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Biophysical Environmental Chemistry: A New Frontier for Chemistry

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Abstract. The paper discusses the position and role of environmental chemistry among the other environmental disciplines. It discusses the various aspects of environmental chemistry and emphasizes the need for developing fundamental studies in biophysical environmental chemistry in order to better understand the functioning of environmental systems. These systems include a large number of various structures in the nanometer to meter range which play key roles on compound fluxes and consequently on the homeostasis of ecosystems and on their disturbance by anthropogenic activities. Both structures and fluxes are presently ill-known and new concepts and methods must be developed in this field. For chemistry, this is a challenging area where supramolecular structures and processes play dominant roles. It is also a challenging field for the development of environmental sciences since detailed and sound physico-chemical processes are needed in macroscopic modeling of compound circulation in ecosystems. In addition, teaching this discipline to chemistry students would allow them to confront complex, structured real systems. This paper also discusses the relationship between biophysical environmental chemistry and the other environmental disciplines within integrated multidisciplinary studies. The structure used at the Faculty of Sciences of the University of Geneva to favour a flexible but efficient integration is briefly described.

'If you ask a chemist to find for you what a dynamo is, the first thing he would do is to dissolve it in hydrochloric acid' (*Albert Szent-Györgyi*, 1893–1986; biochemist, *Nobel price of Medicine 1937*).

1. Introduction

Not all scientific disciplines have reached the same stage in their development. Today, environmental chemistry, as rational discipline, parallels the emergence of biochemistry (formerly called biological chemistry) in the first half of the present century. Achievement of scientific knowledge includes several steps: formulation of concepts, collection, classification, and interpretation of data, and generalization and formulation of new more rigorous and quantitative concepts. Both chemistry and

biochemistry have passed through long descriptive periods in which important discoveries allowed deducing structures and properties of elements and compounds. This led to quantitative formulation of modern concepts allowing predictions to be made on compound reactivity. Whereas descriptive phase in chemistry has probably reached its pinnacle, in biochemistry still a great deal has to be done. This lag is due to the greater complexity of the system studied and, particularly, to the key role played by supramolecular organized structures.

Environmental chemistry deals with even more complicated systems than biochemistry and it is a much younger discipline. Therefore, despite the development of modern sophisticated analytical techniques, it is still at its infancy, *i.e.* much work has still to be done on experimental data collection and classification. Let us think for instance about sediments, soil aggregates or humic compounds which are key environmental components but whose rigorous chemical description is extremely difficult. This enormous difficulty does not mean that rigorous description of environmental systems is impossible: biochemistry has succeeded in de-

scribing in detail the primary to quaternary structures of proteins, polysaccharides or DNA, and of even more complicated structures like biological membranes, even though such achievements were considered as impossible at the beginning of the century. Thus, undoubtedly, environmental chemistry will succeed in describing the components and structures that play key roles in environmental processes. However, to achieve this as much time and effort as have been put in other disciplines will be required and new sophisticated technologies and concepts should be developed. In particular, it is crucial to realize that environmental chemistry (like biochemistry) is more than just an application of 'classical' chemistry concepts and methods. Most of the latter have been developed for chemical systems composed of small molecules, often with only few components. Similarly, most analytical techniques have been developed for homogeneous systems, so that, physically complicated systems should initially be transformed (by preliminary steps such as filtration, dissolution of solid phases or extraction) into well homogenized systems in order that meaningful interpretation of data be possible. Although such a 'classical' chemical approach has been and is still useful in environmental sciences, it is not sufficient to understand the chemical basis of environmental system functioning which largely depends on physico-chemical processes based on the existence of biological and physical structures and of corresponding concentration gradients and fluxes of compounds. This is again exemplified by means of the analogy with biological systems: the chemical analysis of a homogenized biological cell gives some information on its composition, but little on its functioning.

The main goal of this paper is to emphasize this particular aspect of environmental chemistry which may be less familiar to the reader and which is called hereafter 'Biophysical Environmental Chemistry' to suggest the important role of supramolecular physico-chemical structures and their links with biological activity. We believe that this aspect of environmental chemistry should be significantly more developed to allow ultimately efficient environmental protection. To clearly point out the peculiar features of this aspect of environmental chemistry, we compare it with 'classical' environmental chemistry based on the application of well-established general chemistry and chemical analysis concepts to environmental systems. The term 'classical' chemistry is used here for the sake of clarity to distin-

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guish it from 'biophysical' chemistry. This comparison should help to understand the role of environmental chemistry amongst the other environmental sciences as well as one of the chemical disciplines, which may bring new challenges to the development of chemistry. We will discuss here mostly this latter aspect and put 'classical' chemistry and biophysical environmental chemistry in perspective with one another.

2. The Place of Environmental Chemistry in Environmental Sciences

A simplified but useful representation discriminates between three aspects of all environmental natural sciences (Fig. 1): the fundamental understanding of the functioning of unperturbed environmental systems (boxes 1 and 2), and the understanding of anthropogenic perturbations on these systems (box 3). It is essential to make the distinction between aspects 1 and 2 on the one hand and 3 on the other: anthropogenic perturbations cannot be understood and controlled without a preliminary understanding of the behavior of unperturbed ecosystems (see below the analogy with medicine, Fig. 2). A major role of *environmental chemistry*, therefore, is to study the physico-chemical processes occurring in unperturbed environmental systems.

It is also useful to discriminate between environmental 'microprocesses' (occurring at small scales: nm to mm; box 1) and 'macroprocesses' (large scales: mm to km; box 2) corresponding to whole ecosystems. Fig. 1 shows that in both cases their study should be done in close association with microbiology and geochemistry. Although the border between these two scale ranges is rather arbitrary, the nature of the corresponding processes, the techniques used to study them and, consequently, the corresponding conceptual approaches are very different. Traditionally, in many universities, environmental chemistry has been developed in non-chemistry departments (department of soil science or agriculture for soil chemistry, of oceanography for chemical oceanography, of meteorology for atmospheric chemistry, of civil engineering or geology for geochemistry or groundwater chemistry, etc.). Consequently, the development of environmental chemistry has been largely driven by non-chemical disciplines interested in macroscopic aspects of environmental sciences (box 2), and hence 'classical' chemistry concepts, valid for well-mixed systems, as well as 'classical' analysis applicable to homogenized samples, have been and are still by

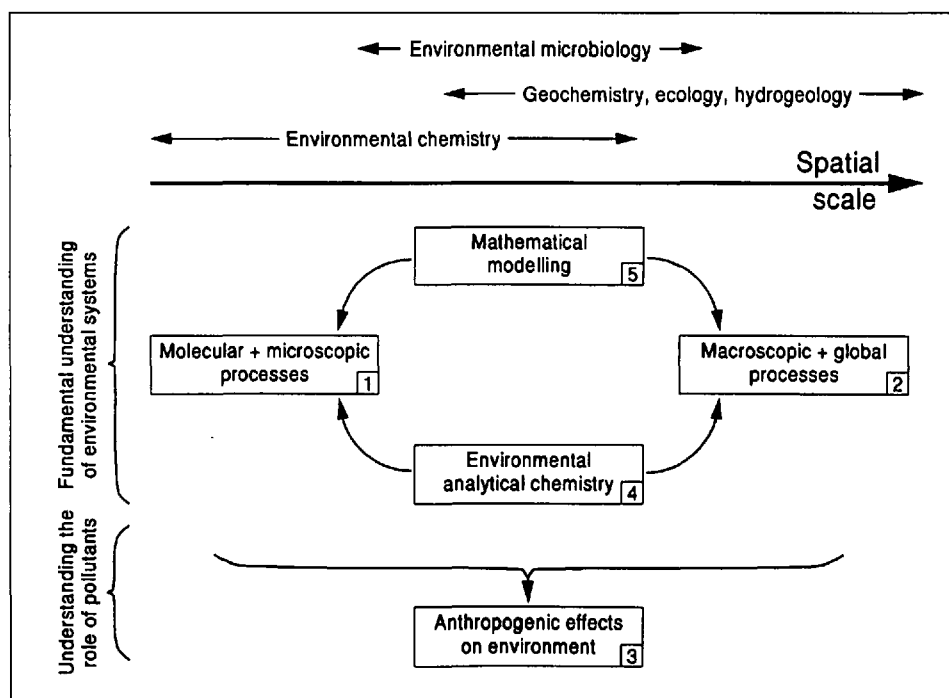


Fig. 1. Different aspects covered by environmental natural sciences

far the most widely used. In particular, such approaches are the ones applied to quality monitoring in governmental institutions. As mentioned above, they have their usefulness but environmental chemistry should not be restricted to this classical approach, as it is not sufficient to provide the necessary concepts and information for developing predictive models of ecosystem functioning. Complementary studies on molecular and microscopic structures and related processes (box 1), *i.e.* biophysical environmental chemistry, are required. They need long-term physico-chemical investigations, with sophisticated techniques and high-level biophysical, biochemical or physico-chemical competence which are generally only available in chemistry and biochemistry departments. Therefore, full development of environmental chemistry should include the biophysico-chemical approach as well as the aforementioned classical aspects. Both branches should be in close contact with non-chemical environmental disciplines. But, while the classical approach can be developed in non-chemical departments since it is based on well-established concepts and methods, the biophysico-chemical approach should be studied and developed in chemistry or biochemistry departments and requires its recognition by the other chemical disciplines as an important branch of applied chemistry, equivalent to biochemistry.

Another major task of environmental chemistry is to develop the *analytical chemical methods* (box 4) needed to study environmental processes (boxes 1 and 2) and allow environmental quality monitor-

ing (box 3). Obviously, since chemistry influences many geological and biological processes, these methods are required not only by chemists but also by most other environmental scientists. Analytical chemistry has thus a key role to play in almost all aspects of Fig. 1. Because of it, a common idea is that the development of analytical methods for environmental quality control is the major role of environmental chemistry. This notion is not correct, as it can be understood by the analogy between environmental and medical sciences discussed below (Fig. 2):

- Although, unquestionably, environmental analytical chemistry is of great importance to all environmental scientists, environmental chemistry should not be confined to it. The study of biophysico-chemical processes is another key component of environmental chemistry, as important for the ultimate protection of environmental health as biochemistry and biophysics are for medicine. Incidentally, the analogy with medical sciences also helps to understand the difference between 'classical' and biophysical environmental chemistry: they parallel physiology, and biochemistry or biophysics respectively. At any rate, the simultaneous development of analytical chemistry and process studies is as vital for solving environmental chemistry problems as for combating diseases in the medical domain.
- The nature of environmental analytical chemistry itself should be discussed. Because environmental chemistry has often grown in non-chemical universi-

ty departments, environmental analytical chemistry has been largely restricted to the application of *classical analytical methods* to environmental samples. Even though quite sophisticated and very useful adaptations of instrumental analytical techniques have been done, *original analytical concepts* or approaches (Sect. 3.2) are only rarely developed specifically for studying environmental processes. In fact, such developments require *i*) long term investigations, and *ii*) tight coupling with detailed physico-chemical process studies which are outside the scope of most non-chemistry departments.

- Because of the urgency of solving pollution problems, most administrations and many research foundations favor the founding of strategic short-term and, therefore, empirical studies. Because of the key role that environmental chemists have to play in developing analytical methods for environmental quality monitoring, they are under a strong pressure to move progressively from fundamental studies onto biophysico-chemical processes to tackle short-term problems related to environmental management. A real danger lies here for the future. Urgent pollution problems must be solved without any doubt, but one should not forget that for the long-term basic research is the most useful and it pays off [1]. Without the results of long term fundamental studies in biochemistry and microbiology, it would not be possible to fight against tuberculosis, diabetes, cancer and many other diseases today. By favoring short term empirical studies on the environment, the authorities discourage thorough-minded scientists

to undertake fundamental studies in this field, thus hampering environmental science to develop into a sound science. This may have dramatic consequences for the future generations, which will be confronted to more serious pollution problems than ours, but who will have no rigorous scientific discipline to solve them.

Sect. 3 gives more details on the type of fundamental biophysico-chemistry studies and advanced analytical chemistry developments which are needed.

3. Specificity of Biophysical Environmental Chemistry as a Chemical Discipline

3.1. Study of Environmental Biophysico-Chemical Processes

As far as physico-chemical processes are concerned, work conducted over the last 20–30 years by Stumm [2][3], Schindler [4] and others have clearly shown that global geochemical cycles of elements are ultimately controlled by the reactivity and physico-chemical properties of compounds at the molecular level and that, without a good knowledge of the behavior of chemical compounds at this level, no prediction will be possible at the global level [25]. The cycling of phosphorous in lakes (with possible concomitant lake eutrophication) is an interesting example of an old important problem, which has been studied for decades, without yet being able to find models giving satisfactory quantitative description of the complete cycle [5]. This is because phosphorous cycling (as that of most chemical compounds) depends on many still largely ill-known physico-chemical mechanisms such as transfer of phos-

phate through biological membranes, oxidation of organophosphorous compounds, phosphate adsorption on iron hydroxide, nucleation of iron phosphate, oxidation of Fe^{II} into Fe^{III} , calcium phosphate crystal formation, growth and dissolution which itself may depend on adsorption of surface active organic compounds, etc. Each of these steps is intricately related to other physico-chemical processes, in a manner analogous to the metabolic cycles in biochemistry (e.g. Krebs cycle for glucide metabolism in organisms). The primary role of biophysical environmental chemistry is to elucidate the most important steps at the molecular and microscopic level, in particular, those which play a rate limiting role in the overall cycle of the element of interest. The aforementioned microprocesses are examples of processes which are rarely studied in detail in macroscopic non-chemical disciplines, as pointed out in Sect. 2, and that would be more easily tackled in chemistry or biochemistry departments. Only then would it be possible to model rigorously the corresponding physico-chemical processes to include them as submodels in global models of ecosystem functioning. Presently, most global models include physical, biological, or geochemical macroprocesses, but they rarely include detailed microprocesses, because of the dearth of available data. As a result, global models often fail to represent adequately detailed spatial distribution or seasonal evolution of chemical compounds [5][25]. Conversely, in cases where such detailed studies of physico-chemical, and/or microbial processes have been made, good concordance between experimental and predictive calculations are obtained, such as that for the fate of herbicides in the Rhine River after Schweizerhalle accident [6].

In contrast to the usual systems studied in chemistry, environmental chemistry systems have the striking feature that many of their properties are closely related to their physical and chemical heterogeneity. The study of environmental physico-chemical processes, therefore, requires using new conceptual approaches combining classical chemistry concepts with additional ones, in particular reactivity probability concepts and supramolecular structural physical models. The main features characteristic of biophysical environmental chemistry are described below.

- The *chemical heterogeneity* of environmental systems is a first major difficulty for non-environmental chemists who are usually trained to think in terms of reactivity of individual, small molecules. According to this approach,

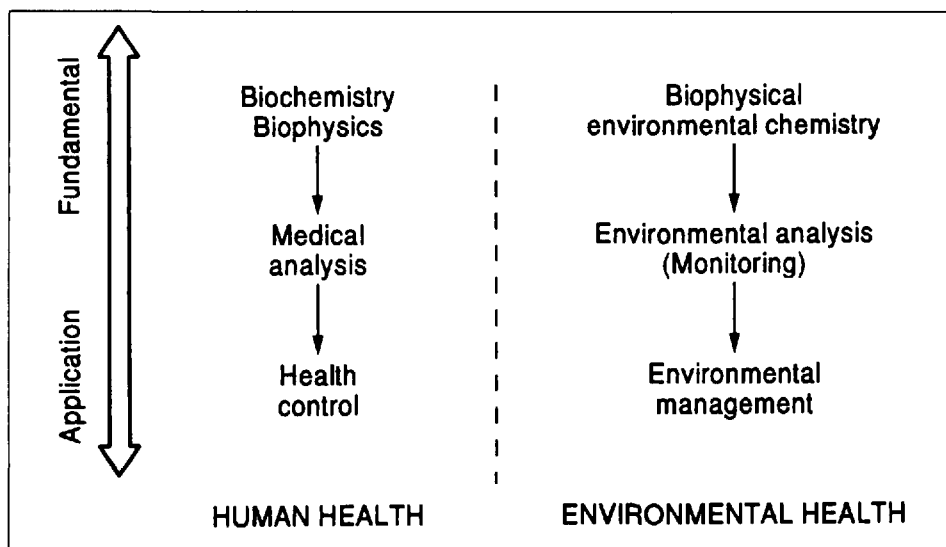


Fig. 2. Analogy between environmental and medical sciences

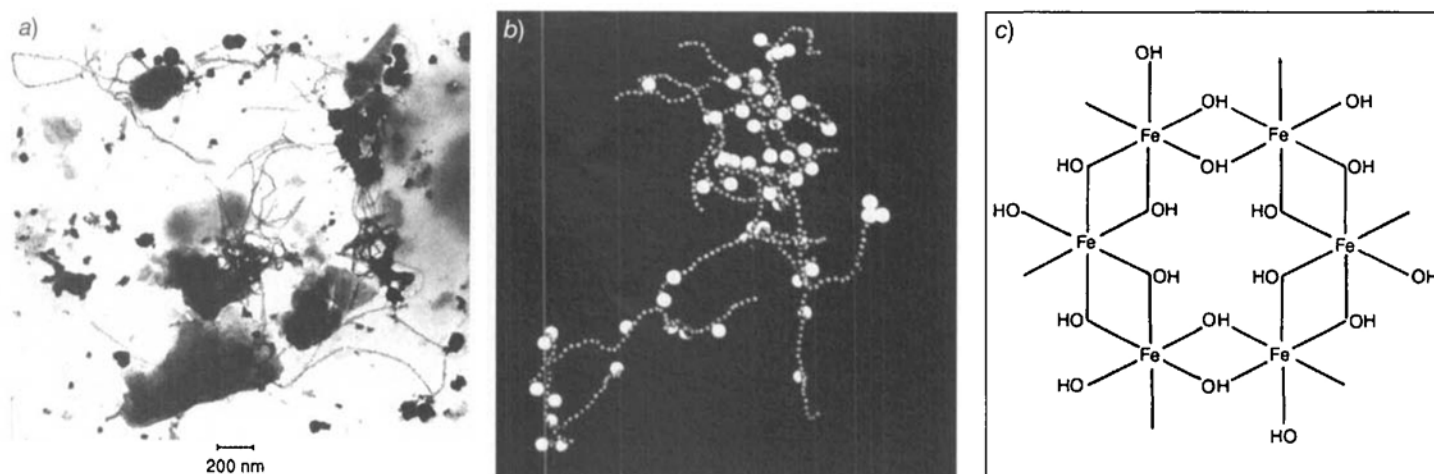


Fig. 3. a) Iron hydroxo-phosphate globules (spherical black particles with size $< 0.2 \mu\text{m}$) formed at the oxic-anoxic boundary layer of a eutrophic lake (Bret, VD, CH) [15]. These globules are aggregated with other colloidal material, filaments, and bacteria (not visible in this figure), which influence the sedimentation rate and bioavailability of iron and phosphate. b) Kinetics of aggregation between spherical colloids and comparatively larger filaments or macromolecules can be simulated by numerical modelling. c) Cyclic hexanuclear precursor which has been shown to be formed in laboratory during the oxidation of Fe^{II} at neutral pH [16]. The iron globules of Fig. 3a have well-defined chemical composition, and transmission electron microscopy shows that they are themselves aggregates of small units (1–2 nm in size), possibly the precursor shown in Fig. 3c.

the study of a complex mixture consists of a first detailed characterization of each component of the mixture. The complexity of environmental systems, however, is huge and complete characterization is never possible. Even if one casts aside the enormous efforts required to study environmental problems in this manner, the solutions to the questions posed are not always obtained. Indeed, this approach ignores that heterogeneity by itself is a key property of the environmental systems of interest. Fulvic and humic compounds of soil and waters provide a good example of such a case. Even after 'purification', fulvic and humic samples are composed of a large number of similar but not identical compounds. As an ensemble, they act cooperatively as a complexing system for metal ions (and small organic molecules), with significant buffering intensities spanning over an extremely wide concentration range of metal ion. As such they play a key role in maintaining acceptable concentrations of vital and toxic metal ions for organisms in soils and waters [7–9]. Alone, none of the individual molecules will impart this property. Hence, they should be thought of as a single chemical system rather than as a mixture of individual compounds. This buffering action due to chemical diversity (or chemical heterogeneity) can be seen as equivalent to the increased stability of ecological niches when the number of biological species increase (biodiversity). It has been shown that the overall properties of heterogeneous chemical systems may be rigorously related to

the properties of individual molecules by introducing the concept of reaction probability [9–11]. Description of such chemical systems should then be based on rigorous statistical concepts, applicable not only to a large number of identical molecules (as usually done in classical thermodynamics), but also to a system consisting of a large number of similar but nevertheless not identical molecules. Similar approaches are applicable to some of the chemical properties of whole soils and sediments.

b) It is now well established that the most important reactions in environmental systems (soil, sediment, ocean, fog droplet) occur in solid-liquid and gas-liquid interfaces [3][12–14]. The electric field and solvent structure are very different at these interfaces (over a thickness of tens of nm) than in the bulk solution and thus may drastically modify the nature and rates of chemical reactions. Unfortunately, a fast glimpse at many chemistry curricula for chemistry students shows that surface reactions (adsorption isotherm, interface catalysis, etc.) are barely (sometimes not at all) taught.

c) The previously mentioned interfaces are the simplest examples of *environmental microstructures*. All environmental systems are physically structured at all levels, from nm to km range. Examples of large structures are soil horizons; lake, ocean or atmosphere stratification; geological layers. Microstructures are those which environmental chemistry is more concerned with. Aggregates between large polysaccharide macromolecules, clays and microorganisms in soils, water, and

sediments or dust particles in the low troposphere are examples of microstructures in the range nm to mm (Fig. 3). They play a key role for example for the circulation of oxygen and water in soils and for that of most nutrients in the whole biosphere, and, therefore, they exert key influences on the maintenance of life. Sediment-water interfaces in lakes and oceans are other example. They are stratified at the μm to mm level (Fig. 4) in successive layers of varying chemical composition, which controls the overall exchanges of chemicals between the bulk water and the sediment. Similarly, the gas exchanges at the ocean/atmosphere interface (such as that of CO_2 with its link to climate change) are predominantly controlled by a diffusion layer of 30–80 μm thickness whose chemical composition is very different from the bulk solution. In all cases, the functioning of living environmental macro, and microsystems is very much dependent on their physico-chemical structure (see d); indeed the functioning of living systems (organisms or ecosystems) is based on pH, redox and other chemical gradients which can only develop with physical heterogeneity [15][18]. A good characterization of environmental microstructures is, therefore, a key task of environmental chemists (as characterization of cell structure is a key aspect in biochemistry). This implies knowledge in colloid chemistry, macromolecular physico-chemistry and biophysical concepts as well as the development of adequate analytical tools. These fields are also rarely included in the usual training of

chemists which is largely focused on homogeneous solution chemistry (see introductory quotation by *Szent-Györgyi*).

- d) The physical structures existing at all scales of environmental systems and the corresponding chemical gradients imply the existence of *fluxes of compounds* within the system of interest (e.g. soil aggregate), or between one compartment and the neighboring one (sediment-water interface). Environmental systems (micro- and macrosystems) are, therefore, dynamic ones. Understanding environmental processes then necessarily implies coupling kinetics of chemical reactions with physical transport processes [18][19]. This often occurs by molecular diffusion in microsystems (e.g. soil or underground pore water), as well as by eddy (turbulent) diffusion and laminar or turbulent hydrodynamic flow, at the macroscopic level (e.g. lakes, rivers, atmosphere). This is an additional lacuna in the training of most chemistry

students. Not only the coupling of chemical and diffusion equations is rarely taught, but often more emphasis is laid on chemical equilibria than on chemical kinetics. The coupling of chemical reactions with hydrodynamic transport processes is also not taught to university chemistry students. With respect to that particular aspect, chemical engineers may have a better training to solve macroscopic environmental chemical problems.

It is essential to realize that properties related to items *a* to *d* above, in combination with classical chemical reactions, are key factors for the maintenance of the *homeostasis* of environmental systems. They also correspond to processes of environmental systems which are particularly sensitive to impacts of anthropogenic activities. These concepts should then be taught in detail to future environmental scientists, and even given at a general level to chemistry students, so that they could take them into account during their professional life.

3.2. Environmental Analytical Chemistry

Analytical chemistry, *i.e.* development of new analytical methods based on new physico-chemical principles, is a well-established branch of chemistry and will not be discussed here. However, environmental sciences definitely need the development of new analytical methods specifically adapted to the physico-chemical nature and properties of the environmental systems under study. Many pollutants or vital compounds in environmental systems are present at trace levels. Concentration levels below the ppb are currently determined. High sensitivity combined to large selectivity (due to the complexity of environmental systems) are, therefore, key characteristics of environmentally useful analytical methods. This also implies much precaution to avoid contaminations and losses by adsorption on vessels. Much work has been done to solve these problems for environmental applications, by combining careful sampling and sample handling to sometimes very sophisticated instrumental techniques, such as ICP-MS, GC-MS, HPLC-MS, Flow Field Flow Fractionation techniques, NMR and FTIR, or Surface analysis techniques (e.g. Particle Induced X-Ray Emission, Laser Microprobe Mass Spectrometry, X-Ray Fluorescence or Electron Energy Loss Spectroscopy, *etc.*). Such analytical developments are extremely helpful for the progress of environmental sciences. In most cases, however, the sample structure is destroyed and/or average analysis is done. Such analysis cannot give any information on the links between chemical composition or properties and sample structure. These analytical developments hence are similar to those made for non environmental fields, and belong to 'classical' analytical chemistry, according to the distinction made in this paper.

As discussed in *Sect. 3.1*, what is more specific to environment is that ecosystems are dynamic and physically nonhomogeneous. Monitoring average concentrations of compounds is then not sufficient for quality control; concentration gradients which occur over distances sometimes smaller than mm are also key parameters for making predictions on chemical fluxes within or between environmental compartments. This implies developing new specific methods enabling to perform *in situ*, remote sensing of these fluxes, without perturbing environmental systems either by chemical contamination or by physical disturbance. This will also allow continuous monitoring of chemical parameters, in real time, which is required for

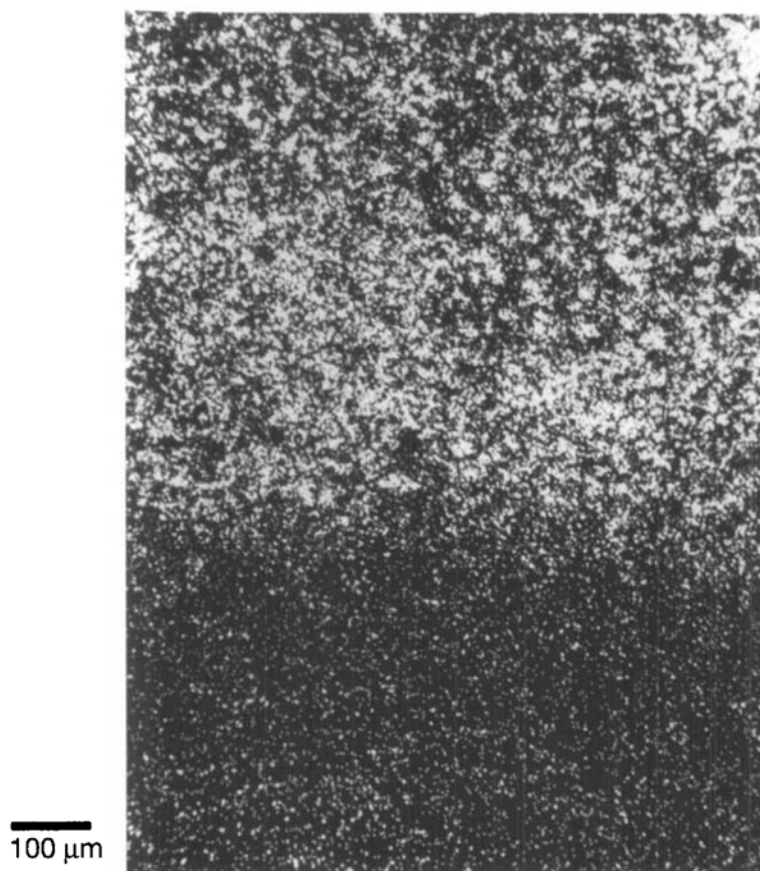


Fig. 4. Fine chemical stratification at the top sediment of sediment-water interface in an anoxic lake. The two layers correspond, from top to bottom, to manganese oxide, and iron oxide formed *in situ* on Teflon plates inserted vertically in the sediment [17]. Picture is obtained by electron microscopy coupled to mapping by energy dispersion spectroscopy. Each sediment layer is a few mm thick and the separation zone between the two layers is 100 μm reflecting very steep vertical redox gradients in the sediment. Transmission electron microscopy shows that the iron oxide layer is composed of either amorphous iron hydroxide globules (similar to those of Fig. 3a) or crystallized lepidocrocite, depending on lake pH (neutral or acid, respectively). The exact nature of these layers influences phosphate and many other trace compound fluxes between water and sediments.

efficient pollution control. The development of such systems became recently feasible, thanks to new technological advances. For instance devices have been built which allow to determine oxygen, anions or trace metal concentration profiles (*e.g.* [20]) at the sediment-water interface, while keeping a resolution of 100 μm , *i.e.* that corresponding to the strata thicknesses on the top sediment layer (*Fig. 4*). Another example is the development of NO_x sensors with very fast response time (fraction of second) for recording fluctuations of NO_x concentrations in the low troposphere. Such fluctuations are directly linked to eddy diffusion processes, and provide more precise estimates of NO_x fluxes than gradients based on classical concentration profile measurements.

Another specific aspect of environmental analytical chemistry is related to speciation [7]. Bioavailability, and consequently, toxicity of any particular element or compound for a microorganism depends both on its flux inside the microecosystem surrounding the organism and on its chemical form (so-called chemical species, *e.g.* redox state, complexation with natural ligands, *etc.*) [21]. Presently, most of the threshold limits of toxic compounds are fixed by rather arbitrary governmental regulations, imposing generally a maximum tolerable average total concentration of the compound in the ecosystem of interest (soil, water, *etc.*). Chemical speciation in particular is often not considered because of the lack of data or adequate analytical technique. Development of non-perturbing speciation analytical methods coupled to detailed biophysico-chemical environmental studies are, therefore, a prerequisite for building sound ecotoxicological regulations.

Such analytical developments are a basic requirement if we wish to solve future environmental problems. But it is also a big challenge. It is becoming feasible thanks to the fast progresses of nano- and microtechnologies and their application to the development of remote controlled microsensors and integrated micro-analytical systems [22]. It should be realized, however, that laboratory development of such systems by analytical chemists (as good as they can be) will not be successfully applicable in the field unless an important research effort is also done to transform the sensors operative in laboratory conditions, into probes working routinely and reliably *in situ*. This requires developments which may be at least as difficult as the sensor development itself. Let us just think for instance of the suspended particles of water samples which

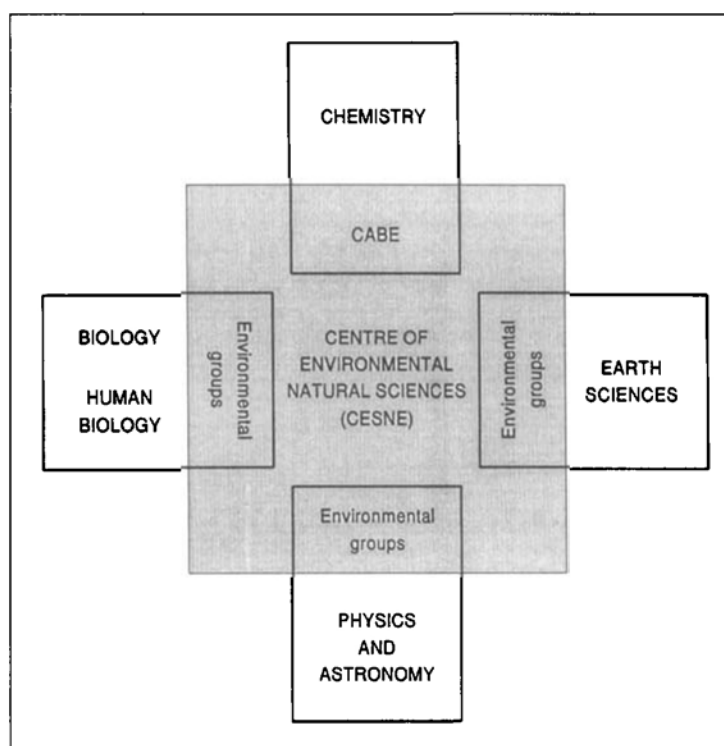


Fig. 5. Links between the various experimental groups of the Faculty of Sciences at the University of Geneva, their basic Departments (Sections) and the Faculty Centre of Natural Environmental Sciences (CESNE)

interfere with most sensors. They can be easily separated by filtration in laboratory but this procedure is not applicable at depths of several 100 m in lakes or oceans: obviously new analytical concepts and methods have to be developed for *in situ* remote analytical methods. Such developments require that analytical developments be done in close cooperation with biophysico-chemical studies and that analytical chemists go to work on the field, with real systems, under natural conditions, in close cooperation with environmental scientists, micromechanic and electronic engineers to consider the constraints of *in situ* measurements. This makes environmental analytical chemistry a challenging multidisciplinary science.

4. Teaching and Research in Environmental Chemistry

4.1. The Position of Environmental Chemistry in a Faculty of Sciences

From the above discussion, in particular *Sect. 2*, it appears that, both for research and teaching, there is a need for two types of environmental chemistry (without clear-cut boundary between them):

- The first type has been called here 'classical' environmental chemistry, including 'classical' environmental analytical chemistry. It may be incorporated in non-chemistry departments. Its role is not to form front-line chemical research but to apply modern though well-established methods and

concepts for solving macroscopic environmental problems, by knitting closely with other scientific disciplines, in a fully integrated manner.

- The second type corresponds to 'biophysical environmental chemistry' and advanced environmental analytical chemistry as discussed in *Sect. 3*. It should be dealt with in biochemistry or chemistry departments, by specialists in biophysical, physico-chemical or biochemical processes, trained to apply these concepts and methods, and develop new ones, to environmental systems. Eventually, these latter will become the concepts and methods used in the above 'classical' approach. This discipline, therefore, is very important also for the improvement of environmental monitoring and management. Although enough interactions should exist between this discipline and other environmental sciences for ensuring the study of environmentally relevant problems, integration with other disciplines may be less stringent than for 'classical' environmental chemistry.

Classical environmental chemistry can be taught at various levels, as one type of applied chemistry to chemistry or non-chemistry students interested in general environmental sciences, with a view to work ultimately on multidisciplinary studies of anthropogenic impacts. Biophysical environmental chemistry should be specifically taught to chemistry and biochemistry students. We believe that such teaching is of vital importance for environmen-

tal chemistry (and environmental protection), and is also a key training for chemistry students since this is one of the few opportunities they have to confront complicated structured systems in the rest of their curriculum.

Various types of organization may be imagined to solve the dilemma of environmental chemistry which should be integrated both in a multidisciplinary institution as far as 'classical' environmental chemistry is concerned, and into chemistry departments for biophysical environmental chemistry. At the *Faculty of Sciences of University of Geneva* (Fig. 5), the environmental group of each scientific discipline (environmental chemistry, environmental biology, etc.) belongs to the department (Section in Geneva University language) of its individual discipline (Chemistry, Biology, etc.) and to a larger structure (CESNE = Centre of Natural Environmental Sciences) directly attached to the Faculty. This for instance allows CAGE (group of Analytical and Biophysical Environmental Chemistry) to perform biophysical chemistry research and to teach to chemistry students in the chemistry department, while contributing by means of 'classical' environmental chemistry to multidisciplinary studies and teaching in the frame of CESNE and its Diploma in Natural Environmental Sciences. This flexible structure is helpful not only to environmental chemistry, but for the same reasons, to all other environmental disciplines.

4.2. Role of Modelling

In recent years, the use of numerical simulation models as a means to evaluate large-scale or complex natural processes has increased sharply. In some cases, the predictions generated by these models are considered as a basis for public policy decisions (e.g. global circulation models to predict Earth climate). There is an over-emphasis on the predictive value of modelling. Even by neglecting the fact that all models are oversimplified compared to natural processes, many natural processes are still unknown and, above all, the primary value of models is heuristic [23]. The prediction capability of models then should never be the main goal of modelling. On the other hand, it is unquestionable that models have enormous importance as educational tools both for students and researchers. They allow in particular *i*) classification of information, *ii*) checking working hypothesis with experimental data, *iii*) formulation of new hypothesis by eliminating unimportant factors, and *iv*) sensitivity analysis.

These considerations apply to all disciplines. But, as a learning mean, modelling is particularly important in environmental chemistry: it is the only tool available to quickly evaluate the indirect but sometimes predominant influence, on the macroscopic evolution of ecosystems, of factors which affect molecular or microscopic processes [25]. Let's take again lake eutrophication as an example: it depends on a number of molecular or microscopic processes such as formation rate of iron hydroxide species like that shown in Fig. 3, its reactivity with phosphate ions, its aggregation processes to form microscopic globules and more complicated aggregates (Fig. 3), and its sedimentation. Although each step must be studied experimentally, only mathematical simulation combining microscopic and macroscopic processes allows understanding the respective role of each of them on the overall evolution of the lake. In general, the time and space domains of chemical processes are very far away from those occurring at the macroscopic or global scale in environmental systems (Fig. 6). It is thus extremely difficult, both for students and researchers, to assess the actual importance of chemical processes on ecosystem evolution. Modelling is an extremely useful tool to do it (Fig. 1, box 5). It is also helpful for non-chemists to learn the importance of using detailed physico-chemical processes instead of empirical parameters to make reliable quantitative predictions.

4.3. Experimental Work

As mentioned earlier, expertise in any scientific discipline can only be acquired by working experimentally in that field for some period of time. This is even more important in environmental sciences because of the complexity of environmental systems and the multidisciplinary nature of the problems involved. As far as environmental chemistry is concerned, the student should be confronted at least with the following three experimental aspects:

- Study of physico-chemical processes *in situ* (in the field). Planning and performing well-controlled experiments in the field is much more difficult than in the laboratory, because of the large number of factors to be considered and controlled in order to allow sound interpretation of data.
- Study of biophysico-chemical processes in the laboratory with model compounds simulating natural systems. Studies on natural systems allow to discriminate between predominant and secondary factors affecting a particu-

lar macroscopic process. However, results of *in situ* measurements cannot provide precise values of physico-chemical parameters. These can only be determined in the laboratory, by using model experimental systems that mimic natural ones. The combination of these two complementary approaches is essential to build environmental chemistry as a rigorous discipline.

- Development in the laboratory and application *in situ* of analytical methods specifically designed for studying environmental processes. Measuring the right parameters in correct conditions is a key issue in order to understand natural processes. This is far to be trivial in complicated and structured natural systems, and often significantly more complicated than with well controlled systems, in laboratory conditions.

4.4. Teaching Environmental Chemistry Concepts

Sect. 3 discusses the basic physico-chemical concepts which are currently missing in many curricula of chemistry and are a prerequisite for understanding environmental chemical processes. The teachers, in the classroom, will be faced with two additional difficulties of a general type, other than those specifically related to the principles, while teaching these concepts to the students. The first is related to the time and space scales covered by environmental sciences (Fig. 6). It is not always easy to make the students to grasp the idea as to how chemical processes occurring at the ns to ms level can affect ecosystem evolutions over centuries or even geological times and again, modeling is a very useful tool here. Another problem is our 'sensitive' time window. Every one understands the meaning of time flow, in the time range from fraction of second to millennia. This type of scales are met in environmental macroprocesses (often biological, geological, physical processes), where the student does not have problems visualizing it. However, the time-space windows in physico-chemical processes are very much different from the above ones and it is difficult to make the students visualize their relevance in environmental chemistry (i.e. the link between chemistry and macroscopic environmental processes). The situation becomes worse if one compares the 'sensitive' space window of man (fraction of mm to tens of km) to the size of plankton (10^{-5} – 10^{-4} m), colloidal particles (10^{-8} – 10^{-6} m), or simple molecules (10^{-9} m). These entities differ in size by orders

of magnitude, and, therefore, behave in a completely different manner. The importance of these differences is not obvious to the students confronted for the first time to these concepts.

A second difficulty of environmental chemistry is that many different concepts have to be integrated to understand the behavior of any particular environmental system. The principles of the various individual chemical reactions (acid-base, redox, complexation, precipitation, hydrolysis, etc.), that may occur in this system, are often easy to understand. It is, however, much more difficult for students to decide which processes to ignore and which ones to consider, *i.e.* which ones play a major role in the evolution of the environmental system of interest, in particular when non-chemical processes have also to be taken into account. In most curricula of chemistry, students learn to understand single processes in depth, but they are not trained to combine many processes together and even less many concepts of different disciplines. At the general teaching level, this may be one of the most important input of environmental chemistry to chemistry students. Even if they do not pursue their studies in environmental sciences, learning how to combine and compare quantitatively many different factors affecting a given process, will be a very fruitful training for any real world applications.

5. Conclusion

The learning of a science in general involves more than the acquisition of new knowledge by a blank mind. Instead it involves a substantial restructuring of pre-existing knowledge, in which new knowledge must compete with the student's previous knowledge and familiar way of thinking [24]. This is particularly true for chemistry students learning environmental chemistry and environmental sciences.

It should also be clearly stated to the students that any curriculum of one to three years in environmental chemistry or environmental sciences is insufficient to make them specialists of environmental processes. The basic requirement for a medical degree is five years, and specialization in a particular field of medicine is required, *i.e.* additional years have to be spent before claiming to be a specialist. Environmental systems are certainly at least as complicated as the human body. There is, therefore, no hope to produce environmental scientists with expertise within 1–3 years. The only thing we can do

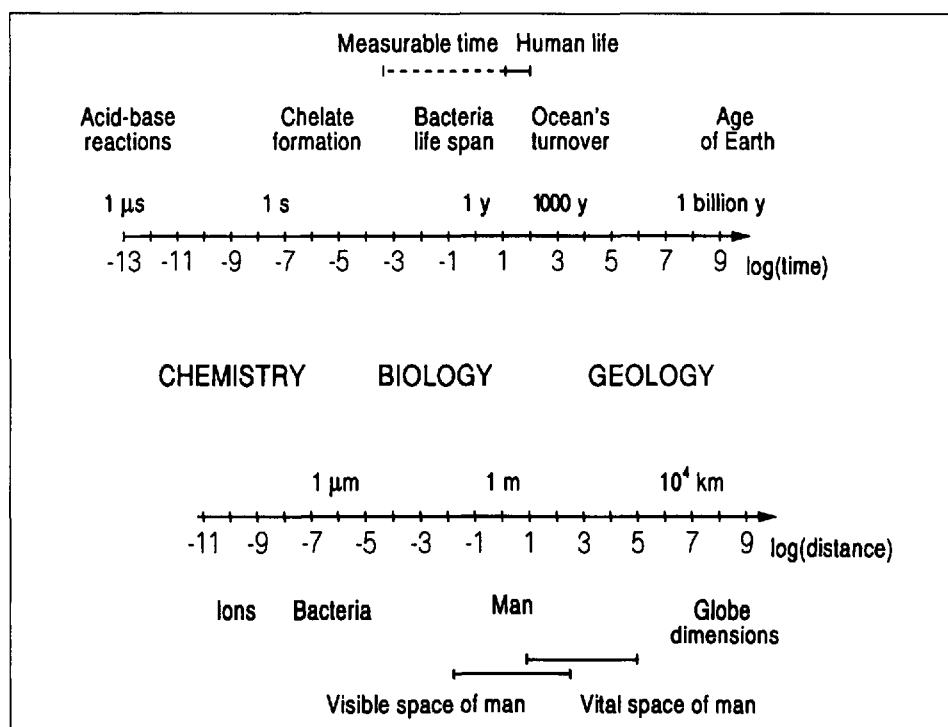


Fig. 6. Time and space domains covered by environmental sciences

(which anyway is a major issue) is to give them the basic concepts necessary to learn and progress by themselves.

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