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Aquatic Modeling: An Interplay between Scales

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***Abstract*—**This paper presents an integrated knowledge-based approach to multi-scale modeling of aquatic systems, with a view to enhancing predictive power and aiding environmental management and policy-making. The basic phases of this approach have been exemplified in the case of a bay in Saronicos Gulf (Attiki, Greece). The results showed a significant problem with rising phytoplankton blooms linked to excessive microbial growth, arisen mostly due to increased nitrogen inflows; therefore, the nitrification/denitrification processes of the benthic and water column sub-systems have provided the quality variables to be monitored for assessing environmental status. It is thereby demonstrated that the proposed approach facilitates modeling choices and implementation option decisions, while it provides substantial support for knowledge and experience capitalization in long-term water management.

***Keywords*—**Aquatic ecosystem, integrated modeling, multi-scale modeling, ontological platform.

I. Introduction

AQUATIC systems modeling, especially when linked to environmental management and policy-making, is often mechanistic, represented by a set of equations that summarize how the modeler perceives the physical, chemical and biological processes driving the dynamic and ever-changing system. As the predictive needs become more long-term over time; the models become more complex as per both, the number of biogeochemical and ecological processes described and their physical framework. Notwithstanding, the limited understanding of the underlying natural processes, especially as regards pollution-ecosystem interactions, along with the insufficient data available restrict modeling either to one scale, usually the macro- or meso-scale, where measurements are feasible [1], or to one scientific domain, usually ecology or hydrogeomorphology, where knowledge is available [2]. Such approaches have been more successful in exploring possible interactions or outcomes of change at one scale rather than predicting outcomes or events of the whole system [3], [4].

A relative example of poor predictability owing to the inability to handle different scales within a single model may be presented by the Sidi Kerair case (Egypt) [5]: extensive coastal erosion due to tidal activity, threatening local flora and economy by the accumulation of floating algae and solid debris at the shoreline, has been addressed at late 1990's by the construction of an artificial lagoon barrier based on the implementation of a physical model; the barrier, however, worsened the problem as it sustained stagnant water pools that supported further algae spreading that, soon, overturned local flora. On the other hand, trusting entirely trophic transfer models might also lead to misjudgments, as it was shown by the early 1980's attempts to preserve the Dogger Bank herring at North Sea: as over-fishing was thought of as the major cause of the population decline, spawn enrichment was carried out, yet to no success [6]; it was soon evident that the existence of sub-optimal hydrogeological conditions, i.e., a physical factor that could be apparent at physical modeling, hindered the recovery of the population.

Inevitably, the optimal model should be *mechanismic,* i.e., multi-scale and integrated. Developing such a model is, generally, much more challenging than building a single-scale model, because the modeler has to determine what scales include and how/where to connect them. Integrating modeling [7] comes at least in three parts: (a) combine models for different processes to link abiotic with biotic parameters at the same space–time scale, (b) combine processes of the same type across space–time scales (e.g. hydrological transport processes from lateral fluxes in upstream catchments to longitudinal buffering in downstream floodplains), and (c) combine processes of different types across different scales (e.g. export of metals from upstream mining areas with organisms exposure in the downstream parts of the river).

Multi-disciplinary modeling teams might serve adequately the first part, since each participant contributes specialized disciplinary knowledge and data acquisition processes to narrow knowledge gaps. Usually, however, collaborative efforts are loosely organized in a hierarchical way (Fig. 1), whereas little attempt is made to maintain the information flow at the required granularity level [8]. The main reason for this lies in the structure of knowledge, which remains context-specific across different disciplines: (i) disciplinary specialization makes it difficult to find a common language in collaborative teams (e.g., the term 'monitoring' is variably defined in different disciplines as period inspection in ecology, continuous detection in metrology, or supervision of activities in management); (ii) existing scientific knowledge may reflect a historical scientific and socio-political context unsuited for the current environmental issues; (iii) mismatches in space and time scales, in forms of knowledge (e.g., macro-systems versus nano-systems), and in levels of precision and accuracy (e.g., qualitative versus quantitative data), may create difficulties in the comparability of results or the flow of information; (iv) disciplinary scopes dictate the way scientists view and study the ecosystems, often favoring certain assumptions over others.

The field of hydrology, for example, is often successful at predicting depositions in relatively small scales where detailed information on small-scale topography exists [9]. The geomorphology field is more concerned with wider areas, yet it uses small-scale data for calibrating large-scale models [10].

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Ecology, using information from hydrological and geomorphological studies, could certainly provide the means to solve environmental problems; yet, it only recently has started to elucidate ecosystem dynamics to produce relatively precise models [1], [2]. Nonetheless, several knowledge gaps exist, the bridging of which requires the collaboration of many disciplines (such as microbiology and nanotechnology) rendering the field trans-disciplinary [7]. Thus, ecological responses to pollution are often considered in qualitative, semi-qualitative or stochastic terms, increasing uncertainty manifold in decision-making [11].

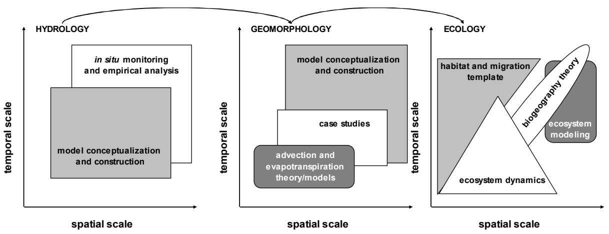

Fig. 1 Schematic representation of the knowledge structures of hydrology, geomorphology and ecology; the arrow indicates information granularity level increase

Using an ontological platform can help putting experts' knowledge in the right perspective, providing, also, spatio-temporal projections for the second part of integrating modeling. Ontologies are considered as appropriate modeling structures for representing complex domains at a knowledge integration platform that handles structured or unstructured information resources [12]. Most platforms developed, however, provide a taxonomic (*is-a*) backbone, built on strict hierarchical (often disciplinary) intra-relations, that is used to detect mereological (*part-of*) inter-relations at the same or adjacent knowledge levels (see, e.g., [13], [14]); but this format cannot satisfy the third part of integrating modeling. In most aquatic ecosystem ontologies (see e.g., [15]-[17]), the scientific domain (and its scale) is drawn first and then the object of interest is represented as a downstream instance of this domain; there certainly exists the risk either to supersede interrelations existing beyond the domain's scale boundaries or to rely on partonomic functions that are not consistent with the site-specific hydrogeobiochemistry.

This paper presents a methodological framework for bridging the gaps between macro- and micro-scales in aquatic ecosystem modeling through a flexible ontological platform, designed/developed to accommodate partonomic functions in and between different knowledge domains and levels. Focusing on the water system *per se* and its processes between its components, ontology building adopts herein a processualist view for capturing the *mechanismic* aspects of the modeled structure: the ontology is built around the (sub-) system of interest and subsequently integrates all relevant scientific domains (and scales), with a view to accurately representing (and, thus, predicting) the processes that are the most likely to take place on site.

II. METHODOLOGY

The integrated approach suggested herein focuses towards the modeling of all physical and (bio)chemical processes that take place in the aquatic ecosystem of interest in order to (i) reveal all possible paths to follow energy or mass (i.e., pollution) entering the system, and (ii) identify a set of key monitoring parameters for each path, the estimation of which will be used to recognize early the processes initiated at the micro-scale so as to predict their propagation at the macro-scale. Modeling follows a four-phase iterative process, briefly presented below.

A. Phase 1: System Description

The identification of water-quality issues and concerns associated with the aquatic ecosystem is necessary to obtain a precise expression of the existing or potential ecological problem(s) that the system faces. Regulators, conservation groups, residents, landowners, industries and other stakeholders should participate in this phase by engaging in focused discussions regarding their interests and needs. It is important to identify key issues and concerns early in the process because such information provides the modeler with a basic understanding of the tradeoffs that need to be supported by the model.

B. Phase 2: Functional Analysis

The purpose of this phase is to define the prioritized set of system functions that the model has to include in order to serve its intended scope, i.e., to support the management of the outcome of the events defined in the first phase. The system of interest is decomposed into autonomous sub-systems based on ecological criteria and/or hydrogeochemical criteria, depending on the prevailing conditions and the nature of the related problems.

The ecosystem is considered as an input–output system with boundaries (Fig. 2). The inputs to the system are energy and mass; whatever energy or mass enters a defined ecosystem must eventually leave. This is always true, although the characteristics of the energy and mass leaving the system may differ from those entering, depending upon interactions within the system. Thus, any ecosystem has three primary components to be characterized: the input mass/energy budget, the system itself, and the output mass/energy budget. The output mass/energy from a system can be changed both in character and in timing. Only two mechanisms can change the output: either the input mass/energy budget has changed or the ecosystem itself has changed. A variety of forces interact dynamically across the time and space scales of the environmental continuum. For any ecosystem domain, this dynamic interplay of forces will be apparent at large variations over time in ecosystem budgets of mass and energy; usually, when budgets are stable there is only one critical variable that greatly dominates the remaining variables/parameters.

The functional analysis is based on structuring a model for each sub-system describing the interactions among its elements, in order to elucidate the propagation of an impact through the sub-system and, also, the secondary processes that

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will be triggered.

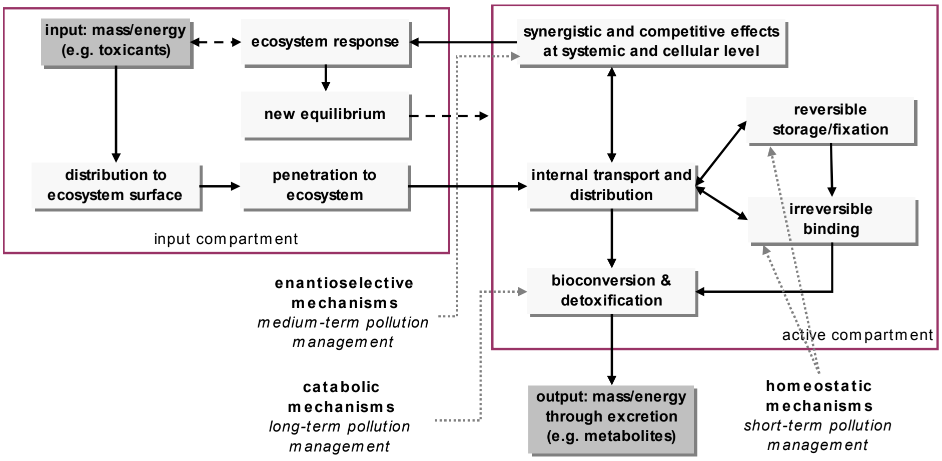

Fig. 2 Simplified compartment model for stressor - ecosystem interactions, used for system decomposition and translation of the requirements into sets of characteristics pertinent to each sub-system (functional analysis)

C. Phase 3: Systemic Analysis

The functional model is reformed into an ontological matrix of intersected elements, where the nodes are the key parameters describing each sub-system; the connection of the nodes represents inter-dependencies in regulation, initiation or propagation. Since the functional model portrays the ecosystem as a system with inter-related parts (sub-systems), the ontological network cannot be built on an *is-a* hierarchy as it is already based on partonomic relations. Therefore, the ontology is built around the sub-system of interest (e.g., the first impacted or the most susceptible), providing extensions to the upstream and downstream links. Ontology merging and alignment tools required have been adopted from [18] and [19].

The matrix is subsequently thinned out for eliminating properties/relations of low significance. Thus, the most critical nodes are identified and set as quality criteria, whereas their interrelations formulate the sub-system constraints. Thinning is performed according to the information-theoretical algorithm of Cheng et al. [20], although more advanced approaches can be considered as those using maximum likelihood estimation (e.g., see [21]). The algorithm has three subsequent steps termed drafting, thickening and thinning. At the first step, the algorithm establishes, from the data, the mutual information for each pair of variables and constructs a draft digraph from this information. During thickening, the algorithm adds arcs between pairs of nodes if the corresponding variables are not conditionally independent given a certain conditioning set of variables. To conclude, each arc of the graph obtained so far is examined using conditional independence tests, and is removed if the two variables connected by the arc prove to be conditionally independent.

D. Phase 4: Physical Analysis

This phase completes functional analysis by identifying the fluxes, the boundaries, and interfaces among the sub-systems. During the implementation of this phase, super-structures may be identified through shared inflows, outflows, or interfaces. In such a case, a re-assessment of phase (2) might be called for (and the phases thereafter), provided that the synergy of the sub-systems of the super-structure is such that can be modeled as a single system.

III. Case Study

A. Implementation Area

Saronikos Gulf is located in the Eastern Mediterranean Sea (Fig. 3). It is a typical semi-enclosed marine environment, which comprises two main sections, the eastern and the western, separated by the Aegina Island; the eastern section has relatively uniform topography, while the western part is deeper (>400 m). At the north of the Gulf lays the Elefsis Bay with maximum depth of about 30 m; the Bay is joined to the Gulf by two narrow and shallow inlets. The Piraeus Port, which is one of the greatest in the Mediterranean Sea, is located about 1 km southern of the eastern inlet. The shoreline is densely populated and heavily exploited, rendering the Gulf one of the most polluted marine regions in Greece; large amounts of industrial and urban sewages end up to its coasts, sometimes without even having been submitted to complete treatment [22].

Actually, urban sewage from the city of Athens reached the Gulf untreated for many years. Only a few years ago a treatment plant was constructed to protect the Gulf, located on the small island of Psitalia near the Piraeus harbor. An approximate 800.000 m^3 of treated wastewater is daily discharged at approximately 62 m depth [23]. Significant amounts of nutrients outfall directly into the Elefsis Bay from more than 30 industries (oil refineries, steel mills, shipyards, etc.). In the main Gulf the effect of the Psitalia outflow is evident, as a plume of nutrient-rich water extending about 20 km south of the Salamis Island. Fishery activities are also important in the Gulf, mainly in the central and its southern side.

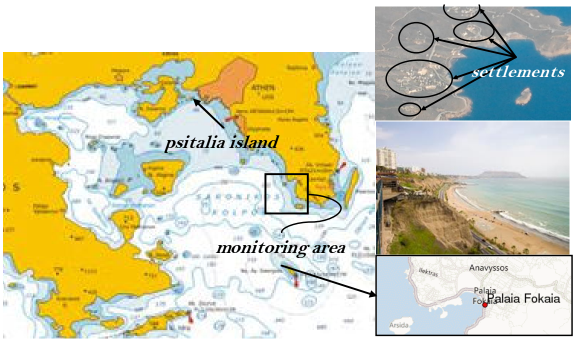

Fig. 3 Saronicos Gulf (right), indicating the Psitalia wastewater treatment facility and the area under study, at a groove before the Sounion Cape, hosting Palaia Fokea and Legrena coasts (bottom left), a rapidly developed region with several ongoing engineering projects (middle left) and a number of settlements (top left)

The Gulf receives low rainfall inputs and some inputs from small rivers and ephemeral streams (Kifissos and Ilissos). The water in the Elefsis Bay is 2-3^{o}C colder than that of the Gulf during winter and the hydraulic flux of the seawater lies from western to the eastern side. Stratification starts during March and is completely developed during August with a thermocline observed at about 15 m depth. During winter, the water column is fully homogenous as a result of wind driven currents. Salinity near the eastern coastal regions is lower due to brackish wastes and sub-water springs that outflow to the eastern shoreline. An area of interest is found in this shoreline, where a natural groove before the Sounion Cape (Fig. 3), is rapidly developed into recreation and aquaculture areas, whereas a number of expanding settlements surround it. The shore has coarse mixed-sediment beaches of sand, granule and pebble. The wave exposure is uniform, and the alongshore and across-beach (perpendicular to the water line) sediment characteristics are relatively homogeneous. Both cross-shore and alongshore sediment transport processes drive changes in shoreline position, however, the along-shore processes act over much longer time frames, giving rise to shoreline variability, especially during spring and summer.

The Gulf endures a considerable accumulation of chlorinated organic pesticides [24], [25], possibly from the central Athens sewage outfall received in the past. Moreover, the neighboring fields, which were cultivated systematically until recently, might have contributed to the enrichment of the sediments with fertilizers through run-offs. The currents and the geology of the monitoring area impart some protection over the chemical burden, keeping seawater at acceptable quality. Despite, the rapid expansion of the near-by settlements some years ago has driven considerable declines over many water quality parameters, including coliform levels, eutrophication indicators (especially increased nitrogen), and heavy-metal resistant bacteria.

B. Modeling

Diverse and complex natural processes within the coastal zone of the Gulf, i.e., waves, littoral currents, agricultural runoffs, industrial wastewater, subsidence, sediment and spill transport, bioinvasion, etc., serve to continually change the physical, chemical, and biological features of the fragile seashore ecosystem. On the other hand, regional conditions and local shoreline characteristics control the differing interactions and relative consequences of these natural processes. Thereby, even small vertical changes in sea level, for example, can impact coastlines dramatically, especially on the gently sloping coast used herein as the implementation case study (Fig. 4).

The functional analysis was narrowed to the local problem of pesticide and fertilizer burden. The produced model revealed, also, a significant increasing trend on phytoplankton blooms, correlated to the expansion of the major settlement towards the seashore and the engineering activities at the front beach.

Land-sea exchanges at coastal areas influence biogeochemical cycles at an extent much more than their coverage might imply. Processes that occur disproportionately in coastal environments, such as organic matter decomposition and burial, mineral formation, and denitrification affect the water balances of many elements [26]. Assuming nitrogen to be the principal nutrient limiting phytoplankton biomass in the system under investigation, an increase in nitrogen inflow might be responsible for the phytoplankton rise, carrying along several organic and inorganic loads (heavy metals, hydrocarbons, etc.) and their microbial paraphernalia (coliforms and bacteria). Evidently, the nitrogen load has been selected as a critical quality criterion (phase 3), the monitoring of which will allow the elucidation of the ecosystem status, since the given inter-relations can provide a sufficient model for other criteria. The physical model developed (phase 4) and the ontological matrix produced, describing the nitrification/ denitrification processes in a vertical section of the physical model, are shown in Fig. 5. The ontological matrix includes external loading of nutrients, surface and bottom fluxes of nutrients due to wind mixing and bottom sediment re-suspension, predicted short-wave radiation and light attenuation, and assimilated water temperature and salinity conditions. The benthos and the water column actually form a super-structure with nitrogen loading as common input and denitrification products as common output.

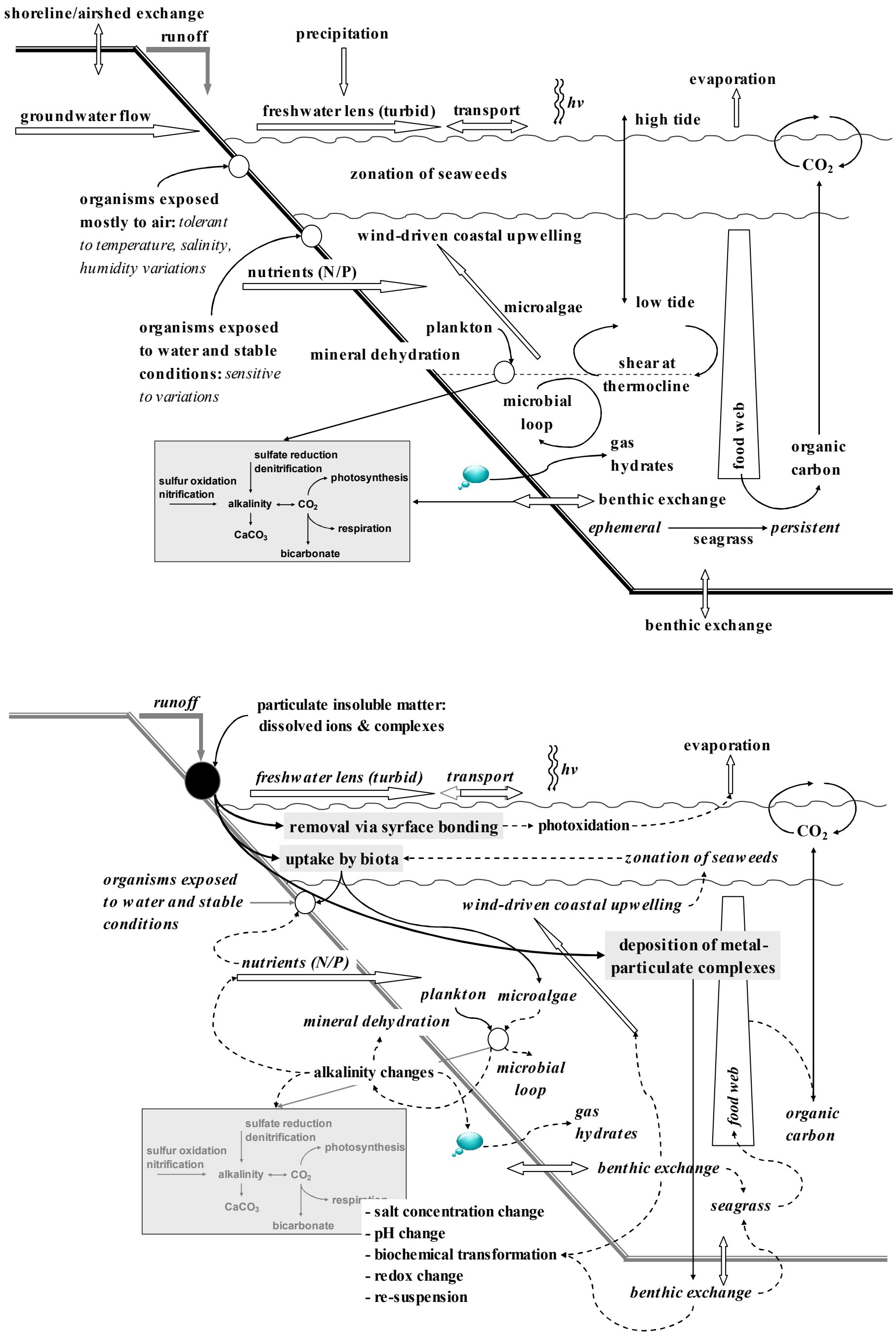

Fig. 4 Drafting of the functional model of the shoreline segment under study using compartmentalization on the basis of ecological and hydrogeochemical criteria. (top) Schematic diagram of the ecosystem, including biotic and abiotic inter-relations; benthic exchange produce is moving towards the surface through the wind-driven coastal upwelling and the food web that start the cycle again. (bottom) An example of how an input (e.g., particulate insoluble matter such as lipiphilic pesticides) affects these inter-relations; bold lines indicate primary mechanisms, straight lines show initial effects and dotted lines show the propagation of these effects to other ecosystem elements: since insoluble, the input is caught up by the turbid zone and is partly removed via surface bonding, photodegradation and evaporation. Vertical diffusion contributes to its uptake by biota, which becomes significant below the low tide zone, where the impacts on the plankton, algae and microbial zones contribute to critical alkalinity changes adversely affecting (by shifting ionization equilibria) energy production (box in gray), mineral dehydration, nutrient availability and gas hydrate supply. Benthic exchange and re-suspension affect ephemeral and persistent sea grass species that propagate the impact to the foodweb and the carbon cycle, while coast upwelling returns the impact back to the surface to restart the impact cycle through the seaweeds.

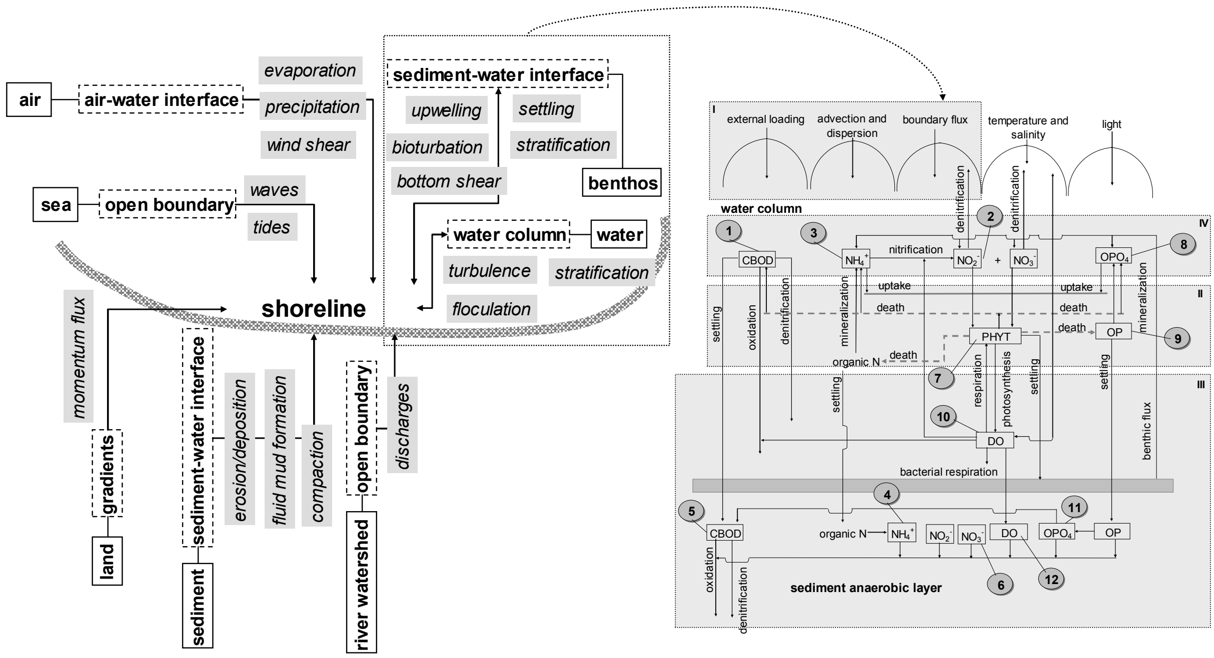

Fig. 5 Part of the physical model drawn for the case study area (left) and the corresponding ontological matrix produced for the benthos and the water column systems (right), actually forming a superstructure. Boxed species are the nodes with the higher in- and out-degrees: DO (dissolved oxygen); PHYT (phytoplankton as carbon); CBOD (carbonaceous biochemical oxygen demand); NH_4^+ (ammonium nitrogen); NO_3^- /NO_2^- (nitrate and nitrite nitrogen); OPO_4 (ortho-phosphorus or inorganic phosphorus); OP (organic phosphorous)

The translation of the quality criterion into a set of characteristics (phase 2) resulted in the following water quality parameters which are linked to nitrogen inflow: dissolved oxygen (DO), phytoplankton as carbon (PHYT), carbonaceous biochemical oxygen demand (CBOD), phosphorus or inorganic phosphorus (OPO_4), organic phosphorous (OP), ammonium nitrogen (NH_4^+), nitrate and nitrite nitrogen (NO_3). In the shoreline system, one source for DO is photosynthesis carbon fixation, which is proportional to the density of phytoplankton and their growth rate [27]. Re-aeration can be either a source or sink for DO; in the usual under-saturation condition, it functions as a source for DO, which is diminishing mainly due to the microbial aerobic processes, sediment oxygen demand (SOD), phytoplankton respiration, nitrification, and oxidation of CBOD.

The ontological matrix developed at phase (3) describes a basic transformation process including photosynthesis, uptake, respiration, nitrification, denitrification, benthic flux, sediment suspension, and external loads, putting emphasis on the water column and the sediment anaerobic layer at the accumulation sub-compartment. After thinning, the nodes with the higher in- and out-degrees are shown in Fig. 5 in descending order of significance; boxed species are the nodes with the higher in- and out-degrees, whereas circled numbers indicate the major points of interactions.

IV. Discussion

The use of the ontological platform is extremely valuable in outlining/elucidating processes and determining control variables in aquatic ecosystems. The high complexity of ecological processes and their inter-relations might (and commonly do) conceal the significant links in mass/energy and other interdependence chains that, actually, drive a constantly changing system responding to seasonal variations and pollution load alterations. Moreover, the profound non-linearity of the quantitative relations that govern the interdependence chains create the pre-requisites for chaotic behaviors that could result in irreversible adverse effects on the ecosystem under consideration, as well as, the wider environment.

In the present work, ecosystem-relevant spatio-temporal parameters at various scales are revealed and linked to support dynamic multi-scale modeling. This scheme enables knowledge to be used not only for representation but also for reasoning at conceptual level, proven to be useful in real-world problem solving; that requires, inevitably, the involvement of domain experts, herein realized by integrating the modeling construction process within a framework of 2nd order cybernetics.

The integrated modeling approach presented herein, as proven by the relevant case study, enables (i) the precise definition of the seashore and related stakeholders needs; (ii) the timely identification of the pertinent critical quality parameters and their variables, feasible by the the drafting of the ecosystem using ontology-based functional modeling and its reviewing using physical modeling; and (iii) resources saving due to the reduction of monitoring parameters to those addressing specific ecosystem needs.

The seashore model was developed through a holistic analysis and a systemic breakdown of the site-specific physical and chemical inter-relations, including optimization and stakeholders' expectations. Throughout model development, uncertainty has been inherently minimized since the modeling objective was precisely defined within the coastal management context, described with the ecosystem elements identified in the functional analysis and accounted for in the quantification of the constraints early in the process. The special attention given to in-depth and dynamic analysis throughout the model facilitates validation of the model, as well as, the search for compromises at both levels; the biochemical and the managerial.

The proposed approach can be considered as a first step towards the qualification and justification of modeling decisions by using the knowledge representation for controlling, internally, the model development process; any data gathered when the monitoring network operates is, also, used to update and, at the same time, assess the model built, assuring reliable ecosystem impact assessments.

V. Conclusions

This paper presented a methodological framework for bridging the gaps between macro- and micro-scales in ecosystem modeling through an ontological platform designed/developed to accommodate partonomic functions in and between different knowledge domains and levels. The implementation of the proposed framework for integrated modeling is expected to aid decision-making in a diverse range of water management activities, including: predictive modeling for wastewater regulation, water allocation decisions and infrastructure operations, marine pollution monitoring (especially at ports where the low depths facilitate wide dispersions), development of ambient guidelines to support water management planning, environmental performance measurement, negotiation of trans-boundary water management agreements, as well as research into a wide variety of issues including aquatic ecosystem contamination, use, impairment, and restoration.

Acknowledgment

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