

A Multi-Scale Agent-based Distributed Simulation Framework for Groundwater Pollution Management

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Abstract— Groundwater is like dark matter – we know very little apart from the fact that it is hugely important. Given the scarcity of data, mathematical modelling can come to the rescue but existing groundwater models are mainly restricted to simulate the transport and degradation of contaminants on the scale of whole contaminated field sites by averaging out the effect of spatial heterogeneity on the availability of the pollutant to the degrading organisms. These coarse-scale mean-field models therefore tend to rely on fitting to data rather than being predictive. Also, they are less suited to incorporate spatial variability and non-linear kinetics and feedbacks. We propose to solve the two mutually exacerbating problems of environmental patchiness and data scarcity by developing a flexible and robust distributed simulation framework that uses an ensemble of small scale simulations running on different processors/computers to scale-up, i.e. to feed the effect of small-scale patchiness into a concurrent site-scale simulation of the dynamics of groundwater pollutant degradation. Our scaling approach solves problem #1 by simulating dynamics also on the small scale where some of the patchiness resides, and problem #2 by enabling rigorous validation of our small-scale model and scaling approach with laboratory data, which are high quality at low cost.

Keywords- groundwater; bioremediation; distributed simulation; multi-scale modelling; agent-based systems; individual-based models

I. INTRODUCTION

Clean groundwater resources are essential from resource development, human health and ecological perspectives, yet groundwater pollution continues to be a problem worldwide. Biochemical processes in groundwater provide important groundwater pollution controls. Biochemical attenuation of pollutants in groundwater occurs naturally but can also be stimulated using remediation technologies.

Current models describing these processes have been developed from laboratory experiments and observations at field scales typically without adequately incorporating the micro-scale behaviour of the microbial communities degrading the pollutants, but see [40] for a good exception. Thus,

existing models have limited predictive capability and rely heavily on calibration against field data and acceptance of significant uncertainty.

Existing groundwater models are mainly restricted to simulate the transport and degradation of contaminants on the scale of contaminated sites by averaging out the effect of spatial heterogeneity on the availability of the pollutant to the degrading organisms. These coarse-scale mean-field models prevent meaningful incorporation of spatial variability across several scales coupled with non-linear kinetics and feedbacks between scales.

This paper aims to explain our proposal for a radical redefinition of the way groundwater pollution models are developed/implemented in order to overcome these limitations.

Recent developments in predictive microbial population modelling using agent-based simulation approaches, e.g. [39], provide the basis for incorporation of the relevant microscale behaviours in a new generation of models. Advances in computational capacity through parallel computing architectures allow the direct coupling of agent-based models to predictive models of macroscale behaviour. This strategy avoids the problems inherent with the traditional large scale averaging of non-linear microscale behaviour and should provide far greater predictive capability. In addition, testing and verifying predictions of a model on the scale of a contaminated site would take decades and cost millions. In contrast, small scale models can be tested and verified with laboratory experiments that allow full control of conditions [32].

This paper presents a novel approach for groundwater management that enables:

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- Multiscale modelling to incorporate heterogeneity on different temporal and spatial scales.
- Incorporation of non-linear pollutant degradation dynamics and patchy pollutant and degrader distributions in reactive transport models of groundwater processes.

The rest of the paper is organised as follows: Section II provides an overview of the groundwater system. Section III discusses the problem of managing groundwater pollution and presents the challenges and solutions proposed so far. Section IV presents our proposed framework while Section V concludes the paper discussing plans for future work.

II. THE GROUNDWATER SYSTEM

Groundwater is the basis of over 50 % of the world-wide drinking water production [13]. Groundwater constitutes the largest reservoir of freshwater in the world, accounting for over 97% of all freshwater available on earth (excluding glaciers and ice caps) [5]. Depending on the region, up to 90% of the drinking water is produced from groundwater [5]. At the same time, groundwater is increasingly threatened by pollution. Almost all pollutants can actually be degraded by some microorganisms at least under some conditions, but this can be a very slow process, and bioremediation seeks to enhance the rate of degradation.

Most groundwater systems are porous, i.e. water flows through the pores among sand, silt and gravel. Some of the groundwater also occurs in rock fissures and caves, but since hydrological processes are very complex in such systems, for the proposed framework we focus on porous media groundwater. Groundwater flow is dependent on permeability, affected by pore sizes and connectivities, and the hydraulic gradient.

Groundwater is habitat to a plethora of organisms: bacteria, archaea, fungi, unicellular animals (protozoa) and multicellular animals such as worms and crustacea (metazoa) [9]. The ecosystem is characterized by three major constraints: (i) confined spaces, (ii) limited supplies of electron acceptors, e.g. oxygen, and (iii) limited supply of electron donors (mostly carbon/energy sources). These three limitations lead to low densities as well

as low activities of groundwater organisms unless contaminations increase the supply of carbon/energy sources. It also means that the transport of electron acceptors and carbon/energy sources is crucial (see e.g. [8]).

Knowledge about the groundwater animals and microbes is scarce – we hardly know who is where let alone what they do and how active they are [35]. The microbial community as known so far consists mainly of species well-known from other habitats, that are characterized by a flexible metabolism (e.g. long periods of dormancy). In contrast, the animal species are mainly endemic (only occur in groundwater of a particular region) and are highly adapted to this extreme environment by having a slow metabolism, longevity, low reproduction rate, as well as low mobility rates [35]. They are therefore outcompeted in areas with better resources by their more agile and vigorous relatives.

Where groundwater is in a near-natural state and far from the surface, one may assume a (pseudo-) steady state without much development in time, but spatial gradients are important. The temporal dimension becomes critical at the interfaces, which are the most reactive zones: e.g. the interface between a contaminant plume and the adjacent pristine water, on which we focus here.

III. MANAGING GROUNDWATER CONTAMINATION

Remediation of groundwater contamination is of great importance because many groundwater contaminations persist even after decades and they still increase in numbers. In 1997, the EC-funded Concerted Action CARACAS identified 750,000 contaminated sites across Europe. Groundwater contamination can also result in surface water pollution through seepage into surface water bodies and thus threaten drinking water production. The timeliness and urgency of at least sustaining the current status of (ground)water systems, if not improve them, is underlined in the recently enacted groundwater directive, GWD [11] complementing the European Water Framework Directive WFD [12].

Most contaminations will only be degraded over very long time spans. Therefore remediation seeks to speed up the rate of degradation. Techniques that have been applied with success to remediate contaminations include physical/chemical measures

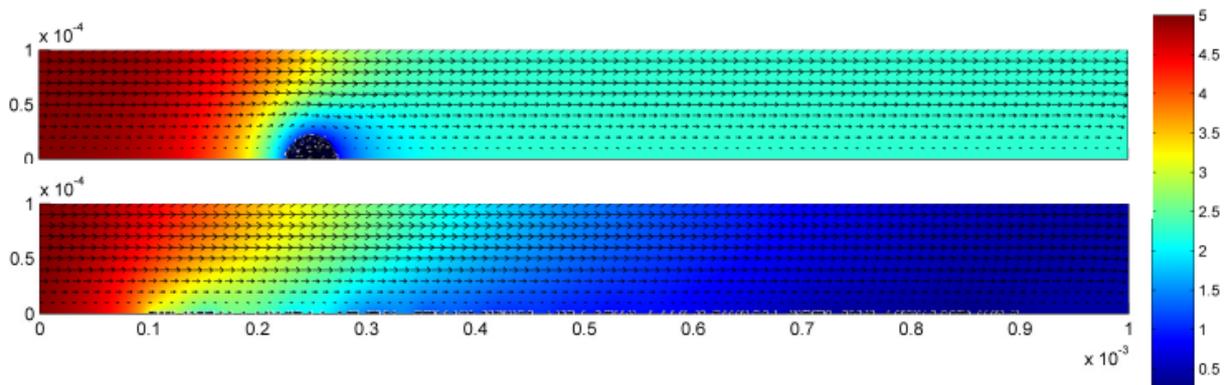


Figure 1: Degradation of a simple compound (acetate) in a tubular pore (2D radial symmetry). Acetate comes in with the flow from the left. Top panel: 200 cells in a single colony results in limited degradation. Bottom panel: 200 cells scattered along the tube surface achieve more extensive degradation. Steady state flow and concentration fields were solved with a combination of Matlab and COMSOL at $10 \mu\text{m/s}$ flow velocity. The length scale is in meters, the flow field is given by the arrows, the acetate concentration is in mM (coloured contours), and the colony and cells are outlined in black.

as well as biological measures [7]. Among the physical/chemical methods, permeable reactive barriers have probably been used most often. They reduce the flux of contaminants with the groundwater flow through placement of a permeable and reactive material, where the reaction leads to less harmful substances. *In situ* thermal remediation technologies use heat to mobilize contaminants so they can be extracted from the ground. *In situ* chemical oxidation is based on injecting aggressive reagents into the contamination to trigger or enhance degradation reactions. The biological methods are centred around two approaches: (1) stimulating native microorganisms by adding nutrients, oxygen, or other electron acceptors (a process called biostimulation) or (2) providing supplementary pre-grown microorganisms to the contaminated site to augment naturally occurring microorganisms (a process called bioaugmentation) [7].

Using predictive mathematical models to evaluate potential bioremediation strategies in order to identify optimal strategies should become the basis for future successful groundwater management and remediation strategies.

A. Why Multi-Scale Simulation - The fallacy of averaging.

There are many reasons why macroscale models can fail to predict contaminant degradation rates, after all, degradation depends on the degrading

organisms coming into contact with the contaminant and an electron acceptor or donor depending on whether the contaminant is being oxidized or reduced. So the transport of these substrates to the biomass, and/or of the biomass to the substrates, is vital. Moreover, the biomass is mostly attached to surfaces in clusters of cells originating from growth and cell division of a single ‘founder’ cell, leading to a heterogeneous distribution of cells on the surfaces. Cells may become motile and leave the surface or become detached by shear. Some of these issues can be avoided by considering e.g. mass transfer limitations in ‘efficiency factors’ when upscaling microscale reaction rates to macroscale rates [22]. However, if microscale reaction rates are based on the classic one dimensional biofilm models which assume uniform biomass and substrate distribution along the biofilm, the upscaling would be based on unreliable microscale rates [22].

Generally, when the response to environmental conditions is not linear, and these conditions vary in time and space, the average of the response to these varying conditions will differ from the response to the average condition [21] [16]. For example, locally high biomass density leads to high rates of substrate consumption resulting in low substrate concentrations locally (Figure 1). This is in contrast to assuming that biomass and substrate are homogeneously distributed, which would

overestimate reaction rates which are typically proportional to both biomass and substrate concentrations at low substrate concentrations. Further, typically 1,000 times more groundwater microbes are attached to surfaces rather than suspended or swimming in the water phase (planktonic) [19], and the growth of attached cells leads to the formation of clusters of offspring rather than a more dispersed uniform random distribution of cells. The outcome are hot spots of activity on a largely deserted surface resulting in less spatial overlap of contaminant and degrader than predicted by mean field models. Moreover, cells might aggregate at hot spots of contaminant concentration due to chemotaxis, a mechanism by which microbes detect and follow concentration gradients, increasing the heterogeneity of biomass distribution. The microbes are grazed on (eaten) by larger organisms, e.g. protozoa. There is a large body of work on "grazing increases productivity" in protozoan ecology that suggests that grazing could enhance degradation rates and should therefore be considered in predictive models and we propose to do so. In fact, laboratory scale experiments have shown that grazing can influence contaminant degradation [4].

To address these issues, this paper's central hypothesis is that allowing for patchiness on the microscale is crucial for robust prediction of contaminant degradation rates under various management scenarios. This pore-scale heterogeneity can be captured through the utilisation of agent-based modelling.

IV. THE PROPOSED FRAMEWORK

As described in the previous section, there are many different length and time scales in a groundwater ecosystem. Upon introducing a new contamination, the abundance of microbes responds to this change within a few months. Since we are interested in the degradation of contaminants, which takes many years, we can neglect the non-steady state transient phase of the response.

Regarding length scales, we have to consider the patchiness on the microscale, e.g. the distribution and transport of contaminants, substrates, and organ-

isms in the pores of the aquifer, and also larger scale heterogeneity, e.g. different geological strata with different pore sizes, different flow rates, and carbon/energy source and electron acceptor concentrations.

We propose to solve the two mutually exacerbating problems of (a) environmental patchiness and (b) data scarcity by means of a flexible and robust distributed simulation framework that uses an ensemble of microscale distributed simulations to "scale-up", i.e. to feed the effect of small-scale patchiness into a site-scale simulation of the dynamics of groundwater pollutant degradation.

Our up-scaling approach solves problem (a) by simulating dynamics also on the small scale where some of the patchiness resides, and problem (b) by enabling validation of the model with experiments. Such experiments have to be done in the laboratory to be well-controlled and feasible, hence they will be short (months rather than decades) and on the small scale (cm rather than km). Yet they will enable us to validate our small scale model rigorously, which is a big step forward towards predictive models compared with the fitting of large-scale models to field data. We propose experiments to validate both the small-scale model and the scaling approach in the laboratory (combining two types of mini-aquifer with different porosity etc.), thereby making sure that our large scale simulations are as reliable as possible – and far more reliable than in the past.

Our proposed solution is illustrated in Figure 2. The framework integrates macroscale (mean field PDE model for contaminated site, scale 100 m up to several km) reactive transport simulation of an aquifer (groundwater body) with an ensemble of small scale agent-based models. It also involves the dynamic partitioning of the site-scale domain into subregions. The novelty here is that instead of evaluating differential equations to obtain the derivatives to step the PDE solver forward, we propose to launch small scale agent-based simulations (corresponding to subregions), initialized to correspond to the current local state of the PDE model, that will return the 'derivatives' to the PDE solver.

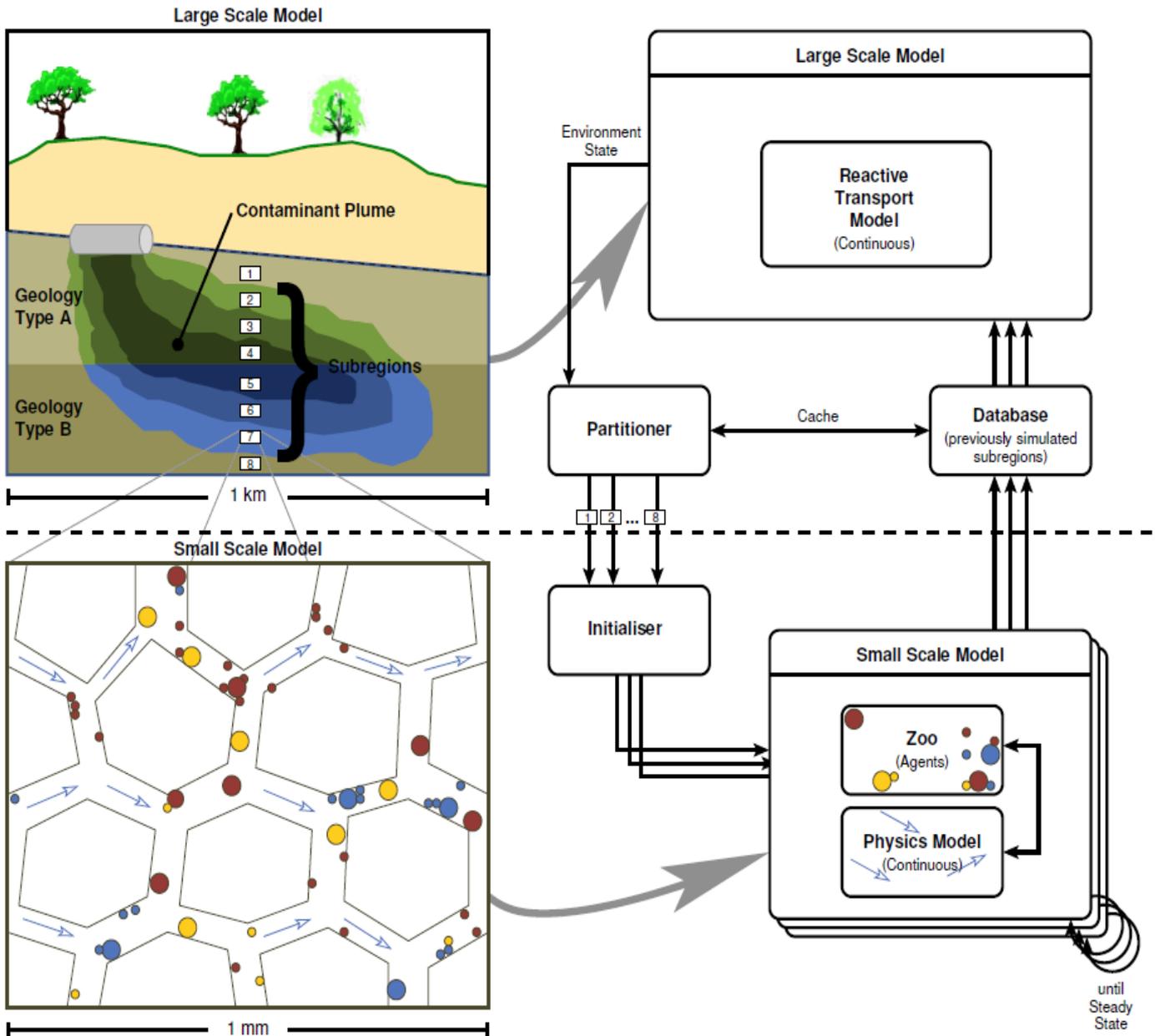


Figure 2: The Proposed Approach

This upscaling approach follows the ideas developed by Ioannis Kevrekidis [20]. The ensemble of microscale simulations (one per subregion, see below) supplies the derivatives (reaction rates, velocities, etc.) to the macroscale model which essentially - like any numerical solver of PDEs - calculates the next time point based on these derivatives. A key feature of this automatic upscaling is that it does not impose any assumptions on ‘efficiency factors’ or constraints in the upscaling as the microscale simulations simply directly supply

derivatives to the macroscale PDE solver. A database of microscale simulation inputs and outputs is meant to prevent unnecessary duplication and can also be used for interpolation, thus improving efficiency.

It should be noted that scaling goes both ways, not just upscaling from small to large scale, but also down from large to small scale as feedbacks go both ways. As the reactive transport macroscale model simulates the flow and degradation of a contaminant plume through various types of porous media, the

contaminant and electron acceptor and degrader distributions can converge/diverge and/or move into different porous medium conditions, which is feeding back into the small scale dynamics.

In the next sections we provide more details of the basic components of the framework.

A. Partitioning

The larger scale heterogeneity necessitates a partitioning of the contaminated site domain into subregions with similar geology, flow regime, carbon/energy and electron donor concentrations. In the model, this involves partitioning the large-scale domain (Figure 2) with the contaminant plume (area of polluted groundwater, which is found downstream from a point source of pollution) into self-similar zones. Each such subregion, being sufficiently uniform in conditions, can then be treated by upscaling from a single representative microscale simulation. In this way, simulations on two spatial scales can capture a lot of the relevant heterogeneity while achieving efficiency by simulating only one microscale model for each subregion.

There are about 5 “dimensions” to consider in partitioning the domain into zones according to self-similarity in the following conditions: available electron acceptor (5 different types), electron acceptor concentration (5 levels), carbon/energy source concentration (5 levels), grain size (5 levels), groundwater flow rate (5 levels). Performing the partitioning presents an interesting research question. Efficient algorithms for unsupervised partitioning of the site-scale domain into subregions are required.

B. Large Scale Model

The macroscale model predicts flow and concentration fields which upon changes trigger repartitioning of the domain though spawning of new small scale simulations only if new subregions have arisen (see next section). The model is based on a standard PDE solver, which encompasses groundwater flow field, solute diffusion and reaction, and porosity as given by grain sizes and biomass accumulation. The PDE model is not computationally demanding and therefore it is anticipated that a sequential simulator should be enough, although standard parallel options do exist.

C. Small Scale Model

The dynamics of all subregions identified by the partitioning component described above will be simulated by an ensemble of microscale agent-based simulations – one per subregion. A zoo of agents will model the various microorganisms inhabiting a network of pore spaces on a cm scale. In contrast, the world these agents inhabit will be treated as a continuum and modelled by a system of PDEs. They will be used to model the transport of groundwater and solutes, which will affect the agents and will in turn be affected by the agents. There are two options to simulate the micro-world these microbial agents inhabit and change.

One could model the geometry of the porous medium as it is, by representing in the simulation the various complex shapes of grains of various types and sizes read in from a computer tomography reconstruction of a core [29] taken from an aquifer. This would obviously lead to a very complex mesh for solving the convection-diffusion-reaction equation, which has of course to be solved also in the microscale model. The complexity of the mesh would limit the spatial scale that could be simulated quite severely, probably to < 1 mm, thereby defeating the objective of representing the heterogeneity of pore spaces and connectivities [29] in the microscale model. After all, the microscale model must be able to simulate a domain sufficiently large to be statistically representative, i.e. a cm scale.

Therefore we favour the second option; using a network of tubes of various lengths and diameters, as illustrated in Figure 2, that captures the pore size distribution without mirroring the actual geometry. As the tubes’ inlets and outlets can be connected to a variable number of other tubes (by itself not a trivial problem), we can also capture the distribution of connectivities of the real system. This coarser approach has been successfully used e.g. by Thullner and Baveye [24].

The agents, when not attached to a surface, are transported with the groundwater flow, or if attached, can be detached by shear forces arising from the flow. The foodstuffs for the agents, i.e. contaminants, other carbon/energy sources, and electron acceptors, are also advected with the flow and diffuse through any boundary layers into the microcolonies or biofilms attached to the surfaces.

Growth of the agents will increase the rates of solute consumption and may lead to changes in water flow and even clogging. These incomplete examples already illustrate the tight coupling between agents and the physical world, which makes it necessary to simulate transport processes both in the microscale and macroscale models.

For our microscale model, the medium in each tube of the network can be modelled as a continuum, rather than simulating all molecules of the liquid as individual agents, because molecules are many orders of magnitude smaller and more numerous than the microbial agents. We anticipate to use the open source software GeoSys/RockFlow [15] or an off-the-shelf PDE solver (such as COMSOL) to solve the convection-diffusion-reaction equations in tubular geometries.

Coming back to the agents, we propose to model each individual microorganism as an agent, represented as an object in the software, as in previous models from which we can learn [37][38]. The agents can attach to surfaces and then become immobilized or detach from the surface and then become suspended in the liquid where they are transported passively but they may be motile (self-propelled) in addition. A single cell attached to a surface will produce offspring that remains attached to the surface next to the mother cell, in this way forming a cluster of cells called a microcolony. All individuals of one species form a population, and populations of several species form a community.

For the degradation of ‘background’ substrates and the contaminant, we need to include in the model the various metabolic types of species relevant for the degradation of the contaminant of interest. These physiological or functional types are called guilds in ecology and we expect that about 5 different contaminant degrading guilds using different electron acceptors and two predatory guilds (one hunting swimming bacteria and the other one grazing the surface attached bacteria) will usually suffice.

The question is which of the plethora of microbes within each guild should be chosen for the model? One aspect of this question is which microbes are actually present in a given aquifer of interest? The other aspect is which of those present would become dominant upon introduction of a contaminant?

For the former aspect, we assume that all types of microbes are present at least somewhere within the aquifer, or migrate into the aquifer frequently enough so we can consider them ‘present’ during the timescale of interest. This idea was first expressed by Bass-Becking in 1934 as “Everything is everywhere – but the environment selects” [14]. The reason for this hypothesis is the fact that microbes are very small and numerous and have short generation times, thus they disperse at a very high rate and therefore get everywhere [17]. Whether this ‘dogma’ is actually true has been hotly debated [23], but the consensus now seems that in most environments, dispersal rates are so high that indeed everything gets everywhere [25][18]. However, some exceptions have been reported, most notably for hot spring organisms [26], probably because there are only a few hot springs on Earth, and thousands of kilometres separate these small islands of habitat, so dispersal rates are actually not sufficient to support a sufficiently frequent exchange between communities which would prevent the evolution of endemic species. Such endemism is typical for groundwater animals. It is not entirely clear whether dispersal rates from surface waters to a groundwater body would be high enough to bring everything everywhere, but it seems a reasonable assumption for all aquifers that are in contact with surface waters over larger areas. Some evidence indeed supports sufficient dispersal rates, e.g. [31], but finding only one bacterium, *Candidatus Desulforudis audaxviator*, in the extreme conditions of fracture water 2.8 km deep down a South African gold mine [33], raises doubts. However, 16S gene sequences similar to “D. audaxviator” have just been found in Finland [36]. Also the gold mines in SA have meanwhile yielded further bacteria [34]. If everything gets everywhere, organisms able to degrade a newly introduced contamination should already be present in the above sense of getting there often enough. Several groundwater studies have indeed found that bioaugmentation, i.e. introducing pre-grown organisms, did not enhance degradation rates [42][41], presumably because organisms capable of degrading the contaminant were already there anyway or because degradation was not limited by the absence of degraders.

The question which of the microbes present would become the dominant degrader that should be included in the model is difficult to answer *a priori*,

but our idea of simulating a zoo of microbes should solve this problem. Seeding the model simulation with a zoo, that is, a range of different species for each guild (metabolic type), means that the most competitive species under given conditions will grow fastest in the simulations and outcompete the other seeded microbes which will no longer be present in the 'steady state', so the answer to the question of who dominates emerges from the simulation, which we intend to run into steady state.

The organisms able to degrade the contaminant will respond to a contamination by growing and multiplying so that soon the pollutant degraders are abundant, led by the degraders which utilize the energetically best electron acceptor because the energetically favourable electron acceptor supports the fastest growth. Ten generations might be enough for a substantial degrader community (1024 cells) to develop from a single, possibly dormant cell. Generation times in groundwater are not very well known, but are thought to range from 10 days to several years [30]. It is therefore to be expected that a microbial degrader community will establish within a few months, led by the more competitive, faster growing species. For the protozoa preying on the degraders, one might expect a longer transient towards the climax community. However, changes in electron acceptor use that will drive changes in consumer community composition do not have to lead to substantial changes in predator community composition and predator numbers. Steady state should be reached after a few months of simulated time for the microbes [30] and probably longer for the protozoa (e.g. [10]). All the available evidence shows that the community composition found in a given place can be predicted from the availability of carbon sources and electron acceptors and that the change upon depletion of the best electron acceptor, oxygen, is in the sequence expected from thermodynamic grounds (in order of decreasing redox potential), further supporting the hypothesis of Baas-Becking [14].

Since the populations respond to contaminations within months, while it takes many years to degrade the contamination, the agent-based simulators should be executed until a quasi steady state of the microscale system is obtained at certain rates of nutrient input given by the macroscale model. This is computationally very intense and therefore calls

for distributed simulation approaches for the hybrid of an agent-based and a continuum model [28]. At the macroscale, simulation of transients is required as at this scale the time course is of interest and a quasi steady state would not usually be reached within decades.

V. CONCLUSIONS

Groundwater is vital as our societies increasingly rely on it as a source of drinking water. At the same time the rate of new groundwater contaminations outpaces the rate of remediation. There is therefore a strong need for efficient and effective approaches to manage groundwater and make accurate and fast predictions about pollution-related problems.

Experimentally, sampling of groundwater is particularly challenging and the typically slow changes require monitoring for quite long periods; as a result data are and will remain very scarce. Scarcity of data and costs of obtaining more make groundwater management one of the particularly challenging frontiers that still remain on Earth. Simulation has therefore a crucial role to play in this realm. At the same time, laboratory experiments and our own preliminary simulation results suggest that the patchiness of pollutant distribution and localization of pollutant degrading microbes crucially impact on the potential for biodegradation (pollutant must meet degrader).

Recent technological advances and research in agent-based systems, multi-scale modelling, distributed simulation and parallel computing provide a unique opportunity to develop groundwater management systems that can predict optimal groundwater remediation strategies. In this paper we take an important step in this direction. We proposed an integrated framework based on a laboratory-validated multiscale model that consists of a reactive transport model for the macroscale, a domain partitioning component, and a microscale model that is a hybrid of an agent-based and a continuum model.

The application scenario we present here is the very first to approach the issue of splitting a large scale simulation in order to support multi-scale modelling. It is a novel way of describing phenomena in groundwater that vary in time and space and over multiple scales. It is our vision that our approach will prove a viable alternative to

existing and established models, and - despite limitations that come with a high demand for parameters that are largely not known yet - might even go beyond existing models. In our approach micro-organisms are used as agents in the model which act and react on each other and their continuously simulated environment within defined reaches of influence. Thus, each simulation step consists of the agents' actions followed by solving the environmental field with finite elements. In each instance of the Agent-based model up to 1M agents will be modelled. The computational complexity of these models requires a parallel approach to simulation to span wider ranges of the ecosystem at the same time. This approach presents the distributed simulation community with some very challenging problems related to the integration of continuous and discrete event models at different temporal and spatial scales and the distribution of agent-based models [27][28]. In the future, we plan to implement the proposed framework, addressing these challenges, and evaluate the framework in realistic scenarios.

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