treatment duration, which are virtually the only required parameter to be inputted by the user. $PEC_{soilinitial}$ is then divided by $PNEC_{soil}$ (predicted no effect concentration) values calculated for the non-target soil organisms; if the resulting risk quotient (RQ) is >1, then CVMP guidelines suggest refinements based on metabolism, excretion patterns, degradation in manure or slurry and degradation in soil. In intensive reared animal two main refinement processes are normally considered: animal metabolism and degradation in manure. The former takes into account the formation of metabolites for a maximum percentage of 10% of the parental a.i.; the latter considers the degradation occurred in manure during the normal storage time (the agronomic management practice) before spreading (see equations from (S2) to (S5) in Supporting information).

2.5. PEC_{gw} calculation

Once evaluated the concentration of a.i. that reaches the soil, guidelines provide a two-tiered approach to identify the PEC_{gw} and therefore the vulnerability of groundwater to the a.i. A set of simple equations taking into account the partitioning coefficient between soil and water represents the first tier. If the resulting PEC_{gw} is >0.1 μg/L, then guidelines suggest to use predictive models (PELMO and PEARL) selected by the FOCUS group in the field of the authorization procedures for PPPs. Models are run using a set of 9 environmental scenarios which were defined by FOCUS group. CVMP guidelines suggest to use the Okehampton scenario as worst case scenario for VMPs leaching; however, also the Hamburg and Piacenza are considered worst case scenarios. In our study, we used the Piacenza scenario (FOCUS Groundwater Workgroup, 2009) instead of Okehampton because the case study simulations were done in an area very near to the city of Piacenza (Northern Italy). Moreover, CVMP guidelines suggest parameterising the scenario with an application date two weeks before emergence of winter cereal because in autumn bigger leaching values are expected. In our generic model application, again in comparison with the case study, we simulated the spread of manure containing residues of VMPs on maize crop at the first of May, 15 days before crop emergence, since maize is by far the most cultivated crop of the area.

For direct comparison with results of the territorial case study, Table 3 shows the classification adopted for PEC_{gw} values using nine vulnerability classes, from PEC_{gw} values <0.0005 μg/L (class 1, no presence) to values above 1 μg/L (class 9), which represents an extreme case of contamination.

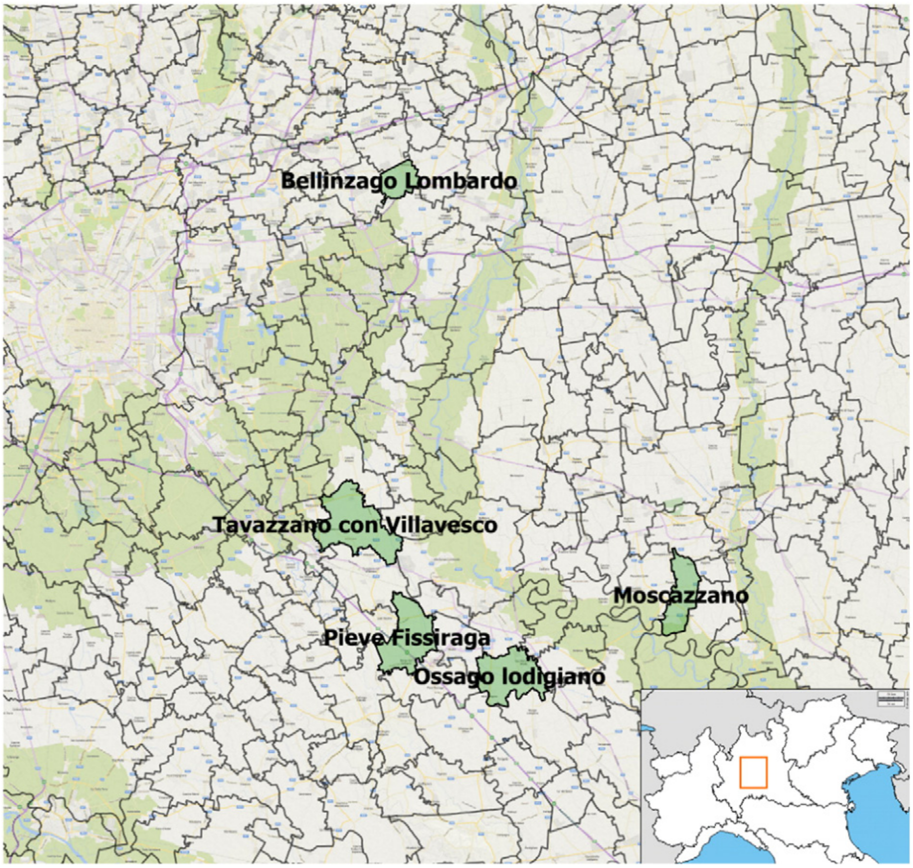

Fig. 2. Position on map of the 5 case study municipalities.

Table 5
$PEC_{soilrefined}$ and corresponding application rates of each active ingredient applying the CVMP guidelines.

	Cows		Pigs	
	$PEC_{soilrefined}$ (μg/kg)	Application rate (kg/ha)	$PEC_{soilrefined}$ (μg/kg)	Application rate (kg/ha)
Amoxicillin	7.2E−02	5.4E−05	0.3	2.6E−04
Chlortetracycline	178	1.3E−01	140	1.0E−01
Florfenicol	1.7	1.3E−03	5.0	3.7E−03
Flumequin	13	1.0E−02	24	1.8E−02
Lyncomicin	5.6	4.1E−03	4.4	3.2E−03
Oxytetracycline	199	1.4E−01	187	1.4E−01
Sulfadiazine	22	1.6E−02	18	1.3E−02
Sulphadimethoxine	67	5.0E−02	63	4.7E−02
Sulfamethazine	89	7.0E−02	70	5.0E−02
Tylosin	0.9	6.9E−04	0.6	4.7E−04
Trimethoprim	5.9	4.4E−03	4.6	3.4E−03
Ivermectin	0.2	1.9E−04	0.3	2.1E−04

2.6. Case study

Our methodology is a modified version of the guidelines procedure above reported, with two clear objectives in mind: the acquisition and use of real case data from external sources avoiding as much as possible the use of default data, and the contextualization of such data in the territory.

It relies on data of livestock consistency and manure management, which are currently put in place by regional authorities to verify agricultural economic subsidies to farmers and the environmental management of Nitrogen fertilisers. These databases are a valuable source of information to transform the generic algorithm of the CVMP guidelines in a site-specific evaluation of groundwater vulnerability to VMPs, because they are localised in a specific area (at different spatial scale) and reflect the current load of VMPs by intensively reared animals. These databases are often linked to payment procedures of European CAP (Common Agricultural Policy) or other agricultural subsidies systems outside Europe and they stock information about number of animals, structures, storage facilities and manure spreading amounts (European Commission, 2016). As case study, we applied the methodology to cattle and pigs farms in five municipalities of the Lombardia Region in Northern Italy (see Table 4). As previously described, Lombardia Region utilized an advanced expert system called ValorE (Acutis et al., 2014). ValorE is constantly updated with data about the entire manure management cycle from animal feeding to field for all kind of livestock farms. Moreover, livestock structures and manure spreading are always referred as spatial entities and therefore it can be easy evaluate manure loads at territorial level.

The five municipalities have a substantial number of cattle and pig farms, as reported in Table 4.

In Fig. 2, municipalities are contextualised within the Lombardia Region and Italy.

2.7. Calculation of VMPs loads reaching the soil

From ValorE expert system we extracted several data that allow us to improve the refined PEC_{soil} equation of CVMP guidelines, such as: (i) livestock size, i.e. the number of animals in livestock ($C_{animals}$), divided into species and way of housing; (ii) the values of animal body weights for each specie; (iii) the so called utilised agricultural area (UAA), i.e. the farm area actually cropped, which changes every year; (iv) the Nitrogen produced by each animal category (depending on the $C_{animals}$) and divided into slurry and dung ($N_{excreted}$); (v) the Nitrogen amount (N_{field}) spread in a year in all the farm fields, divided into slurry and dung; (vi) the storage time (T_{st}) for slurry and dung from each farm storage structure.

Animal weight and number have been extracted from the ValorE database running a query on each livestock structure, manure and slurry amount from each stable structure entity, Nitrogen at the field, storage times and utilised agricultural areas from the farm entity. It's worth to be noted that ValorE takes into account the real manure amount that reaches the fields, removing or adding sold or added quantities.

2.8. PEC_{soil} calculation

With the above data, the $PEC_{soilrefined}$ equation from CVMP guidelines could be modified as below:

$$\mathrm{Mi} = \mathrm{D} \times \mathrm{Ad} \times \mathrm{BW} \times \mathrm{C}_{\mathrm{animals}} \times \mathrm{Fh} \times \mathrm{Fa} \tag{1}$$

$$\mathrm{Mt} = \mathrm{Mi} \times e^{\left(\frac{-\ln(2) \times \left(\frac{T_{st}}{2}\right)}{DT_{50}}\right)} \tag{2}$$

$$PEC_{soilrefined} = \left(\frac{\mathrm{Mt} \times \frac{N_{field}}{UAA}}{1500 \times 10,000 \times 0.05 \times N_{excreted}}\right) \times 1000 \tag{3}$$

Mi is the mass of active ingredient in slurry/manure (mg), *D* is the daily dose of active ingredient ($mg/kg_{bw}d$), Ad is the number of day of treatment (d), BW is the animal body weight (kg), Fh is the fraction of herd treated (between 0 and 1), Mt is the mass of active ingredient in slurry/manure after the mean storage time (mg), T_{st} is the length of time manure is stored (d), DT_{50} is the active ingredient half-life in manure (d), $PEC_{soilrefined}$ is the refined predicted environmental concentration in soil (μg/kg), 1500 is the bulk density of dry soil (kg/m^3), 10,000

Table 6
PEC groundwater calculated with PEARL and PELMO models following CVMP guidelines.

	PEC_{gw} (μg/L) 80th percentile			
	PEARL		PELMO	
	Cows	Pigs	Cows	Pigs
Amoxicillin	0	0	0	0
Chlortetracycline	0	0	0	0
Florfenicol	1.0E−3	3.7E−3	1.0E−3	3.0E−3
Flumequin	5.9E−2	0.12	5.9E−2	0.11
Lyncomicin	1.3E−3	9.3E−4	2.0E−3	1.0E−3
Oxytetracycline	0	0	0	0
Sulfadiazine	2.0E−4	1.4E−4	1.0E−3	0
Sulphadimethoxine	2.1E−2	5.0E−2	1.7E−2	1.5E−2
Sulfamethazine	1.5E−2	1.1E−2	1.4E−2	1.0E−2
Tylosin	4.9E−3	3.5E−3	4.0E−3	3.0E−3
Trimethoprim	0	0	0	0
Ivermectin	0	0	0	0

Table 7
Vulnerability classes of PEC_{gw} calculations in the generic case.

	Vulnerability classes			
	PEARL		PELMO	
	Cows	Pigs	Cows	Pigs
Amoxicillin	1	1	1	1
Chlortetracycline	1	1	1	1
Florfenicol	2	2	2	2
Flumequin	3	7	3	7
Lyncomicin	2	1	2	2
Oxytetracycline	1	1	1	1
Sulfadiazine	1	1	2	1
Sulphadimethoxine	3	3	3	3
Sulfamethazine	3	3	3	3
Tylosin	3	3	3	3
Trimethoprim	1	1	1	1
Ivermectin	1	1	1	1

Table 8
Mean Nitrogen loads per month in the five municipalities (kgN/ha).

	January	February	March	April	May	June	July	August	September	October	November	December
Bellinzago L.	0	22.76	28.07	46.68	75.51	21.24	32.83	15.70	29.48	52.84	39.45	0
Moscazzano	0	34.29	56.87	12.68	60.51	20.29	12.96	11.71	56.49	58.09	1.33	0
Ossago Lodigiano	0	10.59	79.55	28.58	18.77	16.86	9.32	20.68	43.85	36.63	8.82	0
Pieve Fissiraga	0	17.01	80.36	54.78	52.87	4.55	8.48	3.17	28.30	80.77	17.13	0
Tavazzano con V.	0	1.43	98.02	55.11	37.42	20.84	26.78	13.20	64.21	93.80	2.54	0

represent 1 ha in m^2, 0.05 is the penetration depth into soil (m), N$_{\text{excreted}}$ is the total Nitrogen produced from each housing structure, 1000 is a conversion factor (1000 μg/mg).

Compared to CVMP guideline, PEC$_{\text{soilrefined}}$ of the territorial case does not expose the parameter P (animal turnover rate per place) which implies a fixed housing (not used in Lombardia Region) and it adds the total number of animals multiplied for the total Nitrogen produced from each housing structure (N$_{\text{excreted}}$). Moreover, instead of the mean default value of 170 kgN/ha, it has been considered the Nitrogen amount really spread divided by the farm agricultural area (UAA) as the actual Nitrogen load per hectare.

ValorE provides a cumulative value of spreading manure each month and therefore the PEC$_{\text{soilrefined}}$ in the territorial case has been calculated for each type of manure (sludge and dung) of each livestock structure in each municipality for each month. Resulting values have been assigned spatially to the municipality area in which the original manure has been spread.

ValorE provides also Nitrogen spreading month by month in each field; once evaluated PEC$_{\text{soil}}$ for each a.i., species, housing and manure type, results have been converted to obtain the a.i. loads expressed as kg/ha in order to be used as input by leaching models.

2.9. PEC$_{gw}$ calculation: VULPES application

Active ingredient loads in soil have been used as input for the VULPES System (Di Guardo and Finizio, 2015, 2016). VULPES is a regional exposure assessment tool for evaluating the groundwater impact of the use of pesticide at regional level and currently it works at NUTS (Nomenclature des unités territoriales statistiques) 2 level. The calculation unit of VULPES is the so-called UGU (Uniform Geographical Unit) which is a GIS polygon which has a unique set of environmental data, i.e. one type of weather, one map unit of soil types, the presence or not of irrigation.

3. Results and discussion

3.1. Generic model

Applying Eq. (S3)–(S5) in Supporting information, we estimated for each animal category PEC$_{\text{soil}}$ and active ingredients loads (kg/ha) for the twelve VMPs considered, as reported in Table 5.

PEC$_{\text{soilrefined}}$ has been calculated using the default data reported in the CVMP guidelines and application data reported in Table 2, taking into account the animal metabolism (Fa) and the degradation (DT$_{\text{50manure}}$) during the storage time (T$_{\text{st}}$). Application rates of VMPs (kg/ha) have been calculated using Eq. (4), where PEC$_{\text{soilrefined}}$ (μg/kg) has been converted using an incorporation depth of 0.05 m, an average soil density of 1500 kg m^{-3} and a conversion factor of 100,000.

$$\text{Application rate} = \frac{(\text{PEC}_{\text{soilrefined}} \times 0.05 \times 1500)}{100,000} \tag{4}$$

Amoxicillin, chlortetracycline, sulfadiazine, sulfamethazine and trimethoprim have the same application dose for cows and pigs and therefore similar PEC$_{\text{soilrefined}}$ results, with those referred to cows a little higher. In other cases, the difference is due to the different application doses. Chlortetracycline and oxytetracycline have concentrations above 100 μg/kg which is the threshold to trigger a second tier analysis following CVMP guidelines; high concentrations have been reached by application of sulfadiazine, sulphadimethoxine, sulfamethazine and flumequin, in the order of 10^{-2} μg/kg. Other a.i. have PEC$_{\text{soilrefined}}$ below 10 μg/kg and application rates in the order of 10^{-3} and 10^{-4} kg/ha. Due to low degradation times in manure, amoxicillin (DT$_{\text{50manure}}$ = 4 days) and tylosin (DT$_{\text{50manure}}$ = 5 days) are almost all degraded during storage time.

In a next step, PEC$_{\text{gw}}$ was calculated with the PELMO and PEARL models with the standard FOCUS scenario of Piacenza (maize as crop)

Table 9
Mean values and standard deviation data of PEC$_{\text{soilrefined}}$ and application rates for the Tavazzano municipality.

	Slurry		Manure		Total
	PEC$_{\text{soilrefined}}$	Application rate	PEC$_{\text{soilrefined}}$	Application rate	Application rate
	μg/kg	kg/ha	μg/kg	kg/ha	kg/ha
Amoxicillin	1.5 ± 3.8	1E−3 ± 3E−3	0.45 ± 1.0	0 ± 1E−3	2E−3 ± 4E−3
Chlortetracycline	145 ± 53	0.11 ± 0.04	93 ± 107	0.07 ± 0.08	0.18 ± 0.11
Florfenicol	1.8 ± 3.1	1E−3 ± 2E−3	1.6 ± 2.5	1E−3 ± 2E−3	3E−3 ± 4E−3
Flumequin	28 ± 17	2.1E−2 ± 1.3E−2	6.1 ± 6.8	5E−3 ± 5E−3	2.6E−2 ± 1.1E−2
Lyncomicin	4.5 ± 1.6	3E−3 ± 1E−3	2.9 ± 3.3	2E−3 ± 3E−3	6E−3 ± 3E−3
Oxytetracycline	212 ± 62	0.16 ± 4.6E−2	97 ± 109	7.3E−2 ± 8.2E−2	0.23 ± 0.1
Sulfadiazine	18 ± 6.6	1.4E−2 ± 5E−3	12 ± 13	9.0E−3 ± 0.01	2.3E−2 ± 1.4E−2
Sulphadimethoxine	58 ± 20	4.4E−2 ± 1.5E−2	35 ± 40	2.6E−2 ± 0.03	0.07 ± 0.04
Sulfamethazine	65 ± 24	4.9E−2 ± 1.8E−2	42 ± 48	3.1E−2 ± 3.6E−2	0.08 ± 0.05
Tylosin	6.6 ± 16	5.0E−3 ± 1.2E−2	2.9 ± 6.1	2E−3 ± 5E−3	7E−3 ± 0.02
Trimethoprim	4.9 ± 1.7	4.0E−3 ± 1.0E−3	3.0 ± 3.5	2E−3 ± 3E−3	6E−3 ± 4E−3
Ivermectin	0.30 ± 0.1	0 ± 0	0.12 ± 0.14	0 ± 0	0 ± 0

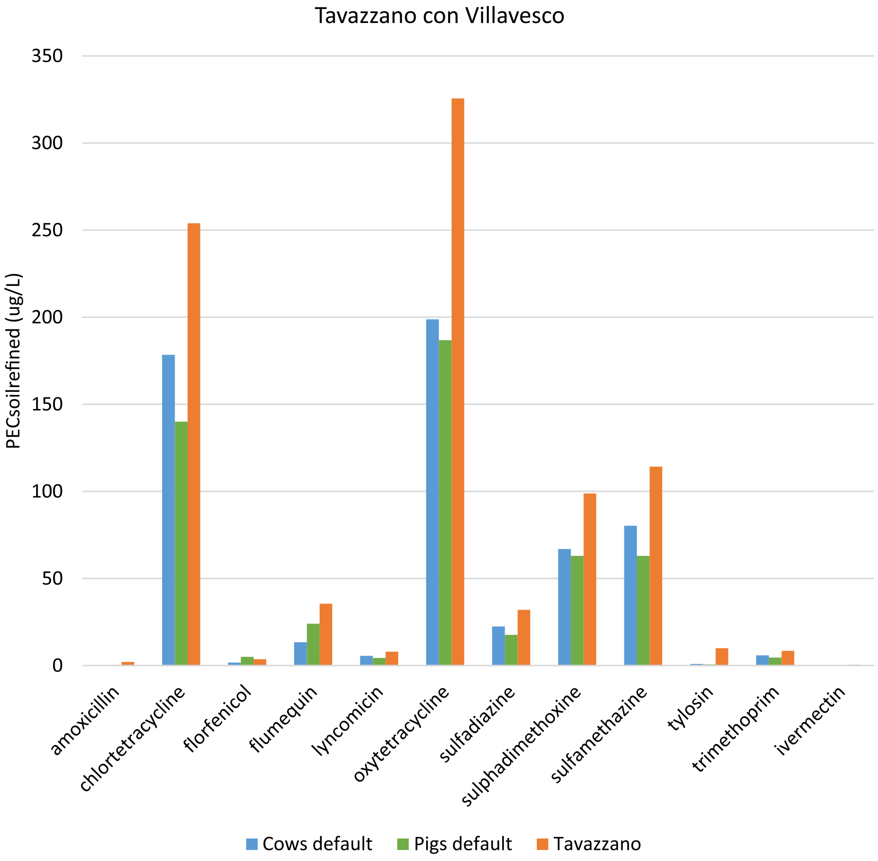

Fig. 3. Comparison between generic case and case study $PEC_{soilrefined}$ (μg/L) calculated for Tavazzano municipality.

and using as input the active ingredient application rates reported above. Results are in Table 6, divided for cows and pigs.

Amoxicillin, chlortetracycline, oxytetracycline, trimethoprim and ivermectin are not leaching compounds in the default scenario (PEC_{gw} are zero μg/L either for cows and pigs manure) either for the rapid degradability in soil (amoxicillin) and the strong sorption (chlortetracycline, ivermectin, oxytetracycline and trimethoprim). PEC_{gw} values of the other a.i. are well below the threshold limit of 0.1 μg/L with the exception of flumequin, where PEC_{gw} from pigs slurry calculated by PEARL is 0.12 μg/L and by PELMO is 0.11 μg/L.

In Table 7, PEC_{gw} values have been transformed in vulnerability classes following rules of Table 3, for direct comparison with results of the case study.

3.2. Territorial case study

Evaluation of $PEC_{soilrefined}$ and PEC_{gw} at a territorial level could give contextualised information about the realistic groundwater contamination and the subsequent vulnerability of an area. To achieve this, evaluations are linked to data availability at territorial level. We extracted from ValorE data referred to farms of the five municipalities, in particular data related to housing facilities (head counts, species and categories of animals, monthly Nitrogen output) and to each farm (agronomic area used, Nitrogen at the field, storage time for dung and slurry). It is useful to note that real data from ValorE depict a situation very far away from default data: for example, the average Nitrogen at the field in each municipality is well above the default value of 170 kg/ha set by CVMP guidelines and in some cases above even to the 340 kg/ha threshold set by EU for spreading in non-vulnerable areas to nitrates (Bellinzago Lombardo, Pieve Fissiraga, Tavazzano con Villavesco). Table 8 reports the average Nitrogen at the field for each month and municipality. Main spreading activities are in spring (March, April and May) and in Autumn (September and October); for January and December data are 0 because national rules do not allow spreading manure in those months.

The main part of farms from the 5 municipalities have only cow livestock, meanwhile the number of pigs outcomes that of cows. Supporting information reports average nitrogen spreading data for each selected farm in Table S2.

3.3. $PEC_{soilrefined}$ calculation

$PEC_{soilrefined}$ have been calculated following the modified version of the second tier of CVMP guidelines and therefore applying Eqs. (1)–(3). $PEC_{soilrefined}$ are calculated for each animal category of each farm taking into account real number of animals for each species and age classes, real monthly Nitrogen loads at the field and farm-specific storage times; $PEC_{soilrefined}$ values are provided separately for dung and slurry, following the data availability in ValorE.

Then, $PEC_{soilrefined}$ are aggregated averaging values from farms in each municipality; as an example, in Table 9 they are reported for each a.i. for the Tavazzano municipality.

From standard deviation data, it could be noted a high variability within the same municipality. Fig. 3 compares average $PEC_{soilrefined}$ values from default data calculation with those obtained in the municipality of Tavazzano.

$PEC_{soilrefined}$ calculated in the case study are generally higher than in generic case; nonetheless, average storage times for farms of the five municipalities are higher than the default parameter (91 days), real case data denote generally higher active ingredient loads due to higher Nitrogen loads at the field. Highest concentrations are in Bellinzago Lombardo and Pieve Fissiraga, which however show in turn the second and third highest load of Nitrogen at the field. Unexpectedly, Tavazzano had limited quantities of active ingredient in spread manure despite it

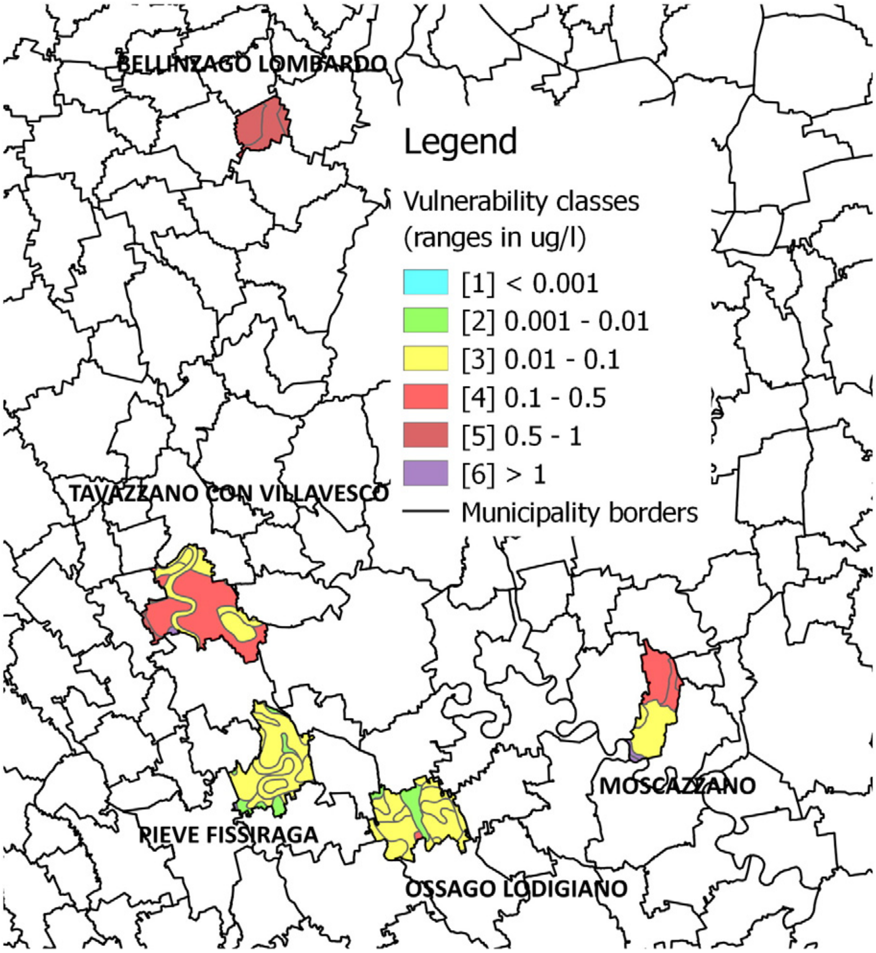

Fig. 4. Vulnerability map to flumequin obtained in VULPES using the PEARL model.

shows the highest value of $PEC_{soilrefined}$, due to the highest annual Nitrogen at the field; this is due to the pattern of N spread among months and the high storage times of farms in that area.

3.4. PEC_{gw} calculation

$PEC_{soilrefined}$ have been transformed into application rates using the agronomic farm area where Nitrogen has been spread; application rates are then used as input for the VULPES system. VULPES results are collected on a vectorial GIS map, where concentration outputs are aggregated into nine classes (see Table 3) according to the potential risk, with the clear characterization of the worst cases (concentration values >0.1 μg/L, corresponding to the regulatory limit for drinking water) in red and violet colours.

As for the generic case, amoxicillin, chlortetracycline, ivermectin, oxytetracycline and trimethoprim do not leach to groundwater due to their physico-chemical properties and were excluded from the analysis.

In Figs. 4 and 5, two vulnerability maps calculated in VULPES with PEARL and PELMO models are presented for flumequin. Maps highlight the leaching behaviour of flumequin in UGUs with different soil structures, even within the same municipality borders, testifying the detailed level of simulations. These maps are the resulting output from the methodology proposed and are intended as a useful tool for risk assessor to identify areas where mitigation or limitation measures are needed to prevent groundwater contamination.

3.5. Comparison between default and territorial cases

In order to compare values of the generic case with those of the case study, values of the UGUs of each municipality have been statistically aggregated using two approaches: a worst case approach using the 95th percentile (see Table S3 in SI) and a standard case using the arithmetic mean (see Table S4 in SI).

Figs. 6 and 7 show vulnerability classes of active ingredients in each municipality compared to the values obtained with the generic case aggregating UGU's values using the 95th percentile for PEARL and PELMO simulations; in Figs. 8 and 9 the aggregation has been done using the arithmetic mean. These figures could be an intuitive method to evaluate the differences between the generic case and the case study simply considering the class jump between them.

Graphs above demonstrate that in almost any case PELMO and PEARL estimates fall into the same vulnerability class, with only one-class differences in two cases of the 95° percentile statistic. This fact demonstrates the reliability of the approach used by the two models and the fact that they are completely interchangeable.

In both statistics, the generic case constantly underestimates the vulnerability classes in comparison with case study applications. The 95th percentile of the generic case is almost always one class below the case study, with the remarkable values of sulfadiazine and sulphamethazine for both the models and sulphadimethoxine for only PELMO, where the generic case is three classes below the Moscazzano municipality application.

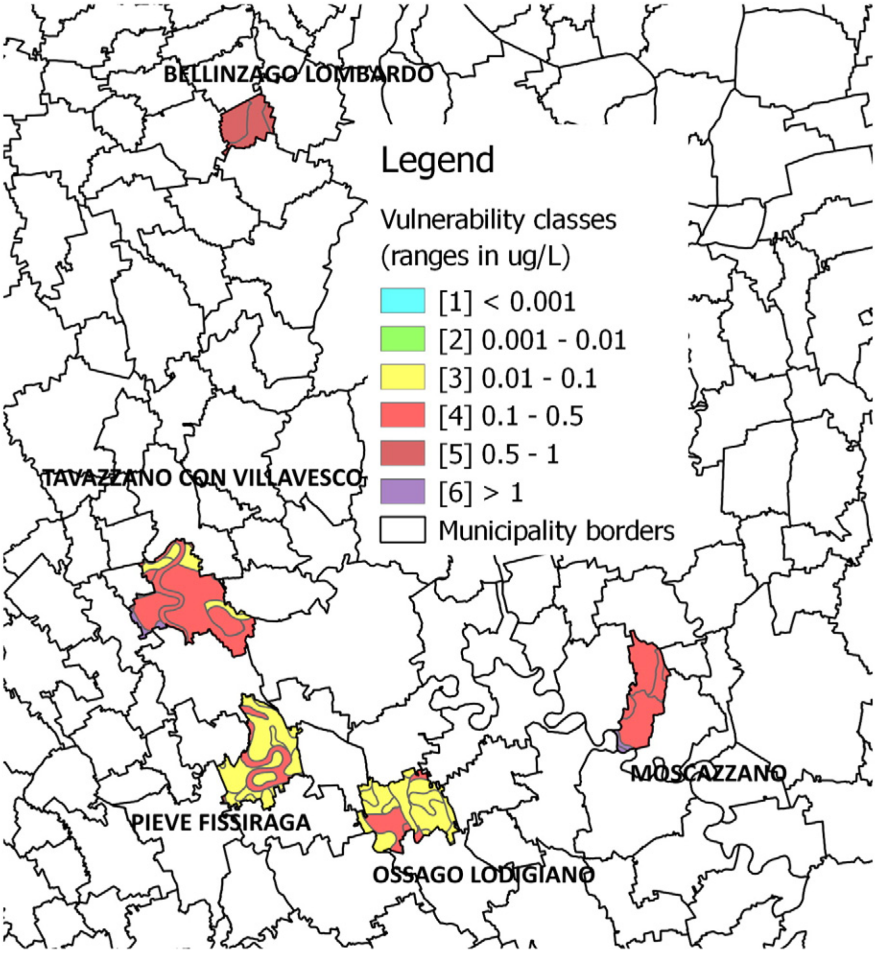

Fig. 5. Vulnerability map to flumequin obtained in VULPES using the PELMO model.

Arithmetic mean values repeat the same pattern, with the generic case underestimating in many cases by one classes the worst municipality application and having sulfadiazine the main difference between the two approaches.

If we consider at risk groundwater which receive values of active ingredients above 0.1 μg/L, i.e. vulnerability classes 4 to 6, we could evaluate in which cases there are differences forecasting dangerous contamination between the generic and territorial cases.

For arithmetic mean statistic, vulnerability class calculated with the generic case approach could not be considered dangerous, being always below the threshold class 4. On the other side, vulnerability classes calculated with the territorial approach reaches class 4 with three active

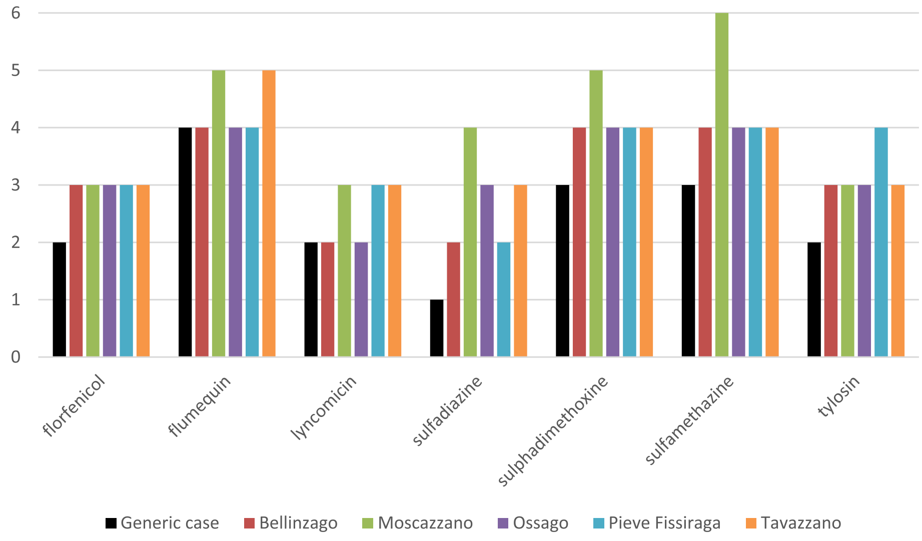

Fig. 6. Vulnerability classes evaluated from 95th percentile of PEC_{gw} values calculated with PEARL model.

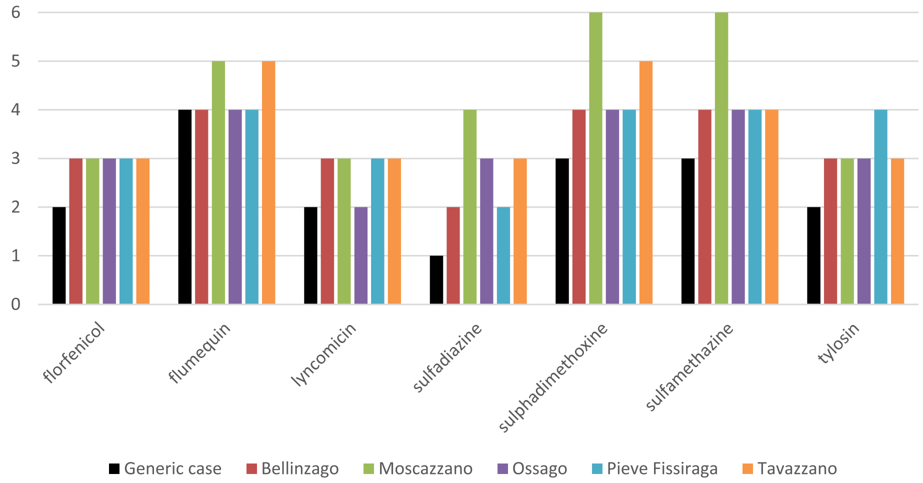

Fig. 7. Vulnerability classes evaluated from 95th percentile of PEC_{gw} values calculated with PELMO model.

ingredients: flumequin in almost all municipalities, sulphadimethoxine in Bellinzago Lombardo, Moscazzano and Pieve Fissiraga, sulphamethazine in Moscazzano (and in Bellinzago Lombardo using the PELMO model).

Results are more markedly different in the 95th percentile statistic aggregation and could be extended to other active ingredients in the panel. Only florfenicol and lyncomicin vulnerability classes fall into non-dangerous values for all the municipalities, here too with an underestimation of the generic approach by one classes in all the municipalities for florfenicol and in Moscazzano, Pieve Fissiraga and Tavazzano for lyncomicin. For flumequin, the generic approach underestimates the vulnerability class in Moscazzano and Tavazzano, where it is one class higher. Main differences could be noted in vulnerability classes of the remaining substances. In particular the generic approach strongly underestimates (3 classes) the worst territorial case for sulfadiazine (3 classes) and for tylosin (2 classes), passing from non-contaminated to contaminated forecast.

As for the arithmetic mean aggregation, sulphadimethoxine and sulfamethazine simulation with the generic approach underestimates contamination (vulnerability class 3, "light contamination"), with the considerable case of Moscazzano municipality where groundwater could reach serious contamination (vulnerability class 6, "extremely contaminated") in at least one UGU.

Considerations set out above show that neither in a standard nor in a worst case logic the generic case could be representative of the groundwater contamination level in comparison with a territorial approach. As explained above, differences are due to the use of realistic manure loads at the field, the environmental conditions of the area and the frequency of distribution of manure during the year. In particular, where the manure is mainly spread in the rainiest months (autumn in our case study), active ingredients are likely to reach the groundwater more than the generic case.

4. Conclusions

Sust-PHarm presented in this work is a pilot experience towards the management at territorial scale of VMPs risk for groundwater. The philosophy underlying the approach is to move from the estimation of the exposure levels in groundwater by running models in predefined environmental scenarios (such as those suggested by the current guidance documents) to site-specific conditions. This is exactly in line with the modern approach for risk management of PPPs and in line with the need of the "sustainable use of veterinary pharmaceuticals". Our approach suggests to link information on typologies of dairy farms, their distribution along the territory, manure management practices (including the spread to land) with predictive models in GIS environment. In this study, we coupled ValorE and VULPES expert systems. The first, together with other information such as quantities of VMPs utilized, metabolic pathways and degradation in manure, allowed us to estimate the potential load of VMPs reaching the soil (kg/ha). The second allowed us

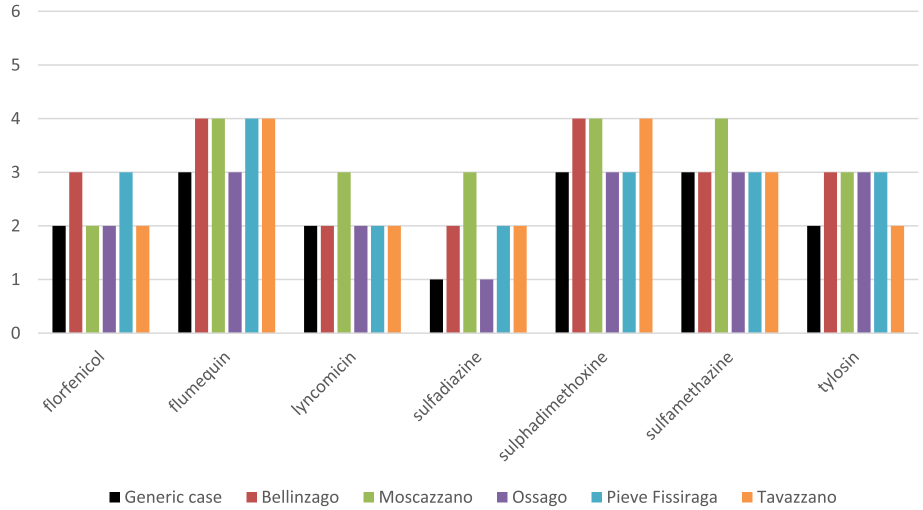

Fig. 8. Vulnerability classes evaluated from arithmetic mean of PEC_{gw} values calculated with PEARL model.

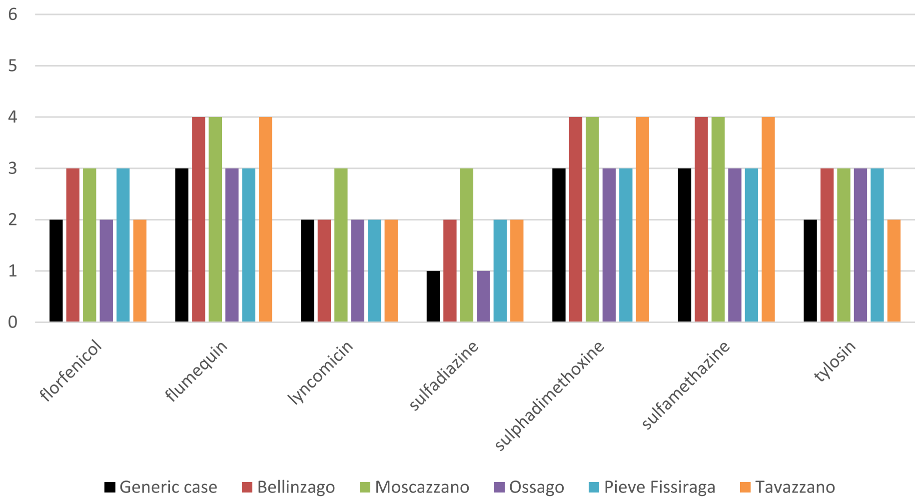

Fig. 9. Vulnerability classes evaluated from arithmetic mean of PEC_{gw} values calculated with PELMO model.

to simulate leaching processes using realistic scenarios (based on the characteristics of the territory) and to identify groundwater areas at risk. However, we would underline that the objective of the work was mostly methodological and that other available tools could be utilized instead of ValorE and VULPES.

The application of Sust-PHarm to 12 VMPs largely utilized in Italy and Lombardia Region clearly highlighted that the generic default scenarios, which are suggested by the current guidelines are not sufficiently protective for groundwater systems of Lombardia Region and this is mainly due to the manure management practices.

Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.scitotenv.2016.09.168.

References

Acutis, M., Alfieri, L., Giussani, A., Provolo, G., Di Guardo, A., Colombini, S., Bertoncini, G., Castelnuovo, M., Sali, G., Moschini, M., Sanna, M., Perego, A., Carozzi, M., Chiodini, M.E., Fumagalli, M., 2014. ValorE: an integrated and GIS-based decision support system for livestock manure management in the Lombardy region (northern Italy). Land Use Policy 41, 149–162.

Ares, J.O., Del Valle, H.F., Olinuck, J.A., 2006. Exploring improved pesticide management in sub-tropical environments with GIS supported fate modeling. Agric. Syst. 91, 189–210.

Ayman, A.A., 2009. Using generic and pesticide DRASTIC GIS-based models for vulnerability assessment of the Quaternary aquiferat Sohag, Egypt. Hydrogeol. J. 17, 1203–1217.

Balderacchi, M., Di Guardo, A., Vischetti, C., Trevisan, M., 2008. The effect of crop rotation on pesticide leaching in a regional pesticide risk assessment. Environ. Sci. Technol. 42, 8000–8006.

Balzer, F., Zühlke, S., Hannappe, S., 2016. Antibiotics in groundwater under locations with high livestock density in Germany. Water Sci. Technol. http://dx.doi.org/10.2166/ws.2016.050 Avail. online 19 April 2016, ws2016050.

Benotti, M.J., Trenholm, R.A., Vanderford, B.J., Holady, J.C., Stanford, B.D., Snyder, S.A., 2009. Pharmaceuticals and endocrine disrupting compounds in U.S. drinking water. Environ. Sci. Technol. 43 (3), 597–603.

Boxall, A., Fogg, L., Baird, D., Telfer, T., Lewis, C., Gravell, A., Boucard, T., 2006. Targeted Monitoring Study for Veterinary Medicines. Environment Agency, R&D Technical Report, Bristol (UK) 73 pp.

Boxall, A.B., Fogg, L.A., Blackwell, P.A., Blackwell, P., Kay, P., Pemberton, E.J., Croxford, A., 2004. Veterinary Medicines in the Environment. In: Whitacre, D.M. (Ed.), Reviews of Environmental Contamination and Toxicology. Springer, New York, pp. 1–91.

Boxall, A.B., Kolpin, D.W., Halling-Sørensen, B., Tolls, J., 2003. Peer reviewed: are veterinary medicines causing environmental risks? Environ. Sci. Technol. 37 (15), 286A–294A.

Copernicus, 2016. Corine land cover 2012. http://land.copernicus.eu/pan-european/corine-land-cover/clc-2012 last accessed on June 2016.

Crane, M., Boxall, A.B.A., Barrett, K., 2008. In: Crane, M., Boxall, A.B.A., Barret, K. (Eds.), Veterinary Medicines in the Environment. Taylor & Francis/CRC Press, Boca Raton, FL, USA/London, UK, p. 224.

CVMP, 2008. Environmental Impact Assessment for Veterinary Medicinal Products in Support of the VICH Guidelines GL6 and GL38. European Medicines Agency, London. EMEA/CVMP/418282/2005-Rev.1.

CVMP/VICH, 2000. CVMP/VICH Topic GL6 (Ecotoxicity Phase I). Guideline on Environmental Impact Assessment (EIAs) for Veterinary Medicinal Products - Phase I. European Medicines Agency, London. CVMP/VICH/592/98-FINAL.

CVMP/VICH, 2005. CVMP/VICH Topic GL38. Guideline on Environmental Impact Assessment for Veterinary Medicinal Products - Phase II. European Medicines Agency, London. CVMP/VICH/790/03-FINAL.

Di Guardo, A., Finizio, A., 2015. A client–server software for the identification of groundwater vulnerability to pesticides at regional level. Sci. Total Environ. 530–531, 247–256.

Di Guardo, A., Finizio, A., 2016. A moni-modelling approach to manage groundwater risk to pesticide leaching at regional scale. Sci. Total Environ. 545, 200–209.

ERSAF, 2016. Carta dei suoli in scala 1:50,000. http://www.ersaf.lombardia.it/servizi/Menu/dinamica.aspx?idSezione=16908&idArea=16915&idCat=17256&ID=28392 last accessed on June 2016.

ESVAC, 2015. Sales of Veterinary Antimicrobial Agents in 26 EU/EEA Countries in 2013, Fifth ESVAC Report. EMA/387934/2015.

European Commission, 2001. Directive 2001/82/EC of the European Parliament and of the Council of 6 November 2001 on the Community code relating to veterinary medicinal products. OJ L 311, 1–66 28.11.2001.

European Commission, 2009. Directive 2009/128/EC of the European Parliament and of the Council of 21 October 2009 establishing a framework for Community action to achieve the sustainable use of pesticides. OJ L 309, 71–86 24.11.2009.

European Commission, 2016. FADN, farm accountancy data network. http://ec.europa.eu/agriculture/rica/database/index_en.cfm last accessed on June 2016.

Farré M., Ferrer I., Ginebreda A., Figueras M., Olivella l., Tirapuc L., Vilanovac M., Barceló D., 2001. Determination of drugs in surface water and wastewater samples by liquid chromatography–mass spectrometry: methods and preliminary results including toxicity studies with *Vibrio fischeri*. J. Chromatogr. A 938, 187–197. DOI: http://dx.doi.org/10.1016/S0021-9673(01)01154-2;

FOCUS Groundwater Scenarios Workgroup, 2000. FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup 2000. EC Document Reference Sanco/321/2000 Rev.2, Pp. 1–202.

FOCUS Groundwater Workgroup, 2009. Assessing potential for movement of active substances and their metabolites to ground water in the EU. Report of the FOCUS Ground WaterWork Group. EC Document Reference Sanco/13144/2010 Version 1, Pp. 1–604.

García-Galán, M.J., Díaz-Cruz, M.S., Barceló, D., 2010. Determination of 19 sulfonamides in environmental water samples by automated on-line solid-phase extraction-liquid chromatography tandem mass spectrometry (SPE-LC-MS/MS). Talanta 81 (1–2), 355–366. http://dx.doi.org/10.1016/j.talanta.2009.12.009.

Halling-Sørensen, B., Jensen, J., Tjørnelund, J., Montforts, M.H.M.M., 2001. Worst-case estimations of predicted environmental soil concentrations (PEC) of selected veterinary antibiotics and residues used in Danish agriculture. In: Kummerer, K. (Ed.), Pharmaceuticals in the Environment. Springer, Berlin Heidelberg, pp. 143–157.

Holman, I.P., Dubus, I.G., Hollis, J.M., 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 (1–3), 73–88.

Huerta-Fontela, M., Galceran, M.T., Ventura, F., 2011. Occurrence and removal of pharmaceuticals and hormones through drinking water treatment. Water Res. 45, 1432–1442.

Jarvis, N.J., 1991. MACRO - a Model of Water Movement and Solute Transport in Macroporous Soils Reps. and Diss., 9 Dept. Soil Sci., Swedish Univ. of Agr. Sci, Uppsala, p. 58.

Klein, M., 2000. PELMO: Pesticide Leaching Model, User Manual Version 3.0.2. Fraunhofer-Institut für Umweltchemie und Ökotoxikogie.

Lewis, K., Tzilivakis, J., Green, A., Warner, D., 2011. Veterinary Substances DataBase (VSDB). http://sitem.herts.ac.uk/aeru/vsdb/ last accessed on June 2016.

Ma, Y., Li, M., Wu, M., Li, Z., Liu, X., 2015. Occurrences and regional distributions of 20 antibiotics in water bodies during groundwater recharge. Sci. Total Environ. 518–519 (15), 498–506.

Ministero della salute, 2016. Prontuario dei medicinali veterinari. https://www.vetinfo.sanita.it/j6_prontuario/public/ last accessed on June 2016.

Pence, H.E., Williams, A., 2010. ChemSpider: an online chemical information resource. J. Chem. Educ. 87 (11), 1123–1124.

Tiktak, A., De Nie, D.S., Van der Linden, A.M.A., Kruijne, R., 2002. Modelling the leaching and drainage of pesticides in the Netherlands: the GeoPEARL model. Agronomie 22, 373–387.

Tiktak, A., van den Berg, F., Boesten, J.J.T.I., Leistra, M., van der Linden, A.M.A., van Kraalingen, D., 2000. Pesticide Emission Assessment at Regional and Local Scales: User Manual of FOCUS Pearl Version 1.1.1. RIVM Report 711401008Alterra Report 28. RIVM, Bilthoven, p. 142.

Wexler, P., 2001. TOXNET: an evolving web resource for toxicology and environmental health information. Toxicology 157 (1), 3–10.

Wilson, J.P., Inskeep, W.P., Rubright, P.R., Cooksey, D., Jacobsen, J.S., Snyder, R.D., 1993. Coupling geographic information systems and models for weed control and groundwater protection. Weed Technol. 7, 255–264.

Wishart, D.S., Knox, C., Guo, A.C., Cheng, D., Shrivastava, S., Tzur, D., Gautam, B., Hassanali, M., 2008. DrugBank: a knowledgebase for drugs, drug actions and drug targets. Nucleic Acids Res. 36-1, 901–906.

Worrall, F., Besien, T., Kolpin, D.W., 2002. Groundwater vulnerability: interactions of chemical and site properties. Sci. Total Environ. 299, 131–143.

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A novel fuzzy expert system to assess the sustainability of the viticulture at the wine-estate scale

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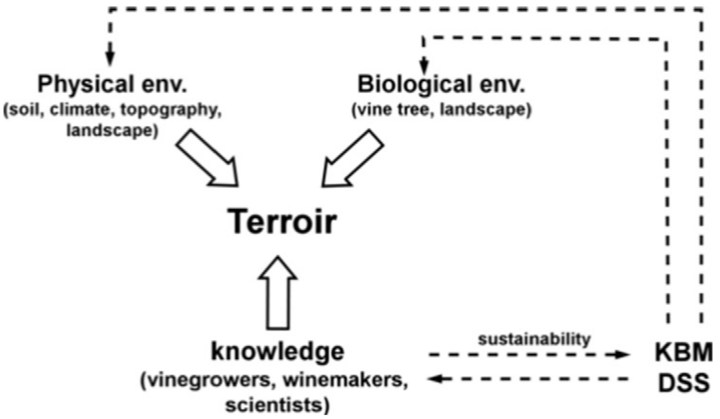
HIGHLIGHTS

- A new multidimensional indicator has been developed to evaluate the sustainability of management options adopted at vineyard scale.
- The indicator considers the main agronomic aspects, related by a hierarchical fuzzy logic and implemented in web GIS software.
- A cross validation approach has been performed on four different wineries.
- Soil and fertility management are the main issues concerning sustainability in viticulture.

GRAPHICAL ABSTRACT



Role of Knowledge Based Model (KBM)/Decision Support System (DSS) like "Vigneto" in the transfer of the sustainability science.

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ABSTRACT

The wine industry is definitely committed in sustainability: the stakeholders' interest for the topic is constantly growing and a wide number of sustainability programs have been launched in recent years. Most of these programs are focusing on the environmental aspects as environmental sustainability indicators, greenhouse gases emissions and the use of Life Cycle Assessment methodology. Among the environmental indicators the carbon and the water footprint are often used. These indicators, while being useful to assess the sustainability performance of the winegrowing farms, do not take into account important aspects related to the agronomic management of the vineyard. To fill this gap a new indicator called "Vigneto" (Vineyard in Italian language) has been developed. "Vigneto" is a multidimensional indicator to evaluate the sustainability of management options adopted at field scale. It considers the main agronomic aspects, which can have an impact on the environment. These include (i) pest management, (ii) soil management (erosion and compaction), (iii) fertility management (soil organic matter management and fertilizer application), (iv) biodiversity management. Those aspects have been related by fuzzy logics and implemented in web GIS software. The application of the model allows obtaining a general judgment of the agronomic sustainability of the vineyard management: the judgment varies from "A" (excellent) to "E" (completely unsustainable). The produced model was validated and tested by four Italian wine estate. The model output reports that the tested wineries have different management strategies: producers

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manage vineyards in different ways, depending on the different geographical position. The main differences are related to the soil management and to the presence of natural areas different from vineyard.
The developed model can be defined as an environmental decision support system that can be used by wine companies' technicians to define the vineyard practices sustainability performance and support them in the definition of more sustainable management practices.

1. Introduction

Sustainable agriculture could be defined as a set of agronomic practices that are economically viable, environmentally safe, and socially acceptable with the aim to create a system that is capable of persisting preserving the same characteristics. In 2004, OIV (Organization Internationale de la Vigne et du Vin, OIV, 2004), defined sustainability as a “global strategy on the scale of the grape production and processing systems, incorporating at the same time the economic sustainability of structures and territories, producing quality products, considering requirements of precision in sustainable viticulture, risks to the environment, products safety and consumer health and valuing of heritage, historical, cultural, ecological and aesthetic aspects”. This definition emphasizes the relationship between the sustainability and the “terroir” concept (OIV, 2010). The “terroir viticole” is as an area in which collective knowledge of the interactions between the identifiable physical and biological environment and applied vitivinicultural practices have been developed, providing distinctive characteristics for the products originating from this area. “Terroir” includes specific soil, topography, climate, landscape characteristics, biodiversity features and common knowledge and this concept is strictly linked to the definition of the protected designations of origin and to their promotion. Therefore, “terroir” and sustainability are strongly related concepts.

Presently different wines which have “sustainability-sounding” names and adjectives (such as sustainable, organic, natural, free, eco-friendly) are offered to the consumer and a large number of different strategies, guidelines and practices are available (Corbo et al., 2014, Santiago-Brown et al., 2014). From the consumers point of view the term sustainability is mainly associated with the environmental dimension and in some cases only with the carbon footprint (Szolnoki, 2013). From the corporate perspective sustainability is subjectively interpreted and the existing programs cover more or less completely the sustainability areas. Sustainability being based on three generic pillars (environment, society and economy) is difficult to measure and the risk of drifts and commodification of its principles are present (Parr, 2009). Strategies for measuring the sustainability in an objective manner are necessary for limit the use of sustainability as mere marketing leverage. The introduction of sustainability indicators and direct measures, such as field experiments, although being time-consuming and not always completely understood by all the stakeholders are required to analyze complex systems. Most sustainability approaches focus only on pesticide impact, carbon emissions or water use. In fact several works are present in the literature focused on the carbon and water footprint of the Italian wines (Bonamente et al., 2015, 2016). Organic carbon, potentially mineralizable nitrogen, and microbial biomass are the most important among soil indicators (Cardoso et al., 2013; Riches et al., 2013), whereas biodiversity indicators are often related only to species richness (Büchs, 2003).

The aim of this work is to develop a multidimensional (space and time) indicator to evaluate the sustainability of management options adopted at field scale. “Vigneto” indicator is an indicator which considers the main agronomic practices which have an impact on the environment. These include (i) pest management, (ii) soil management (erosion and compaction), (iii) fertility management (soil organic matter management and fertilizer application), (iv) biodiversity management.

The paper details a fuzzy expert system connected to web GIS software, which is a useful instrument for measuring the environmental impact of viticulture in a holistic way. The easy-to-use software could be used by farmers and other decision makers to perform a sustainability assessment at vineyard scale, and help to improve their performance, adopting effective measures to improve the sustainability of the wine estate.

“Vigneto” was developed in the framework of the “V.I.V.A. sustainable wine” project, launched in 2011 by the Italian Ministry for the Environment, Land and Sea. The final output of the project is a sustainability label that signals to the consumers the sustainability attributes of the products and provides easily interpretable information about four selected indicators. The wine label shows the V.I.V.A. logo and through a QR code it is possible to consult the results obtained in the four selected indicators: in addition to “vigneto” the other indicators are “Aria” (Carbon Footprint), “Acqua” (Water Footprint, Lamastra et al., 2014), and “Territorio” (a selection of quality indicators to evaluate the socio-economic aspects of sustainability).

2. Material and methods

“Vigneto” indicator has been developed following agronomist expertise rules instead of implementing complex mathematical models The model temporal scale was set to the agricultural year (from pruning to harvest), the model spatial scale was set to the farm and the modeling boundary was the exit of the grape from the vineyard. “Vigneto” is based on six sub-indicators with different spatial scales: five of them are field scale indicators (pest management, fertilization management, soil organic matter, and soil compaction and soil erosion indicators) and one of them is working as a farm scale indicator (landscape quality indicator). The development of the six indicators (Table 1; Fig. 1) was based on validated models available in the literature (Table 1), new indicators were developed for soil erosion, soil compaction and landscape quality due to the lack of simple indicators required by the definition of the fuzzy index (Wieland and Gutzler, 2014).

In the indicator “Vigneto” sustainability was modeled by a logic-based knowledge-based model (KMB) where knowledge is encoded into a database. An inference engine uses logic to infer conclusions and the models are expressed as a series of facts formalized according a logic system. KBM requires that the knowledge is elicited from viticulture and sustainability experts and encoded in facts and rules that can be used to explain the deductions based on chains of rules application (Kelly et al., 2013). The integration of experts and stakeholders' knowledge into the impact assessment process was reached by fuzzy simulation of environmental systems (Wieland and Gutzler, 2014). The elicitation process (Page et al., 2012) started with the development of the idea and required the determination of the processes and of the impacts of agricultural practices on environmental compartments defined by stakeholders. The final output of the elicitation process was a single indicator made from six separate sub indicators related by two levels of fuzzy logic (Fig. 1). The indicators are initially calculated at the field scale and after adjusted to the wine estate scale giving the wine-estate judgment (Fig. 2). An intermediate level called “product” was developed responding to the need of the certification procedure. In fact, a producer can ask to certificate only one or few labels of his product

Table 1
Indicators used and their goals.

Indicator	Source	Environmental compartments (and processes)	Goal
Pest management indicator (PMI)	PDMI of EPRIP (Balderacchi and Trevisan, 2010; Padovani et al., 2004; Trevisan et al., 2009)	Water (pollution of surface water by runoff and drift and of groundwater by leaching) Air (pollution), Soil (pollution), Living organisms (loss of biodiversity) Society (safe water, not polluted environment)	Reduction of the environmental risks related to the pesticide use
Fertilization management indicator (FMI)	FMI of EIOVI (Fragoulis et al., 2009)	Water (release of nutrients into the environment, pollution of surface and groundwater) Living organisms (change in biodiversity) Society (pure water)	Reduction of the environmental impact of fertilizer evaluating the nutrients supply by the fertilizer compared with the vineyard need.
Soil organic matter indicator (SOMI)	I_{om} (Bockstaller et al., 1997; Fragoulis et al., 2009)	Soil (quality) Living organisms (change in biodiversity)	Maintenance of a satisfactory level of soil organic matter evaluating how the management practices have an effect on the soil organic matter level.
Soil compaction indicator (SCI)	New indicator	Soil (quality) Living organisms (change in biodiversity) Society (security)	Restraint of the soil compaction evaluating the effect of the rain, of machinery use, and of soil susceptibility on the soil structure.
Soil erosion indicator (SEI)	New indicator	Water (quality) Soil (quality) Living organisms (change in biodiversity) Society (security)	Prevention of soil erosion assessing how the soil management can affect it.
Landscape quality indicator (LQI)	New indicator	Living organisms (biodiversity quality) Society (tourist exploitation and quality of life)	Maintenance of a quality landscape to ensure an ecosystem rich in biodiversity and a tourist exploitation of the rural areas.

range. At the product level, only the vineyards that are involved in the production of a certain label are evaluated.

EIOVI (Environmental Impact of Organic Viticulture Indicator; Fragoulis et al., 2009) was used as substrate for developing the novel model. EIOVI is a fuzzy field-scale indicator developed for organic viticulture, based on six modules (pest and disease management, fertilization management, water management, soil management, soil organic matter management and biodiversity evaluation). The introduction of new dimensions in the EIOVI model has resulted in an increase in the model complexity: a new definition of the indicators and of the inputs required by the new model was required. The information provided by the six identified indicators output were fuzzified, transforming indicator output values in degree of belonging to the sustainability set by a membership degree, based on S shaped membership functions where alpha (α, sustainability fully reached) and gamma values (γ, unacceptable condition) are the border cases (Zadeh, 1965). The value 0.0 represents the fully sustainable belonging, and 1.0 represent the unsatisfactory case, based on the stakeholder request (Fig. 3). The different sustainability sets were aggregated by a hierarchical-structure-based algorithm and a final judgment was calculated.

2.1. Pest management indicator (PMI)

The adopted indicator is EPRIP (Indicator of Potential Environmental Risk for Pesticides; Balderacchi and Trevisan, 2010; Padovani et al., 2004; Trevisan et al., 2009). It is based on the Exposure Toxicity Ratio (ETR), the ratio between a predicted environmental concentration (PEC) and a toxicological end point. The PECs are estimated in four environmental compartments (surface water, groundwater, soil, and air) following the EPRIP methodology and the toxicological end points are selected as follows. Short-term toxicity is the selected parameter for different reference organisms: for surface water, *Daphnia magna*, fish, and algae have been selected as representative non target organisms; for the soil compartment, the earthworm is used. EC50 for the rat (inhalation)

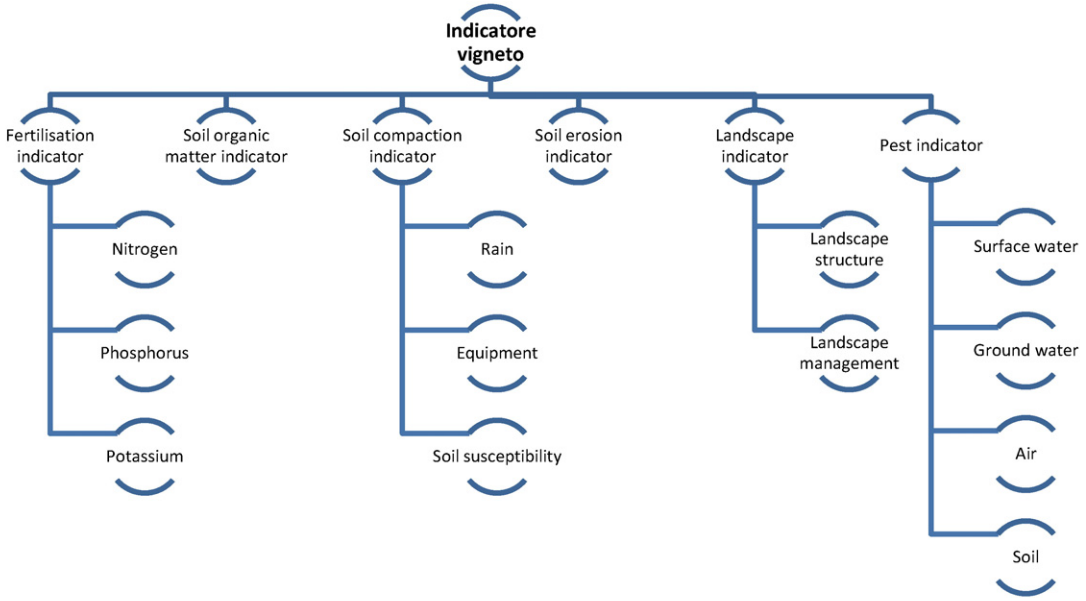

Fig. 1. Hierarchical structure of "Indicatore Vigneto".

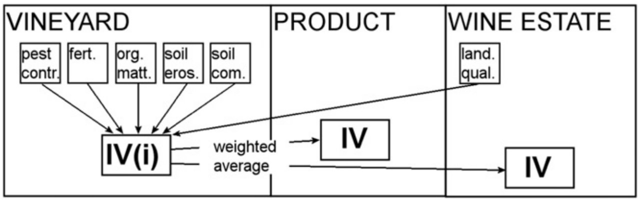

Fig. 2. Scales of the "Vigneto" indicator (IV).

is considered as threshold values for the air compartment. The toxicological endpoint for the groundwater compartment is equivalent to the legal limit for the active substances in the groundwater ($\mu g\ L^{-1}$). ETR is converted into risk points (RP) using a numerical scale (from 1 to 5) to estimate the probability of exceeding a trigger score. The trigger score was set equal to 2 for sensitive areas, such as houses, wells or wineries and 4 for the other areas. The probability of not exceeding the trigger score is calculated assuming a Poisson cumulative function. α and γ values were attributed considering the probability of not exceeding the selected trigger score: the probability of not exceeding the trigger score (4 or 2) in 10% of cases was set as fully sustainable (α value), while the probability of not exceeding the trigger score (4 or 2) in 90% of cases was set as fully unsustainable (γ value).

2.2. Fertilization management indicator (FMI)

The model uses the fertilization component of the EIOVI model (Fragoulis et al., 2009) where a balance sheet of the nutrients is carried out. This consists of three sub indicators that take into account the impact of the three main macronutrients: nitrogen (N; indicator compost or fertilizer nitrogen indicator CMFNI), phosphorus (P; compost or fertilizer phosphorus indicator CMFPI) and potassium (K; compost or fertilizer potassium indicator CMFKI).

2.2.1. CMFNI

The total available nitrogen (NAT) component considers the nitrogen input from mineral fertilizer (available nitrogen from mineral fertilizer; NAF) and organic fertilization (available nitrogen from organic manure; NA).

$$NAT = NAF + NA \tag{1}$$

Where:

$NAF = 0.01 * X * FUR * 0.8$

FUR = *amount of fertilizer* [$kg\ ha^{-1}$]

X: *fertilizer nitrogen content* [%]

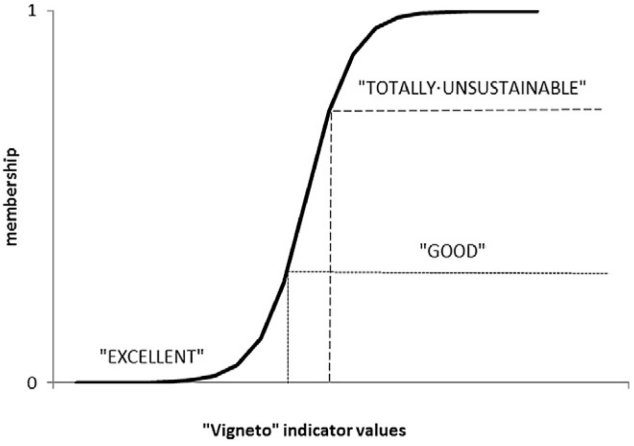

Fig. 3. Sigmoidal function is appropriate for representing concepts like the different degree of membership to the "totally unsustainable"set.

$$NA = \sum_{a=0}^{-4} 0.01 \times 1000 \times CUR_a \times N_a \times NAC_a \tag{2}$$

Where:

CUR = *amount of manure* [$t\ ha^{-1}$]

N = *manure nitrogen content* [%]

NAC = *Nitrogen availability content* (Table 2)

a = *application year* [0 = *actual year*]

2.2.2. CMFPI

The total available phosphorous (PAT, $kg\ ha^{-1}$) is the sum of the available phosphorous from organic fertilizer (PA) and from mineral fertilizers (PAF):

$$PAT = PAF + PA \tag{3}$$

Where:

$$PAF = 0.01 \times y \times FUR \times 0.8$$

Y = *phosphorous fertilizer content (as* P_2O_5*)* [%]

$$PA = 3.5 \times CUR \times P$$

P = *phosphorous manure content (as* P_2O_5*)* [%]

2.2.3. CMFKI

The total available potassium (KAT, $kg\ ha^{-1}$) is the sum of the potassium coming from manure (KA) and of the potassium from mineral fertilizers (KAF)

$$KAT = KAF + KA \tag{4}$$

Where:

$$KAF = 0.01 \times z \times FUR$$

z = *potassium fertilizer content (as* K_2O*)* [%]

$$KA = 7.5 \times CUR \times K$$

K = *potassium manure content (as* K_2O*)* [%]

The three sub indicators have been combined into the fertilization indicator giving 50% of the relative weight to the CMFNI indicator and 25% to the others two indicators (CMFKI, CMFPI). α and γ values were calculated considering plant and cover crops uptake.

For the all indicators α has been set equal to the minimum nitrogen/phosphorus/potassium demand by fertilizer (NDF_{min}, PDF_{min}, KDF_{min}), and γ twice the difference between the maximum nitrogen phosphorus/potassium demand by fertilizer (NDF_{max}, PDF_{max}, KDF_{max}) and the minimum nitrogen/phosphorus/potassium demand by fertilizer (NDF_{min}, PDF_{min}, KDF_{min}) (more information in the supplementary data).

Table 2
Nitrogen availability content based on C/N ratio.

C/N	NAC (if a = 0)	NAC (if a ≠ 0)
<10	0.5	0.05
10–15	0.25	0.1
16–20	0.1	0.1
21–25	0.05	0.1
>25	0	0.05

2.3. Soil organic matter indicator (SOMI)

The indicator assesses the effect of the management practices on the evolution of soil organic matter and it is based on the indicator I_{om} (Bockstaller et al., 1997) also implemented in the EIOVI model (Fragoulis et al., 2009). Its calculation is based on the comparison between the organic matter input from compost and cover crops residues with the recommended levels of input for the vineyard. The recommended levels of organic matter input for vineyards are the levels of inputs that are expected to maintain a satisfactory level of soil organic matter in the long term and are function of the clay and loam content of the soil. The α and γ values are calculated in order to promote conservative soil management in which the presence of grass and the distribution of organic matter in the vineyard are rewarded. The α value has been set equal to 0.6 and γ has been set equal to 1.6: in fact, the supply of more organic matter than recommended has been set as fully sustainable, where the supply of 60% less than recommended has been set as unsustainable.

2.4. Soil compaction indicator (SCI)

Soil compaction is one of the main processes that obliges the farmer to restore optimal hydrogeological conditions. A large number of factors promote or prevent the compaction of soil; therefore three sub-indicators were developed and combined: (1) the action of rain, (2) the passing of farming equipment, and (3) the evaluation of soil features. Greater importance was given to soil susceptibility, according the findings Horn and Fleige (2003). This approach informs the farmer about the importance of the process. The relative weight of the three compaction sub indicators is indicated in the following table (Table 3).

Table 3
Relative weight of three compaction sub indicators.

Indicator	Relative weight
Rain Indicator (RI)	0.10
Farm Equipment indicator (FEI)	0.30
Soil Susceptibility indicator (SSI)	0.60

2.4.1. RI

The mechanical action of rainfall promotes soil compaction while soil cover crops or roof trilling systems have a protection function. The indicator rain (RI) is calculated as:

$$RI = \sum_{1}^{12} (P \times (1 - SC)) \tag{5}$$

Where:

P = average monthly rainfall [mm]

SC = degree of soil cover [−] In the presence of grass the value is: 0.67, in presence of "tendone" or "pergola" trilling system the value is function of the phenological stage expressed in terms of BBCH-scale (BBCH, 2001) as reported in the (Table 4).

Table 4
Soil coverage factor (SC) and BBCH code.

BBCH code	SC
0–10	0.2
11–64	0.3
65–94	0.8
94–99	0.6

α has been set equal to 250 and γ to 800, to reward the soil management practices that intercept rainfall such as the presence of cover crops or roof trilling systems.

2.4.2. FEI

Farming equipment frequently passes over the same vine rows causing localized soil compaction. The indicator is calculated as:

$$FEI = \sum_{t=1}^{m} \sum_{e=1}^{n} (W/A_t) \tag{6}$$

Where*:*

W: weight of the machine [Mg]

A_t: contact area of the wheel / track [m^2]

e: number of journeys per year

t: type of farming equipment

α has been set equal to 30,000 and γ to 500,000 with the aim to reduce the passages on the vineyard and to promote the use of track tractors.

2.4.3. SSI

The soil susceptibility indicator is based on the equations developed by Horn and Fleige (2003) which focuses on the soil pre-compression stress considered as the limit at which soil has an elastic deformation and there are no changes in its porosity and functions. This indicator is depending on the physical and hydrological characteristics and on the organic matter content of the soil. Horn and Fleige (2003) developed a series of "pedotransfer" functions for estimating the pre-compression stress (P_v) at different soil water tensions (pF 1.8 and 2.5), starting from the soil texture, classified according the German nomenclature. The model uses values for pF 2.5, and corrects them taking into account the amount of soil skeleton. The available water content, wilting point, air capacity and water speed at the saturation level were estimated according Saxton and Rawls (2006). The internal friction angle (Gamma) was adapted from literature data (Geotechdata.info, 2013) and the cohesion (C) was adapted from EUROSEM (Baets et al., 2008; Morgan et al., 1998; Supplementary data).

$$SSI = Pv_{2.5} \tag{7}$$

α has been set equal to 30 and γ to 90, according to the Horn and Fleige (2003) pedotransfer function. Pedotansfer functions are reported in the supplementary data.

2.5. Soil Erosion indicator (SEI)

Soil erosion is a major problem in vineyards, especially on slopes, and a large part of Italian viticulture is carried out on hills or low mountains. The erosion indicator is based on the "C" coefficient (Table 5) of the RUSLE indicator (Renard et al., 1997). In fact "C" is the cover-management factor and could be easily used to reflect the effect of cropping and management practices on erosion rates. The other factors of the RUSLE equation are more related to the specific soil features than to the management options. The α and γ values vary from 0.22 corresponding to a perennial cover crop on the 100% of the vineyard surface to 0.39 corresponding to a completely worked soil between rows.

$$SEI = 0.22 \times \text{Grass} + 0.31 \times \text{WinterCoverage} + 0.39 \times \text{Tillage} \tag{8}$$

Where*:*

Grass: % row with grass [−]

Winter Coverage: % row with winter cover [−]

Tilled: % row tilled [−]

Table 5
C values according Wall and Cereal, 2002.

Soil management	C
Cultivated between rows (γ value)	0.39
Winter cover	0.31
Grassing (α value)	0.22

2.6. Landscape quality indicator (LQI)

Usually biodiversity assessment within a vineyard is based on two main factors: (1) the number of species present and (2) the uniformity of their distribution (Cluzeau et al., 2012; Gerlach et al., 2013; Košulič et al., 2014; Trivellone et al., 2014). The evaluation of sustainability at vine estate scale makes the assessment of biodiversity based on the accounting of species practically impossible; therefore the biodiversity indicator was linked to the landscape quality. Several indicators are related to agro-environmental aspects and are useful to evaluate biodiversity and landscape in terms of crop prevalence, crop allocation and field size at farm or regional scale (Bockstaller and Girardin, 2008; Acutis et al., 2014). Anyway, the use of structural indicators is not recommended as wine estate have a landscape composed mainly of vineyards. A similar approach has been followed to develop a novel indicator, taking into account the presence of areas with natural vegetation, the landscape heterogeneity and the conservation efforts made to maintain the farm landscape. The indicator is based on two sub-indicators: (1) landscape structure and (2) landscape management. Both have the same relative weight in the formation of the landscape quality indicator.

2.6.1. Landscape structure indicator (LS)

The developed indicator is based on the following assumptions: (1) natural areas have the highest quality in terms of landscape, (2) agricultural areas can be considered quality areas only if there is crop diversification (3) the artificial areas have no quality in terms of landscape. Natural, agricultural and artificial areas have been defined following CORINE land cover nomenclature (European Environment Agency, 2007). The farmer should devote at least the 5% of the farm surface to the natural areas, while full sustainability is reached when at least the 15% of the farm surface is represented by a natural area: α is set to 0.62 and γ to 0.79.

$$LS = 1 - \left(\frac{Ag}{Ar + Ag + Vit + An} + \sqrt{\frac{An}{Ar + Ag + Vit + An}} - \frac{Ar}{Ar + Ag + Vit + An} \right) \tag{9}$$

Where:
Ar: artificial areas [ha]
Ag: agricultural area not vineyard [ha]
Vit: vineyard area [ha]
An: natural areas [ha]

2.6.2. Landscape structure management

This indicator considers the effort of the producer to maintain the farm landscape and rewards it if in the farm management does not outsource. At least 5% of the working time of the farm employees should be dedicated to the maintenance of the natural areas: alpha is set to 0.85 and γ to 0.95.

$$LM = 1 - \frac{HIA + 0.75 \times HEA}{HIV + 0.75 \times HEV} \tag{10}$$

Where:

HIV: hours directly used in the production of grape and worked by staff partner or employees [h].

HIA: hours spent in the maintenance of accessory vineyard areas and agricultural areas worked by staff members or employees [h].

HEV: hours directly used in the production of grape and worked by staff outside the company [h].

HEA: hours spent in the maintenance of accessory vineyard areas and agricultural areas and staff outside the company [h].

Table 6
Relative weight of the modules given for the creation of the final judgments.

Module	Relative weight
PMI	0.2
FMI	0.15
SOMI	0.2
SCI	0.2
SEI	0.1
LQI	0.15

2.7. Fuzzification and defuzzification

The Sugeno's inference method (Sugeno, 1985) was used to aggregate the indicators and the aggregation process was achieved by combining weighted fuzzy values (Bellocchi et al., 2002; Fragoulis et al., 2009). This indicator, being an expert system, requires knowledge from different fields (Krueger et al., 2012; Page et al., 2012); therefore expert opinion was used to define the relative weight of each module (Table 6).

The final indicator was defuzzified into judgments according an A–E scale (Table 7). Values were classified considering simulations carried out on hypothetical cases. The reported best performances are when the indicator is below 0.3.

2.8. The software

The software for the “Vigneto” indicator is a client-server system based on a web platform, which make use of an advanced web GIS component. The usability, the widespread use of GIS cartography and the logical subdivision of farm data based on the update frequency make “Vigneto” new among the existing indicators.

2.9. Structural data

Structural data refers to the territorial configuration of the estate, some environmental data and the composition of the equipment fleet. For each vineyard identified on the first map, the cartographic component automatically acquires the minimum distance to the nearest ditch, river or lake, by intersecting it with an internal shape file of the hydrologic elements (CISIS, 2013). In the same way, each vineyard feature is intersected with a DTM (Digital Terrain Model; Ministero dell'ambiente, 2001) of Italy in raster format, to automatically calculate the mean slope angle of the vineyard. Other information related to the vineyard could be acquired by the imported shape file or input directly by the user. Among the data that have to be filled by the user there are irrigation use (Boolean flag), water table depth, vineyard management within rows (grass, cropped, winter cover), and the trilling system. Meteorological variables could be uploaded taking them from private meteorological station or from on line available data. All the information about the equipment fleet have to be filled by the user.

Table 7
Indicatore Vigneto scores.

IV value	Judgment	Comment
0–0.3	A	Excellent
0.31–0.55	B	Good
0.55–0.75	C	Acceptable
0.76–0.9	D	Not acceptable
>0.9	E	Totally unsustainable

2.10. Management data

Vineyard management data could potentially change each year. The web portal allows the user to create a new evaluation each year, saving the previous one and preventing new modifications for the past years.

A complete list of the input data required to complete “Vigneto” is reported on Table 8. All data included in the following table (Table 8) are required to assess sustainability using “Vigneto” indicator and therefore cannot be omitted or estimated.

When the user finishes data input, the software runs calculations for each sub-indicator, implementing the models described in Section 2.2 and aggregates the six results with a fuzzy logic model. The software also provides detailed information about each sub-indicator.

3. Results

Sensitivity analysis on pedoclimatic and socioeconomic conditions of the different case studies provide useful information for the redefinition of some of the indicator modules. The model was evaluated on four wineries from different geographical areas of Italy with different soil, climate conditions and management practices was performed (Tables 9–12. The model was developed on real cases because literature on sustainability assessment in vineyard is scarce. Initially the first model attempt was tested and its sensitivity, robustness, and uncertainty were assessed on the first farm. This was repeated on every project partner vine estate underlining the interactions among model and farm characteristics. Following this approach several model changes have been made because some equation was not robust or because of lack of sensitivity were present. Data input and additional information are reported in the supplementary data section. The cross validation approach was done as a qualitative evaluation of the model. This process led to an iterative and adaptive approach and required the redefinition of some modules due to the different pedoclimatic and cultural conditions on the sensitivity and robustness of the implementing modules. The involvement of the stakeholders also allowed the identification and clarification of the impacts and solutions about several issues and improved the user-friendliness of the software (Krueger et al., 2012; Voinov and Bousquet, 2010). In fact, being a knowledge based model, the expert judgment is required to evaluate the reliability of the system (Giordano and Liersch, 2012).

The model output reports that all the results of the tested wineries are different: three of them are in A class, and one in C class. The PMI was always fully sustainable. In fact, European directive for a sustainable use of pesticides (EC 128/2009), reinforce the requirement for vine-growers to engage in more environmentally friendly farming practices and, according current regulation, the available plant protection products have low toxicities (Balderacchi and Trevisan, 2010). Moreover most of the Italian winegrowers have since the early 1990s followed European programs for organic or integrated pest management. The greatest number of vine-growers follows the integrated pest management approach that appears most accessible. In the selected farms individual strategies have been developed combining ‘end-of-pipe’ innovations, based on input substitution and savings, and pollution prevention and control technologies. The individual choices are related on the investments that vine-growers intend to implement in the short or middle and long term. Although in the selected farms the pest and disease management indicator gives no impact as result it was not possible to exclude this indicator from the model because acknowledging

Table 8
Structure of the web GIS input.

Sub-indicator	Data required
PMI	Different strategies of pest control, and for each strategy a set of applications. For each application, the required data are: - active ingredient - phenological stage of application - number of applications - interval between applications (d) - rate (kg/Ha) - -type of application (traditional, tunnel sprayers, precision tools, anti-drift nozzles)
FMI	Fertilization is described by the use of organic matter, mineral fertilizers and by the presence of cover crops. Organic matter data are: - type of organic matter supplied - amount of organic matter distributed (kg/Ha) If a cover crop is used, annual perennial should be selected. Mineral fertilization data are: - type of mineral fertilizer - amount of mineral fertilizer applied (kg/Ha) - - Nitrate, Phosphorous, Potassium content (%)
SCI	Soil compaction is characterized by each management operation based on machinery used. Data required for each operation are: - name of operation - name of machine - - mean number of journeys over soil
LQI	Four questions have been identified to characterize biodiversity management of the estate: - hours directly used in production of grapes and worked by company staff - hours directly used in production of grapes and processed by external staff - hours spent in the maintenance of the vineyard and other agricultural areas by company staff - - hours spent in the maintenance of the vineyard and other agricultural areas by external staff

Table 9
“Vigneto” results for winegrowing farm 1.

	Farm 1					
Vineyard	PMI	FMI	SOMI	SCI	SEI	LQI
Vineyard 1	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 2	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 3	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 4	0.00	0.00	1.00	0.01	0.13	0.96
Vineyard 5	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 6	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 7	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 8	0.00	0.00	0.00	0.01	0.13	0.96
Vineyard 9	0.00	0.00	0.00	0.01	0.13	0.96
Overall score/judgment	0.19/A					

Table 10
“Vigneto” results for winegrowing farm 2.

Winegrowing farm	Farm 2					
Vineyard	PMI	FMI	SOMI	SCI	SEI	LQI
Vineyard 1	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 2	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 3	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 4	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 5	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 6	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 7	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 8	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 9	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 10	0.00	0.00	0.00	0.69	0.13	0.50
Vineyard 11	0.00	0.00	0.00	0.76	0.13	0.50
Vineyard 12	0.00	0.00	0.00	0.76	0.13	0.50
Vineyard 13	0.00	0.00	0.00	0.76	0.13	0.50
Vineyard 14	0.00	0.00	0.00	0.76	0.13	0.50
Overall score/judgment	0.23/A					

Table 11
"Vigneto" results for winegrowing farm 3.

Winegrowing farm	Farm 3					
Vineyard	PMI	FMI	SOMI	SCI	SEI	LQI
Vineyard 1	0.00	1.00	1.00	0.90	0.18	0.50
Overall score/judgment	0.62/C					

the negative impact of cultural practices, and the possible pesticide effects could represent a progressive greening strategy.

The FMI and the SOMI usually perform well, most of the vineyards has impact equal to 0 in both the indicators. In fact, viticultural macronutrient demand (N, P, K, Mg, Ca) is lower than that of annual crops (Bellon-Maurel et al., 2015) but not negligible to eutrophication. The low use of fertilizers in viticulture is unusual due to restrictions on integrated management schedules and because the most of the quality wines regulations (Italian – Ministry of the agriculture) limits the grape yield production for increasing the wine quality. The zero values of the fertilization management indicator are due to not fertilized vineyards, while in the fertilized the result is function of the fertilizer applied (rate, kind of fertilizer) and of the soil features. However, in some wineries the FMI and the SOMI indicators give a value of 1, underlining an unsustainable management of the fertilization. When FMI value is 1 the amount of fertilizer applied is higher than the actual need of the vineyard, making possible the leaching of the nutrients, while, when the SOMI is 1 the organic matter supply is 60% less than recommended considering the presence of grass and the distribution of organic matter. For instance in the vineyard 4 of the farm 1 and in the farm 3 no organic matter is returned to the soil through the use of organic fertilizers.

SCI (0.01–0.90) indicator shows that winegrowers manage soil in different ways. Grass-cover favors the accumulation of stabilized forms of soil organic matter, enhances soil C and N storage, protects the soil surface from water and wind erosion and remediates soil compaction but the presence of cover depends on the geographic location of the vineyards. In the North, there is higher rainfall, and the presence of permanent grass or cover crops in the vineyard is common. At the same time, in the North because of the higher rainfall and thus greater equipment transit for pesticide application soil compaction risk is higher. The higher value is obtained by farm 3 in which a high number of passages (17) with a heavy machinery (8000 kg) is done. Slightly better farm 2 in which 8 passages have been done with a machinery of 4485 kg of weight. Rainfall in the North exacerbates erosion risk as Italian viticulture is mainly in hilly areas but the presence of cover crop effectively reduces the risk.

The LQI score value is affected by the location of the vineyards which are often in vineyard districts in which the vine is the dominant or the unique crop and therefore with low biodiversity (0.12–0.96). Moreover the vineyards of multi-functional farms have a better indicator value due to the more diversified landscape and to the fact that the company staff is naturally involved in different activities, and not only in the vineyard management. The worst result is obtained by the farm 1, situated in a vineyard district in which crop diversity is low. In this farm, in fact, agricultural areas different from the vine are not present, and also natural areas represent less than the 10% of the overall surface. Moreover farm 1 completely outsources the works of maintenance of the vine and of the additional areas. The better result is obtained by farm 4 in which 34,723 m^2 of agricultural areas different from vine exist. The 10% of the time of the farm and external employees is due to the management of the additional area and internal workers satisfy the 43% of the work of maintenance of vineyards and other areas. LQI stands at 0.50 for farm 2 and 3 but results depend on different management options. In the farm 2 the works of maintenance are completely outsourced (LM: 0.998), but the farm has a high biodiversity due to the presence of 508,599 m^2 of agricultural areas (not vine) and of 203,437 m^2 of natural areas (LS: 0.469). In the farm 3 landscape biodiversity is high (LS: 0) and any work is done by external employees but very low time is spent in the maintenance of additional areas (LM: 0.998).

Table 12
"Vigneto" results for winegrowing farm 4.

Winegrowing farm	Farm 4					
Vineyard	PMI	FMI	SOMI	SCI	SEI	LQI
Vineyard 1	0.00	0.13	0.00	0.15	0.00	0.12
Vineyard 2	0.00	0.00	0.00	0.28	0.00	0.12
Vineyard 3	0.00	0.00	0.00	0.29	0.00	0.12
Vineyard 4	0.00	0.00	0.00	0.29	0.00	0.12
Vineyard 5	0.00	0.00	0.00	0.29	0.00	0.12
Vineyard 6	0.00	0.00	0.00	0.29	0.00	0.12
Vineyard 7	0.00	0.00	0.00	0.19	0.00	0.12
Vineyard 8	0.00	0.00	0.00	0.19	0.00	0.12
Overall score/judgement	0.07/A					

The SEI usually performs well. The vineyards on steep slopes are always covered with grass. The best value is obtained by farm 4 in which cover crops cover the 100% of the soil surface, the worst value is obtained by farm 3 in which the perennial grasses cover the 70% of the soil surface.

Comparing the results obtained from the same farms using the three quantitative V.I.V.A. indicators (Table 13) appears that sustainability can be easily assessed only considering a multidisciplinary approach. For instance winegrowing farm 3 has the lower impact in terms of greenhouse gases emissions (GHGs; "Aria") compared to farms 1, 2 and 4 but the higher impact in the "Vigneto" assessment. This result underlines a non-optimal management of the agronomic practices in the vineyard as discussed before. Winegrowing farms 1 and 2 despite their high impacts on "Aria" and "Acqua" indicators have a sustainable agronomic management as highlighted by the results of "Vigneto" indicator.

3.1. Uncertainty analysis

Uncertainty is present in the sustainability science because several concerns are related to intrinsic vagueness of the sustainability concept itself (Ciuffo et al., 2012).

Uncertainty sources were identified in:

- data collection from field;
- derivation of indicator input parameters from the software forms;
- modeling process itself.

A procedure was identified for reducing and for characterizing the uncertainty:

1. Characterize the model robustness and the model sensitivity of each indicator
2. Calibrate the input with higher uncertainty
3. Ask to experts and collaborate for the unclear issues
4. Assess the user performances
5. Reiterate the modeling process using the experience gained from the first attempts.

Table 13
Comparison of the results obtained by winegrowing farms by using the quantitative V.I.V.A. indicators.

Winegrowing farm	"Vineyard" (overall score)	"Air" (kg $CO_{2\ eq}$/0.75 L of wine)	"Water" (L of water/0.75 L of wine)
1	0.19/A	1.69	708
2	0.23/A	1.41	785
3	0.62/C	0.884	755
4	0.07/A	1.11	424

In the present paper were discussed only the uncertainty sources of sub-indicators not previously presented in literature. In particular, was discussed the uncertainty related to the data input of the new selected sub-indicators. Fertilization management, soil organic matter management and pest and disease management indicators uncertainty was not characterized because those indicators have previously been published by other authors. Sensitivity and uncertainty analysis was performed for the landscape quality indicator. Landscape quality uncertainty is mainly related to the difficulty to compute the working time related to the grape production from the one related to the natural areas' maintenance. Landscape indicator was judged by developers as the most simple, robust and easy-to-use among the biodiversity indicator options. Only an input defines erosion indicator, in substance the uncertainty is related to the attribution of grass/soil management to the correct class. Soil compaction balances structural data (soil susceptibility and rain indicators) with management data (equipment and soil cover management). The most sensitive input management parameters are the equipment drive and the grass/soil management. As for erosion indicator case, the soil management is the most uncertain parameter.

Modeling process was reiterated several time for identifying the unclear issues, several indicators that were identified from the first attempt were discarded. Robust pedotransfer functions were introduced to reduce the uncertainty related to the soil input difficult to measure and GIS calculations reduces the input entries required from the end user. However, the use of external datasets (i.e. maps) increasing uncertainty but its characterization can be performed only in each single case.

4. Conclusions

From a theoretical point of view, sustainability requires a holistic approach that means that the different compartments, the relations and the processes, are managed as a whole, and not as collections of parts (Nieto, 1996). However from a modeling point of view this approach is not possible and therefore here, the holism is considered as an "integration" in which the system components are described simultaneously as integral parts of the whole (Voinov and Shugart, 2013). This manuscript demonstrates that sustainability can be easily modeled using only expert knowledge bases starting from a simple statement and toward the definition of an indicator of environmental performance. Simplicity (Gambrel and Cafaro, 2010) is an approach that minimize the risk of drifts and excesses and promotes sustainability and that can be used for modeling the sustainability.

The starting idea "sustainability is a pathway that starts from the presence of grass in the vineyard, from the reduction of the equipment journeys passages over the soil and focuses on the care for the landscape and working staff" was transformed into indicators and algorithms and was implemented iteratively into the software.

The developed model can be defined as an environmental decision support system to support policy and management decision-making (McIntosh et al., 2011). It satisfies two of the five main purposes that Kelly et al., (2013) identified: (1) management and decision-making under uncertainty and (2) social learning. The result of this iterative and adaptive process is a judgment that can be effectively used when communicating with the consumer and for social learning. This integrated environmental model (Laniak et al., 2013) differentiates between different management options indicating which is more sustainable. It integrates knowledge from a broad range of fields (economics, ecology, agronomy, chemistry, and physics) and gives a summary of the environmental impact. This helps with communication of the sustainability assessment to the user. It also addresses the implementation of new technologies in the productive process and can be used as a learning tool for all the stakeholders and scientists.

The learning process also involves software development: the initial sustainability idea was improved iteratively and adaptively by the improvement of the indicators. Some facts were unknown at the beginning of the project, in particular:

- the farmer does not consider the role of organic matter,
- pesticides and nutrients which usually have high environmental impact, could, in viticulture do not have relevant impacts.
- soil management is the main issue concerning sustainability in viticulture.

This confirms that knowledge is the main driver of sustainability and could be considered a main component of the "terroir", which can be framed as the development of a shared knowledge for adapting to social and pedoclimatic conditions and for maximizing and assuring grape and wine production. Therefore "terroir" is not a static concept but evolves with the progress of science and can be driven by the search for sustainability.

A new indicator update will be necessary when:

1) New knowledge is developed and the current implemented idea is obsolete.
2) The "terroir" is modified by the current version of the software and the proposed goal is reached.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.scitotenv.2016.07.043.

References

Acutis, M., Alfieri, L., Giussani, A., Provolo, G., Diguardo, A., Colombini, S., Bertoncini, G., Castelnuovo, M., Sali, G., Moschini, M., Sanna, M., Perego, A., Carozzi, M., Chiodini, M.E., Fumagalli, M., 2014. ValorE: an integrated and GIS-based decision support system for livestock manure management in the Lombardy region (northern Italy). Land Use Policy 41, 149–162. http://dx.doi.org/10.1016/j.landusepol.2014.05.007.

Baets, S.D., Torri, D., Poesen, J., Salvador, M.P., Meersmans, J., 2008. Modelling increased soil cohesion due to roots with EUROSEM. Earth Surf. Process. Landf. 33 (13), 1948–1963.

Balderacchi, M., Trevisan, M., 2010. Comments on pesticide risk assessment by the revision of directive EU 91/414. Environ. Sci. Pollut. Res. 17 (3), 523–528.

BBCH Monograph, 2001. Growth Stages of Mono- and Dicotyledonous Plants. Federal Biological Research Centre for Agriculture and Forestry.

Bellocchi, G., Acutis, M., Fila, G., Donatelli, M., 2002. An indicator of solar radiation model performance based on a fuzzy expert system. Agron. J. 94, 1222. http://dx.doi.org/10.2134/agronj2002.1222.

Bellon-Maurel, V., Peters, G.M., Clermidy, S., Frizarin, G., Sinfort, C., Ojeda, H., Roux, P., Short, M.D., 2015. Streamlining life cycle inventory data generation in agriculture using traceability data and information and communication technologies - part II: application to viticulture. J. Clean. Prod. 87, 119–129.

Bockstaller, C., Girardin, P., 2008. Mode de calcul des indicateurs agri-environnementaux de la méthode Indigo. Agriculture 119.

Bockstaller, C., Girardin, P., van der Werf, H.M.G., 1997. Use of agro-ecological indicators for the evaluation of farming systems. Dev. Crop. Sci. 329–338.

Bonamente, E., Scrucca, F., Asdrubali, F., Cotana, F., Presciutti, A., 2015. The water footprint of the wine industry: implementation of an assessment methodology and application to a case study. Sustain. 7, 12190–12208. http://dx.doi.org/10.3390/su70912190.

Bonamente, E., Scrucca, F., Rinaldi, S., Merico, M.C., Asdrubali, F., Lamastra, L., 2016. Environmental impact of an Italian wine bottle: carbon and water footprint assessment. Sci. Total Environ. 560, 274–283. http://dx.doi.org/10.1016/j.scitotenv.2016.04.026.

Büchs, W., 2003. Biodiversity and agri-environmental indicators - general scopes and skills with special reference to the habitat level. Agric. Ecosyst. Environ. 98 (1–3), 35–78.

Cardoso, E.J.B.N., Vasconcellos, R.L.F., Bini, D., Miyauchi, M.Y.H., dos Santos, C.A., Alves, P.R.L., de Paula, A.M., Nakatani, A.S., Pereira, J.M., Nogueira, M.A., 2013. Soil health: looking for suitable indicators. What should be considered to assess the effects of use and management on soil health? Sci. Agric. 70 (4), 274–289.

CISIS, 2013. DBPrior10K. Centro Interregionale per i Sistemi Informatici (G.e.S., ai sensi della L. 633/41 e s.m.i. (Ed.)).

Ciuffo, B., Miola, A., Punzo, V., Sala, S., 2012. Dealing with uncertainty in sustainability assessment. Report on the Application of Different Sensitivity Analysis Techniques to Field Specific Simulation Models. EUR. 25166.

Cluzeau, D., Guernion, M., Chaussod, R., Martin-Laurent, F., Villenave, C., Cortet, J., Ruiz-Camacho, N., Pernin, C., Mateille, T., Philippot, L., Bellido, A., Rougé, L., Arrouays, D., Bispo, A., Pérès, G., 2012. Integration of biodiversity in soil quality monitoring: baselines for microbial and soil fauna parameters for different land-use types. Eur. J. Soil Biol. 49, 63–72.

Corbo, C., Lamastra, L., Capri, E., 2014. From environmental to sustainability programs: a review of sustainability initiatives in the Italian wine sector. Sustain. 6 (4), 2133–2159.

European Environment Agency, 2007. CLC2006 technical guidelines. EEA Tech. Rep. http://dx.doi.org/10.2800/12134.

Fragoulis, G., Trevisan, M., Di Guardo, A., Sorce, A., Van Der Meer, M., Weibel, F., Capri, E., 2009. Development of a management tool to indicate the environmental impact of organic viticulture. J. Environ. Qual. 38 (2), 826–835.

Gambrel, J.C., Cafaro, P., 2010. The virtue of simplicity. J. Agric. Environ. Ethics 23 (1–2), 85–108.

Geotechdata.info, 2013. Angle of Friction.

Gerlach, J., Samways, M., Pryke, J., 2013. Terrestrial invertebrates as bioindicators: an overview of available taxonomic groups. J. Insect Conserv. 17 (4), 831–850.

Giordano, R., Liersch, S., 2012. A fuzzy GIS-based system to integrate local and technical knowledge in soil salinity monitoring. 36, 49–63. http://dx.doi.org/10.1016/j.envsoft.2011.09.004.

Horn, R., Fleige, H., 2003. A method for assessing the impact of load on mechanical stability and on physical properties of soils. Soil Tillage Res. 73 (1–2), 89–99.

Italian Ministry of agriculture, available at https://www.politicheagricole.it/flex/cm/pages/ServeBLOB.php/L/IT/IDPagina/4625)

Kelly, R.A., Jakeman, A.J., Barreteau, O., Borsuk, M.E., ElSawah, S., Hamilton, S.H., Henriksen, H.J., Kuikka, S., Maier, H.R., Rizzoli, A.E., van Delden, H., Voinov, A.A., 2013. Selecting among five common modelling approaches for integrated environmental assessment and management. Environ. Model. Softw. 47 (0), 159–181.

Košulič, O., Michalko, R., Hula, V., 2014. Recent artificial vineyard terraces as a refuge for rare and endangered spiders in a modern agricultural landscape. Ecol. Eng. 68, 133–142.

Krueger, T., Page, T., Hubacek, K., Smith, L., Hiscock, K., 2012. The role of expert opinion in environmental modelling. Environ. Model. Softw. 36, 4–18.

Lamastra, L., Suciu, N.A., Novelli, E., Trevisan, M., 2014. A new approach to assessing the water footprint of wine: an Italian case study. Sci. Total Environ. 490, 748–756.

Laniak, G.F., Olchin, G., Goodall, J., Voinov, A., Hill, M., Glynn, P., Whelan, G., Geller, G., Quinn, N., Blind, M., Peckham, S., Reaney, S., Gaber, N., Kennedy, R., Hughes, A., 2013. Integrated environmental modeling: a vision and roadmap for the future. Environ. Model. Softw. 39, 3–23.

McIntosh, B.S., Ascough Ii, J.C., Twery, M., Chew, J., Elmahdi, A., Haase, D., Harou, J.J., Hepting, D., Cuddy, S., Jakeman, A.J., Chen, S., Kassahun, A., Lautenbach, S., Matthews, K., Merritt, W., Quinn, N.W.T., Rodriguez-Roda, I., Sieber, S., Stavenga, M., Sulis, A., Ticehurst, J., Volk, M., Wrobel, M., van Delden, H., El-Sawah, S., Rizzoli, A., Voinov, A., 2011. Environmental decision support systems (EDSS) development – challenges and best practices. Environ. Model. Softw. 26 (12), 1389–1402.

Ministero dell'ambiente, 2001. Modello digitale del terreno 20 metri (m_amte:8HCH2C:a5ca714e-8d43-46c8-cb09-13936ceb3254 ed).

Morgan, R.P.C., Quinton, J.N., Smith, R.E., Govers, G., Poesen, J.W.A., Auerswald, K., Chisci, G., Torri, D., Styczen, M.E., 1998. The European soil erosion model (EUROSEM): a dynamic approach for predicting sediment transport from fields and small catchments. Earth Surf. Process. Landf. 23 (6), 527–544.

Nieto, C.C., 1996. Toward a Holistic Approach to the Ideal of Sustainability.

OIV, 2004. Resolution OIV/CST 1/2004. Definition of Sustainable Vitiviniculture.

OIV, 2010. Resolution OIV/VITI 333/2010. Definition of Vinitivicultural "Terroir".

Padovani, L., Trevisan, M., Capri, E., 2004. A calculation procedure to assess potential environmental risk of pesticides at the farm level. Ecol. Indic. 4 (2), 111–123.

Page, T., Heathwaite, A.L., Thompson, L.J., Pope, L., Willows, R., 2012. Eliciting fuzzy distributions from experts for ranking conceptual risk model components. Environ. Model. Softw. 36, 19–34.

Parr, A., 2009. Hijacking Sustainability. MIT Press Cambridge, MA.

Renard, K.G., Foster, G.R., Weesies, G.A., McCool, D., Yoder, D., 1997. Predicting soil erosion by water: a guide to conservation planning with the revised universal soil loss equation (RUSLE). Agric. Handb. (Wash.) 703.

Riches, D., Porter, I.J., Oliver, D.P., Bramley, R.G.V., Rawnsley, B., Edwards, J., White, R.E., 2013. Review: soil biological properties as indicators of soil quality in Australian viticulture. Aust. J. Grape Wine Res. 19 (3), 311–323.

Santiago-Brown, I., Metcalfe, A., Jerram, C., Collins, C., 2014. Transnational comparison of sustainability assessment programs for viticulture and a case-study on programs' engagement processes. Sustain. (Switz.) 6 (4), 2031–2066.

Saxton, K.E., Rawls, W.J., 2006. Soil water characteristic estimates by texture and organic matter for hydrologic solutions. Soil Sci. Soc. Am. J. 70 (5), 1569–1578.

Sugeno, M., 1985. An introductory survey of fuzzy control. Inf. Sci. 36 (1–2), 59–83.

Szolnoki, G., 2013. A cross-national comparison of sustainability in the wine industry. J. Clean. Prod. 53, 243–251.

Trevisan, M., Di Guardo, A., Balderacchi, M., 2009. An environmental indicator to drive sustainable pest management practices. Environ. Model. Softw. 24 (8), 994–1002.

Trivellone, V., Schoenenberger, N., Bellosi, B., Jermini, M., de Bello, F., Mitchell, E.A.D., Moretti, M., 2014. Indicators for taxonomic and functional aspects of biodiversity in the vineyard agroecosystem of Southern Switzerland. Biol. Conserv. 170, 103–109.

Voinov, A., Bousquet, F., 2010. Modelling with stakeholders. Environ. Model. Softw. 25 (11), 1268–1281.

Voinov, A., Shugart, H.H., 2013. 'Integronsters', integral and integrated modeling. Environ. Model. Softw. 39 (0), 149–158.

Wall, G., Cereal, E., 2002. RUSLEFAC: Revised Universal Soil Loss Equation for Application in Canada: a Handbook for Estimating Soil Loss from Water Erosion in Canada. Eastern Cereal and Oilseed Research Centre, Agriculture and Agri-Food Canada.

Wieland, R., Gutzler, C., 2014. Environmental impact assessment based on dynamic fuzzy simulation. Environ. Model. Softw. 55, 235–241.

Zadeh, L., 1965. Fuzzy sets. Inf. Control. 8, 338–353.

Conclusions

The three years PhD course has been focused on the analysis, development and test of Environmental Decision Support Systems for evaluating the impact of chemical substances used in agriculture.

Three main characteristics of the EDSS definition could be observed in the tools here presented: the spatial representation of the context analysed; the dynamicity of the environmental variables studied; the complexity of interaction with physico-chemical and biological processes.

VULPES (Vulnerability to Pesticide) EDSS has been developed with a focus on determining the specific vulnerability of groundwaters to chemical substances at territorial level. In a first release, it was developed to evaluate vulnerable areas to Plant Protection Products (PPPs), dividing the territory in so-called Uniform Geographical Units (UGU), characterised by an unique set of environmental parameters (pedology and meteorology) and irrigation amount for a specific crop; UGU's parameters together with physico-chemical parameters and rate of application of the pesticide become the input for a simulation with PELMO or PEARL models. Results from each simulation (1 UGU = 1 simulation) are then collected on a vectorial GIS map which gives the immediate representation of potential vulnerable areas, where risk assessors could implement further investigations or monitoring activities.

Results from mathematical model simulations are essential for the identification of potential groundwater vulnerability. This is only half of the story, because risk assessors could count on monitoring campaign results, to disclose the present contamination status and assess the impact of newly implemented measures. But each method (monitoring and modelling), taken alone, has consistent flaws (as reported in chapter 4), that could be, in our opinion, overcome putting aside the two approaches. This intuition leaded to the definition of the Moni-modelling methodology, where the combined use of monitoring and simulation models could identify vulnerable areas, lower the costs of monitoring, and identify possible shortcomings of models, as field data can be used to improve the quality of simulation models.

VULPES has then be adapted to evaluate the territorial vulnerability to veterinary medicinal products (VMPs), which imply substantial differences with PPPs in application pattern and scheduling: while spraying of PPPs could be theoretically inferred by the product label, the load of VMPs contained in manure could not be assessed without specific knowledge of VMP use and animal consistency on the territory. In order to overcome these potential weaknesses, we coupled VULPES with ValorE, an EDSS partially realised within the PhD course and used in the Lombardy region to address all the major components of manure management. ValorE contains data from each livestock farm in Lombardy concerning amount of manure exctreted, treated, stocked and distributed in the field, together with their spatial georeferencing. Hence, one could trace the path of each VMP administered until it reaches the field; afterwards, its transport into groundwater could be simulated with VULPES. The methodology here described (called Sust-Pharm, sustainable use of veterinary pharmaceuticals in livestock farms) is the first attempt to evaluate the environmental fate of VMPs in groundwater at a territorial level, making use of the best knowledge of manure management available at the time being.

Every EDSS or methodology realised during the PhD courses has been tested in Lombardy region which represents one of the most important agricultural areas in Europe, intensively cropped with cereals and grass and with the highest number of livestock farms in Italy (and hence in Europe).

Therefore, the choice of Lombardy region is paradigmatic, both for impact of chemical substances from agriculture (nitrogen, pesticides and veterinary medicine products) and for data availability.

Decision Support Systems here presented have been developed to give prototype tools for the implementation of next generation software for public or private risk assessors which could benefit from this methodologies in order to test new policies, investigate more in details specific areas, build new and more efficient monitoring campaign where problems arise. This should be seen in a logic of agriculture sustainability, either in environmental and economic terms, for preventing water and territorial pollution but also for avoiding useless limitation to chemical use without proven evidences.

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