SURFACE WATER QUALITY ASSESSMENT THROUGH THE APPLICATION OF wPRISMA INTERACTIVE TOOL

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ABSTRACT

In the framework of the SWITCH-ON project water concerns and untapped potential of open data for improved water management across the EU, are addressed. The overall goal of the project is to establish a "one-stop-shop" for European water information that make use of open data, and add value to society by repurposing and refining data from various sources. While focusing on water, the project is expected to inspire a much broader environmental and societal knowledge domain and many different end-users. The vision of the project is to improve public services and to foster business opportunities and growth by establishing new forms of water research and facilitating the development of new products and services based on principles of sharing.

Our goal, through wPRISMA, which is one of the products developed within SWITCH-ON that focuses on water quality issues, is to produce a science-based tool that will aid the policy makers and environmental agencies that implement the Water Framework Directive to identify areas that experience significant pressures from selected pollutants, through the web-mapping visualisation.

wPRISMA uses a water quality model in order to predict the spatial and temporal variation of concentrations of selected pollutants in surface water bodies. Several open datasets, like European Pollutant Release and Transfer Register, Corine Land Cover, Digital Elevation Models are used in order to retrieve the pollutant loads. Hydrological data are obtained from E-HYPE, an open hydrological model that enables the calculation of river discharges in catchment level, while procedures developed by FOCUS SW (FOrum for the Co-ordination of pesticide fate models and their Use, Surface Waters) group, are used in order to estimate the quantity of plant protection products from agricultural land uses entering surface water bodies. Data on urban wastewater treatment plants with the use of emission factors for selected metals and also industrial pollution loads from the ePRTR inventory are incorporated in the pollution load dataset.

The results of the water quality simulation are presented in a web-map application where the user is able (1) to compare the simulated concentrations with the EQS and identify areas or water bodies that experience significant pressures from diffuse and point source pollution, (2) to perform simulation of extended hydrological periods and produce maps indicative of the likelihood of EQS exceedance in water bodies and (3) to identify the contribution of upstream areas to the predicted concentration at a specific water body.

Keywords: wPRISMA, Water Framework Directive, Environmental Quality Standards, water quality model, environmental management

1. Introduction

wPRISMA is an interactive map application which aims to quantify the impact of point and diffuse pollution sources into surface water bodies for different hydrological scenarios, by comparing the anticipated concentrations with the Environmental Quality Standards and to spot water bodies that are likely to be negatively affected in case of accidental or uncontrolled pollution incidents such as treatment plant malfunction.

2. Methods and tools involved

2.1. Models employed

In order to describe the fate of a pollutant in the surface water bodies the advection-diffusion-reaction equation has to be solved for every pollutant, which in 1d is written

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} + R \qquad (1)$$

where C pollutant concentration [ML^{-3}], D the diffusion coefficient [L^2T^{-1}], u the stream velocity [LT^{-1}] and R the external sink or sources of the pollutant [$ML^{-3}T^{-1}$].

wPRISMA is intended for large scale application, so complex model with increased data requirements and large computational times should be avoided. Short computational times are also essential for the responsiveness of the web application since the model will be invoked upon user request and will be executed at the web server. Under these considerations the rivers are simulated as 1 dimensional bodies (1d) while lakes and reservoirs are considered as fully mixed cells. Furthermore the steady state solution is sought so this eliminates all time derivatives from the equation. However in order to account for the seasonal variation of river discharges and pollutions loads, the model is applied in a monthly basis in order to obtain representative results about the anticipated concentrations in every water body.

River water bodies are discretized as a network of finite, completely mixed cells connected only by convective terms while dispersion is neglected. This assumption could be valid for small rivers where the dispersive terms could be safely ignored especially at steady state conditions. The elimination of the dispersive terms, which propagate information (concentration) in both directions (from upstream to downstream, but also from downstream to upstream), allows for the analytical solution of the advection reaction equation to be calculated in every segment.

Under these assumptions the general steady state solution for the concentration of a first order decay pollutant can be expressed as

$$C_i^X = \left(UM_i^X + SM_i^X\right)\cdot A_i^X \quad (2)$$

where C_i^X the concentration of pollutant *X* in cell *i* [ML^{-3}], UM_i^X the mass rate [MT^{-1}] of the pollutant *X* entering the cell *i* from all upstream cells calculated from $UM_i^X = \sum_m^{m \in U_i} C_m^X \cdot Q_{m\to i}$, SM_i^X all external sources of pollutant *X* entering the cell expressed as mass rate [MT^{-1}], A_i^X a factor [$L^{-3}T$] for each cell and pollutant calculated from $A_i^X = \left(Q_i^{out} + k_i^X \cdot V_i\right)^{-1}$, Q_i^{out} the total discharge from cell *i* to all downstream cells [L^3T^{-1}] calculated from $Q_i^{out} = \sum_n^{n \in D_i} Q_{i\to n}$, k_i^X decay rate for pollutant *X* in cell *i* [T^{-1}], V_i the volume of cell *i* [L^3], $Q_{m\to n}$ the discharge [L^3T^{-1}] from cell *m* to a downstream cell *n*, D_i the set of cells downstream of cell *i* and $\mathcal{U}_i$ the set of cells upstream of cell *i*.

A constraint arising from the upwind scheme used for the spatial derivative, is that when applying the analytical solution technique at a specific segment all upstream conditions must be known beforehand. Therefore this technique must be applied sequentially from upstream to downstream segments. The model automatically determines which (upstream) water bodies must be simulated and the solution order in order to calculate the pollutants concentrations in an area of interest selected by the user.

Simulated Substances and Processes: The water quality model is applied for suspended sediments, selected heavy metals and plant protection products (PPP). An appropriate lumped first order decay rate is used in order to account for biodegradation, volatilization and oxidation of each heavy metal and PPP inside the water column.

Suspended Sediments: Settling velocities are used in order to describe the transport of suspended sediment and the absorbed metal from the water column to the sediment bed. The sediment bed is not explicitly simulated therefore the amount of solids and the absorbed metal content that are transferred to the sediment bed are permanently removed from the system.

Decay rate for SS can be calculated as $k_i^{SS}=\frac{v_i^{settling}}{h_i}$ where $v_i^{settling}$ [LT^{-1}] and h_i [L] the settling velocity of suspended sediment and the water column depth in cell *i* respectively. Typical values for settling velocities used in the model are 1 m/d.

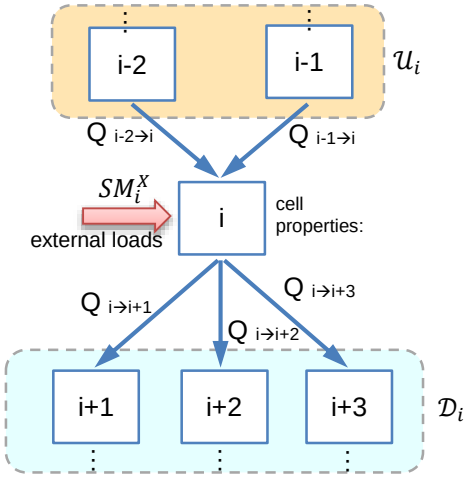

Figure 1: Representation of a river network with mixed cells.

Heavy Metals: Regarding heavy metals, the effect of sorption i.e. bonding onto solid phases, which greatly affects their dissolved concentrations, is taken into account by introducing a metal partition coefficient which is expressed as the sorbed metal mass (in mg metal per kg sorbing material) to the dissolved metal concentration (in mg metal per L of water). The partitioning of the metal to the soluble and solid phase is assumed to be instantaneous, which is regarded as a realistic assumption (Table 1). The same applies for desorption which although slower than sorption, it is assumed fast when compared to other simulated processes. Equations 3 and 4 describe the distribution of metal between dissolved and particulate phase.

$$C_i^{M\ diss}=\frac{C_i^{M\ tot}}{1+P\cdot C_i^{SS}} \quad (3) \qquad C_i^{M\ part}=C_i^{M\ tot}-C_i^{M\ diss} \quad (4)$$

where $C_i^{M\ diss}$, $C_i^{M\ part}$, $C_i^{M\ tot}$ the dissolved, particulate and total metal concentrations [ML^{-3}], P the partition coefficient in [L^3M^{-1}] and C_i^{SS} the suspended sediment concentration [ML^{-3}].

When applying equation (2) for a heavy metal (as total concentration) the decay coefficient k is expressed as $k_i^{M\ tot}=k_i^0+\frac{P\cdot C_i^{SS}}{1+P\cdot C_i^{SS}}\cdot\frac{v_i^{settling}}{h_i}$, where k_0 [T^{-1}] the metal decay rate due to oxidation and volatilization. As it can be seen metals are depended from SS concentration and must be solved after equation for SS has been solved in the entire domain.

Table 1: Range and typical values of partition coefficients for heavy metals used in wPRISMA (US EPA, 2005)

Metal	Partition coefficient between suspended matter and water (L water/kg SS)	
	Typical value	Range
Cadmium	0,050	0,0006 – 2,00
Chromium	0,126	0,0079 – 1,00
Copper	0,050	0,0016 – 2,00
Zinc	0,126	0,0032 – 7,94
Nickel	0,040	0,0031 – 0,50
Lead	0,398	0,0025 – 3,16

Plant protection products: wPRISMA deals with two PPP Dimethoate and 2,4 - Dichlorophenoxyacetic acid (2,4 D). The decay of PPP in the water column is described with a first order reaction. When applying equation (2) for PPPs the decay coefficient k is expressed as $k_i^{PPP} = \frac{ln(2)}{DT50}$ where DT50 [T] the half-life in aqueous environment (Table 2).

Table 2: Typical decay rates for plant protection products used in wPRISMA (University of Hertfordshire, 2013)

PPP	Typical DT50 values in water (days)
Dimethoate	45
2,4-Dichlorophenoxyacetic acid	7,7

2.2. Technical data

wPRISMA is an interactive web map application accessed through a web browser. The water quality model and its main functionalities are implemented in C#. PostgreSQL is used for data storage along with PostGIS for spatial data. The front end application is written in HTML5 with Bootstrap and Leaflet. Data exchange with the custom models is achieved through JSON standard format.

3. Data processing

3.1. Hydrological data

The HYPE model is used for the calculation of river discharge of the main, surface water bodies of the sub-basins defined in the Greek National River Basin Districts. HYPE simulations provide daily discharges at each subbasin for an extended hydrologic period. These discharges are then averaged to produce average monthly discharges which are used by the water quality model. Further statistical processing enables the production of synthetic hydrological years.

When flows are known for every river segment, the velocity and the wet area are calculated assuming uniform flow. The slope is estimated from DEM in a sub basin or water body level and not in a segment level, due to limitations arising from the DEM scale and precision. Manning coefficients are estimated for every water body according to its typology available from RBMPs. In mountainous areas where steep gradients may result from the DEM (e.g. >3%), manning coefficients may be increased internally, in order to account for cascade (step-pool) flow conditions. For lakes and reservoirs relevant data for their depths and volumes are obtained from the River Basin Management Plans.

3.2. Pollution Loads

Regarding point source pollution from industrial facilities wPRISMA uses open data from the European Pollutant Release and Transfer Register (E-PRTR). Since E-PRTR contains limited data for Greece, an attempt to supplement these data could be based on the IPPC inventory of Greek facilities and data included in the RBMPs. Another source of heavy metal quantities entering surface water bodies is Urban Wastewater Treatment Plants. An inventory of Greek UWWTPs with operational data (e.g. discharge, served population, effluent characteristics) is available from Special Secretariat for Water in the context of the implementation of Directive 91/271/EC. When metal concentrations are not being measured on a regular basis, typical metal concentrations (UKWIR, 2014) are used in order to estimate UWWTPs contribution in metal loads.

The pressures on surface water bodies, as a result of diffuse pollution from the Plant Protection Products (PPPs) used during the agricultural activity in Greece were estimated by Ziogas et al., 2015. The pressures are quantified and expressed as loads from the PPPs' active substances that enter surface water bodies by implementing the methodology presented by the FOrum for the Co-ordination of pesticide fate models and their Use (FOCUS Surface Waters).

4. Product functionalities and results visualisation

Map and Monitoring results. wPRISMA creates maps with the anticipated concentrations of the selected pollutants. The user selects a pollutant, an area of interest, and a hydrological year either actual or statistically processed and the model run in a web server and returns a map with concentrations expressed as values or as percent of EQS (Figure 2). The user can also browse results from existing monitoring programs and compare with the simulated results.

Statistics. In this mode the model provides a way to assess the effect of different discharges in the anticipated pollutants concentrations in the water bodies. The model keeps the point and diffuse loads constant and repeats the simulation for all available hydrological years and presents the results as a cumulative probability function. The user can examine the effect of different hydrological years in the anticipated pollutants concentrations (Figure 3).

Figure 2: Web environment of wPRISMA - Results expressed as EQS exceedance.

Figure 3: Likelihood of EQS exceedance.

Contribution. This functionality enables the calculation of upstream areas contribution in the pollutants concentration in a specific water body segment. Knowing where the pollution originates from is useful while designing the measures program. The contribution of an upstream cell *i* $C_{i\to p}^{X}$ in terms of concentration [ML^{-3}] of the pollutant *X* at a given point of interest *p* is calculated by

$$\mathrm{C}_{\mathrm{i}\to\mathrm{p}}^{\mathrm{X}}=\mathrm{SM}_{\mathrm{i}}^{\mathrm{X}}\cdot\mathrm{B}_{\mathrm{i}\to\mathrm{p}}^{\mathrm{X}} \quad (5)$$

where $B_{i\to p}^{X}$ [$L^{-3}T$] contribution factor calculated from $B_{i\to p}^{X}=A_{i}^{X}\cdot\left(\sum_{n}^{n\in\mathcal{D}_i}Q_{i\to n}\cdot B_{n\to p}\right)$. As it can be seen the equation of contribution factor B contains in RHS the evaluation of B for the downstream cells in a recursive way, which means that the equation has to be solved beginning from downstream cells. For the point of interest itself the contribution factor B is defined as $\mathrm{B}_{\mathrm{p}\to\mathrm{p}}^{\mathrm{X}}=\left(\mathrm{Q}_{\mathrm{p}}^{\mathrm{out}}\right)^{-1}$, while for every other downstream boundary cell *b*, other than the point of interest we set $\mathrm{B}_{\mathrm{b}\to\mathrm{b}}^{\mathrm{X}}=0$.

Risk. This functionality enables the risk assessment of the upstream point and diffuse sources by evaluating how likely is a point source to cause an EQS exceedance in a downstream given point of interest. This results in a map where every point source is characterized by a factor which essentially expresses how many times could its current pollution loads be increased without causing an EQS exceedance in the selected area of interest. Point sources with a risk factor close to 1 are considered potentially dangerous, since a slight increase in their pollution loads could cause an EQS exceedance in the given point of interest. A similar approach can be adopted in order to evaluate the risk factor of a specific point source. This time the model evaluates how likely is a specific point source to cause an EQS exceedance not in a given point of interest but in any downstream water body. Both approaches are easily implemented using the contribution factor described in the previous paragraph.

5. Conclusions

wPRISMA is a dynamic tool with high potential which could aid water authorities and policy makers to identify appropriate measures for the protection of the water bodies and also establish specific water quality objectives. Furthermore, wPRISMA could serve as guidance to the competent authorities during the design of the monitoring programme and need for either a surveillance or an operational monitoring protocol.

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