The Water Framework Directive requires new tools for a better water quality monitoring

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Abstract:
Our goal is to demonstrate the need to design a new type of environmentally friendly instrumentation to face the challenges of the Water Framework Directive. Rivers are spatially and timely structured ecological systems exhibiting hot spots and hot moments that contribute to their overall health status. However, current programs for monitoring water quality (grab samples and laboratory analysis) are based on sampling strategy that do not take into account the spatial and temporal heterogeneity of a water body. To reflect their actual dynamics, a paradigm shift is essential. This requires the development of new monitoring strategies and therefore new instrumentation.

This new instrumentation must be able to measure at time scales appropriate to phenomena monitored and at a cost low enough to allow a sufficiently dense deployment in water bodies. We propose to enhance developing wireless networks of autonomous micro-sensors associated with mathematical processing of the collected data. The distinctive feature of this kind of smart sensor comes from the complete monitoring network expected, associating surface- and ground- waters chemistry, electronics and energy harvesting with smart data processing aiming to represent dynamic of basic ecological functions.

Introduction
A clean and healthy environment is essential for human well-being. To limit environmental threats to human health, the EU took actions and made progress in various fields during the last decade, such as the implementation of the REACH chemicals legislation and the Water Framework Directive 2000/60/EC (WFD), and the agreement reached on the Industrial Emissions Directive. Environmental monitoring is the cornerstone of any policy for managing,
Protecting and restoring surface water and groundwater resources. The WFD requires that an integrated monitoring programme has to be established within each river basin district. Specifically, to meet the requirements of the WFD, two primary monitoring programmes are required: the Surveillance Monitoring (SM) and the Operational Monitoring (OM). This latest is used to determine the status of water bodies identified as being at risk, and to establish a programme of measures. Unfortunately, rivers being mistakenly conceived as homogeneous well-mixed systems, and also because the water quality data are expensive, these programmes are based on a few grab samples analysed at laboratory, despite wide recognition by scientists of spatial heterogeneity and temporal variability of rivers. [1-5]. Only for France, the Programme of Measures is estimated to 24.4 billion euros, over the period 2012-2015, or more than 6 billion euros a year [6]. And it’s a safe bet that if our monitoring methods are not well suited to actual quality measurement of water bodies, this money will be spent in vain.

**Hot spot & hot moment**

In rivers, rates of biogeochemical processes vary in space and time to produce both hot spots and hot moments of elemental cycling. Indeed, at the intersection of hydrological fluxes with substrates or other fluxes containing complementary or missing reactants, some patches show disproportionately high biogeochemical reaction rates, relative to the surrounding. These areas of high activity are called hot spots. In a same way, at some periods of time, biogeochemical processes are enhanced and exhibit disproportionately high reaction rates relative to longer intervening time periods, when episodic hydrological fluxes reactivate and/or mobilize accumulated reactants: hot moments occur. Hot spots and hot moments often overlap and coincide with natural or anthropic disturbances. They need to be understood as a source and sink for N and organic matter. These conditions often occur in riparian zones, stream channels and hyporheic zones, and several investigators have measured high rates of denitrification and nitrate decline in these locations [7].

In order to a mechanistic understanding, it is necessary to identify biogeochemical hot spots at broader spatiotemporal scales and to factor them into quantitative models. In particular, the water managers must incorporate both natural and anthropic created biogeochemical hot spots into their water quality management plans. However, an actual visualization and an adapted water sampling are essential to river quality management. Also, we need new robust and flexible tools able to detect the ephemeral nature and the particular locations of these hot moments and spots, to assess their importance in biogeochemistry of bioactive element cycles, to improve our ability to predict their occurrence, and finally to better manage water resource.

**Chemical status**

Nowadays, the state of the art with regard to the physicochemical and biological monitoring of rivers, that is to say what is technically applicable and available for the majority of water managers, is still dominated by the conventional protocol: the grab sampling, that is “send a technician; take an isolated sample, send it to the laboratory and analyse it” with at best, in conventional water chemistry, a daily average flow proportional composite sample. The ecological pertinence of such a procedure is more than problematic [8]. Indeed, this kind of protocol only provides information on pollutant contents at time t (usually during working hours) ignoring the hourly or daily variations in a pollutant discharge and the functioning of
the natural environment itself, and is unable to provide information on the ecological or even chemical status of a water body [9]. Furthermore, the high cost of this protocol makes it impossible to obtain any satisfactory spatial representativeness. The average sample also obscures the essentially dynamic character of a polluting event and the average contents are devoid of any ecological realism. Biocenoses in rivers are never exposed to average contents, which have no actual existence as far as they are concerned. They are in reality exposed to changes in their physicochemical ambiences. The greater and more sudden these changes, the more disturbance they cause. In terms of toxicology, fluctuation is a more important parameter than the average level and, in the present case, the peak maximum concentration reached by the pollutant is more important than the average concentration.

In fact, almost all transient polluting events do not fit the conventional protocol, whether these be urban discharges during rainy periods, and in particular those from combined sewer overflows, or polluting rural runoff generated during storm events, which are particularly destabilising for biocenoses. The time scale of many important water quality processes is on the order of minutes to hours (and not weeks to months), and ecological status is more the result of the dynamics of pollutant flows and especially of the contents of paroxysmal pollution peaks than of daily, fortnightly or even monthly average concentrations, as measured by integrative passive samplers [10-12]. Understanding the process linkage between watershed hydrology and stream water chemistry requires measurements on a time scale that is consistent with these processes [13]. Thus, continuous monitoring is essential for properly determining the chemical and ecological statuses of a water body [14]. Note that definition of the chemical status of water bodies, sensu WFD, is normative, as the texts call for a list of priority substances to be monitored. The scheduled revision will probably increase the number. However, the pertinence of such standardisation may be questioned. While it is true that a laboratory analysis deploys a wide range of analytical techniques for determining the exact content of specific analytes, in view of the high cost of the laboratory analyses required and the potential artefacts that may be introduced during the conventional sampling sequence, viz. collection-packaging-transport, it does not meet the ecological realism requirements prescribed by the WFD.

Ecological status

As far as ecological status is concerned, species lists alone cannot judge the biological quality in highly dynamic and anthropogenically impacted water bodies [15-16]. But it should be stressed that the WFD defines ecological status (Art. 2, § 21) as "an expression of the quality of the structure and functioning of aquatic ecosystems" and does not enumerate any specific parameter in annex V. Rather, the "quality elements" used for classifying the ecological status are functional, such as "oxygenation conditions" instead of oxygen concentration, or "acidification status" instead of pH [17]. On the one hand, this opens up the field to integrated technological innovation in terms of environmental monitoring, and on the other it may be interpreted as the need to access more complex information that a simple discontinuous record of more or less relevant parameters. Thus, measurement of driving pressures (physical and biochemical parameters continuously measured and with a greater accuracy than biological ones) as surrogates or proxies of ecological states, can be automated and used to produce, through data processing and modelling, synthetic quality indices or classes of water bodies [18-19], this is the avenue that we propose to explore.

The functional approach to aquatic environments is not a new concept. All the major conceptual river models published in the past three decades take such an approach.
Examples include the 'River Continuum' [20], 'Resource Spiraling' [21-23], 'Flood Pulse' [24], 'River Health' [25], or 'Riverine productivity model' [26] and reviews published on the subject [27-30]. The expression of a recycling distance in the river corridor, as described in the "telescoping ecosystem model" [22] and validated in several publications, demonstrates that it is possible to determine the spatial and temporal dimensions of biodegradation processes in a river or stream, where the largest material fluxes come from organisms involved in the sediment food web [31].

To do this we propose to adopt the concept of “ecological ambience” developed by Michel Lafont [32] (Figure 1) and based on the ranking of nested factors, with abiotic factors (functional unit) supporting the function (biocenosis). A functional unit is a physical-chemical coherent assembly supporting generic metabolic processes operating in a specific physicochemical context. The working hypothesis is therefore based on the existence of physicochemical ambiances, specific to each functional unit, that support a specific biocenosis (ecological ambience) and are modulated by trophic or toxic inflows. A precise description of this physicochemical context must therefore enable the various involved processes to be identified and the likely causes of any variations or alterations to be inferred.

Figure 1: concept of ecological ambience, which breaks down a biotope into functional ecological units, themselves viewed as a sequence of three nested logics: forms (geomorphology), fluxes (hydro-chemistry) and functions (biology).

Over the last 25 years, stream ecosystem theory has expanded to include explicitly the vertical dimension of surface–groundwater linkages via the hyporheic zone or hyporheon, defined as the saturated interstitial spaces below the streambed and adjacent stream banks that contain between 10 and 98% of channel water [33]. This functional unit plays a major role in overall stream metabolism [4] and it can be viewed as a stream bed living reactor where hydrological, ecological, and biogeochemical processes interact. These interactions influence key stream ecosystem processes, such as primary productivity and nutrient cycling, and more especially in the sediments that harbour microbes and invertebrates and are used by some fish for spawning. Unfortunately, this major functional unit is not accessible to conventional analyses without disruption or modifications. Its study thus demands new
measurement tools [34]. We will focus on this key unit, indicator of the global metabolism in hydrosystems [35-36] that will contribute to a better knowledge of the functioning of water bodies.

We propose to work on an elementary ecosystem referred to as a functional unit, that is to say a set of coherent interrelations between a biotop and a biocenosis. This functional unit will be chosen from environments that are in contact with the aquifer and are subject to unexpected anthropogenic or natural variations. Owing to the functional coherence inherent in any ecosystem, variations in physicochemical conditions (or physicochemical ambience) within a functional unit may be viewed not as random but as the responses of a structured environment adapting to modifications in environmental conditions. This coherence in environmental parameters due to the intrinsic dynamic balance of an ecosystem thus makes it possible to deduce a particular status from a set of measurements without necessarily having to measure it directly. In other words, it is to focus on elements acting as surrogates for ecosystem functioning. A good ecological status may therefore be defined as an initial approximation as that in which all levels of organisation of the system under study are working correctly, i.e. no malfunction, such as a drift in one or more parameters or an accumulation of protons or electrons can be observed at any level at all. Indeed, cell energy metabolism may ultimately be schematised as a self-regulating cybernetic system built on the flows of electrons and protons carried and exchanged by molecules such as ATP, NAD, NADP or FAD and other cytochromes. Biological parameters that are difficult to measure would thus be estimated indirectly by investigating the structure of physicochemical data via non-linear statistical data modelling tools. The principle of this biomimetic approach is: a signal pattern from a sensor array, with different selectivities, is processed with multivariate data analysis for recognition and learning. This approach is an emerging technique also referred to as the virtual sensor [37-38], which bio-mimics the functioning of central nervous systems. Indeed, knowledge generation can be seen as data processing through transfer data from sensors into the brain where they are further processed and related to other information. There are already promising applications of sensors networks in the area of water resources management [39] or the definition of environmental condition indicators [40].

Statistical analysis of the structuring of continuously acquired data could thus lead to a relatively detailed typology of ways of functioning and alterations therein that could be extended to the characterisation of toxic metallic or organic ambiences. Analysing hydrobiological data as a function of physicochemical data is not original in itself. However, for two metrics to be compared they must have the same spatial and temporal representativeness. Indeed, because of the limits referred to above, the physicochemical data usually collected are localised in space and time (grab sampling). Comparing them with biological data that integrate the functioning of the environment over a period of weeks usually leads at best to tautologies: the biological data well explain the biological data [41]. Given that, the distribution of aquatic organisms is closely subservient to physicochemical parameters [42]. Our approach will therefore permit to compare comparable metrics, i.e. continuous physicochemical records and biological organisms, which by their nature, include physicochemical conditions experienced.

A real need of new tools

From 2004, Kirchner et al. pointed to the absurdity of some monitoring methods as stupid as trying to understand a symphony if one could only hear one note every minute or two! That is what we are trying to do when we infer the hydrochemical functioning of a catchment from weekly or monthly grab samples [14]. Given this situation, automated monitoring systems are starting to be proposed. But, because of their complexity, cost and a few specific limitations
(reliability and representativeness), they are not yet used as much in water management as their potentials would allow. The deployment of networks of sensors covering all sensitive or nodal points for monitoring a water body involves miniaturising the sensors and lowering their unit cost. While current research into micro-sensors is leading to the emergence of many measuring principles, validation in real field conditions is still very rare. Furthermore, the micro-sensors that are marketed are based for the most part on UV-Visible technology and data processing, are generally controlled by proprietary programs that are totally unintelligible to the user and do not allow measurements to be optimised [43]. Thus the specific requirements of remote water quality monitoring are not satisfied by existing micro-sensors [44-45].

Consequently, faced with the magnitude of this metrological challenge and the urgency of the situation, a paradigm shift is required in order to imagine a new approach to the problem of water monitoring. A possible avenue that merits further exploration involves the deployment of low-cost instrumentation allowing massive data logging, as well as tools for subsequent data validation, management and interpretation. However, while this new type of instrumentation is possible, and even desirable, such deployment of sensors cannot at the present time cover all the WFD parameters.

An innovative feature of the WFD is its focus on ecological effects, which goes beyond the conventional notions of water quality estimating based on potentially harmful physical-chemical criteria. The quality of a particular environment, equivalent to its ecological status, is explicitly defined in terms of ecosystem structure and functions. This innovative framework calls thus for creativity and makes it essential to develop new approaches and new tools for monitoring the status of rivers at a reasonable cost (WFD, appendix III). To this end, we must develop a new environmental chemistry suitable for providing information on the quality and function of rivers and adapted to the geomorphological and dynamic characteristics of the water bodies monitored. Forsaking the vague expressions “undisturbed conditions” or “reference state” and others “pristine states” [46], associated with good ecological status in the WFD, we propose to focus on the trophic structure, its function, and the changes induced by disturbing factors, in terms of the physical-chemical indicators.

Instead of taking individual and sporadic measurements of chemical and biological quality values, we propose a systemic approach in order to diagnose ecological states, by means of a wireless network of autonomous micro-sensors. The objective of its research phase is to establish rules for integrating the various types of information measured, followed in its industrial phase by the design of an automated warning and decision support system aiming at minimising environmental impacts. Thus, by using a bank of simple robust sensors, coupled to a mathematical data processing system, our aims are to identify critical zones and moments in order to guide and focus mitigating efforts specifically on these sensitive zones and at exactly the right time. Such a tool will also greatly facilitate our understanding of the ecological processes in water bodies in general and the water body management, in particular. There are some technological constrains to address as wireless, self powered, remote transfer of data and no harmful components for the environment. All these features are required to facilitating their implementation on field and creating observation networks.

We think that we need a Wireless Real-Time Monitoring System for continuous monitoring of water bodies, in the sense of the WFD, associating surface chemistry, electronics and energy harvesting with data processing and ecohydrology [47-48], a theory based on dual regulation of river health of water link flux of energy and biocenosis activity. Based on both currently available and new technologies, we will lay the groundwork for a new type of tool for surveillance and operational monitoring of water bodies. Its development will help to make
significant improvements in real-time knowledge of their ecological status and help to quantify the results of efforts made to restore and rehabilitate rivers. From a more fundamental point of view, by bridging the gap between physicochemical determinants and biochemical functioning, we will pave the way for physical actions and biogeochemical stimulation measures with a view to restoring a good ecological status. Formally speaking, the aim is to support the field of restoration ecology for water systems, which involves studying their functioning and developing specific ecological engineering.

Conclusion

As environmental parameters present strong coherence due to the dynamic balances inherent in an ecosystem, a structured group of parameters can be exploited to deduce a particular quantity of them without necessarily measuring them directly. Also, there is emerging a new global approach, which, avoiding development of a more specific sensor, is centred on mathematical processing of signal from sensor network with the aim of deducing the monitored variable indirectly. This virtual sensor, otherwise known as “soft sensor” or “smart sensor”, comprises an array of simple and reliable sensors that are not analyte specific but can be linked by a computer program to process certain sample features and build a proxy of the “unsensed” parameter. Virtual sensors will soon be able to measure a ‘fingerprint’ that can be analyzed by a pattern recognition system. Any sensor can be integrated into a virtual sensor system and its data pooled and processed. By deferring the sensor specificity to mathematical processing, smart sensor technology leads to a simplification of sensing elements and to a more robust sensor network.

The quality of this approach lies in how the data from the sensor networks is mathematically processed. These processing steps span chemometrics to artificial neural networks (ANNs) and genetic algorithms, and can be clustered under two main objectives:

1) Determine structure and data correlations using principal component analysis (PCA) and/or canonical analysis;

2) Establish a model from the data that can be used in predictive mode. In this second approach, the techniques used are projections to latent structures and partial least squares (PLS) regression that generalize and fuse the PCA, and the multiple regression methods, or ANNs.

Nowadays, the majority of the statistical treatments used bring only qualitative information, and not quantitative.

At present, the virtual sensor technology is still under development. But already, and despite the expected difficulties associated with this strongly transdisciplinary approach, some promising results have been obtained.

Sensor technologies have emerged from environmental sciences in the last couple of decades as a promising tool and are still in their infancy. They now require validation. Water quality monitoring is currently based on standardized laboratory methods. Sensors, despite being developed more recently, do not have the same recognition capacities and are only seldom used, despite their advantages. Field validations are needed in order to boost their credibility. ISO standard 15839 (released in 2003) provides a consistent protocol for characterizing these sensors, and should facilitate their adoption for routine use by regulatory bodies. Further work is required to increase their operational period, and particularly to prevent bio-fouling and clogging. Other technological challenges include miniaturization of
on-chip modules, cutting energy consumption, developing in situ fuelling, eco-design, geolocation, communication checking, and data validation and transmission. It is equally imperative to improve data management. Clearly, there is plenty of room for progression.
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