A coupled subsurface-flow and metabolism model to study the effects of solute fluxes in the hyporheic zone

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Abstract

The hyporheic zone and the streambed host a great part of the energy and material fluxes through river ecosystems. However, the role of heterogeneities in the hyporheic zone in metabolism is not clearly understood. This paper proposes a new way to approach the question by using a coupled subsurface-flow and metabolism model for investigating the role of heterogeneities in the hyporheic metabolism. Our results show that (i) our coupled model is feasible for investigating solute fluxes in the hyporheic zone under heterogeneous set-ups, and (ii) the incorporation of heterogeneities seems be of relevance for hyporheic metabolism estimations

1. Introduction

Projects in hydro-ecological sciences are often multidisciplinary in nature and involve cooperation from engineers and scientists from different backgrounds. A variety of different models are employed by them e.g. measurement models, laboratory models, simulation models, etc. In multidisciplinary projects, these models need to be integrated into a single system for solving a common problem. One such problem involves studying the effects of hydrogeomorphological heterogeneity on streambed and hyporheic metabolism.

The hyporheic zone (Hz) is a spatially fluctuating ecotone between the surface stream and the deep groundwater where important ecological processes take place [3]. In fact, Hz and the streambed host a great part of stream metabolism, e.g. 97% of whole stream denitrification [2] and 40–93% of whole stream respiration [7]. Metabolism is one of the most integrative ecosystem-level functions in rivers since it gives clues about the energy and material fluxes through ecosystems [6]. Despite the recognition of this fact, there is still a lack of understanding of complex responses of biological processes to the hydromorphology of the Hz [5] and in consequence research tends to consider Hz as a hydrogeomorphologically homogeneous black box. At reach scale, previous research has tried to combine heterogeneity with metabolism, for instance [1] distinguished several zones within the transient storage zone depending on their metabolic activity or [4] differentiated among different zones of the streambed based on their residence time. But a more complex model with heterogeneous hydrogeomorphology is still needed [4]. We propose a bottom-up approach that helps to clarify whether Hz heterogeneity has to be considered when studying stream metabolism. We propose that while aerobic metabolism (respiration) will be accurately represented in a homogeneous approach, anaerobic processes (e.g. denitrification, methanogenesis) will be neglected.

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In combination with measurements in percolated sediment microcosms, we estimate the relevance of heterogeneous hydrogeomorphology on the physical and biological processes in the Hz by coupling a subsurface-flow model with a model simulating the Hz metabolic processes.

2. Laboratory Model

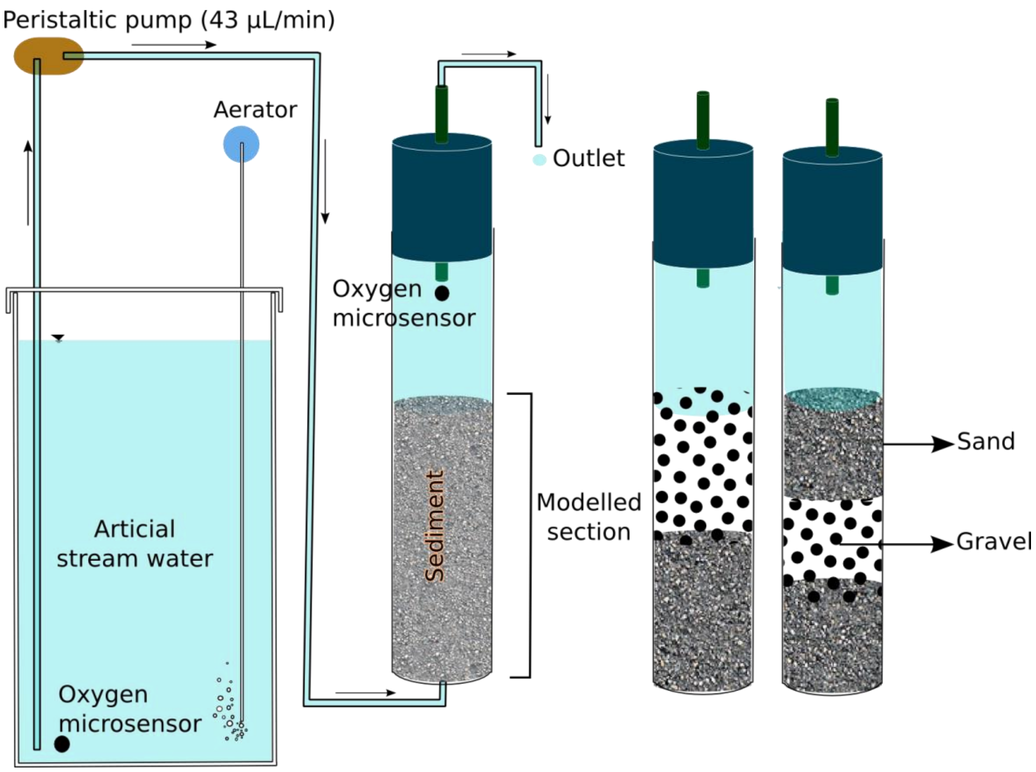

Figure 1: Schematic representation of the experimental set-up: example with one percolating microcosm filled with uniform sediment, and the different combinations of gravel and sand measured (uniform, 2- and 3-layers perpendicular to flow direction).

A portion of the Hz was simulated in a laboratory set-up (Figure 1) consisting of a set of percolating microcosms (20mL glass syringes, diameter 2.01cm, Fortuna Optima, Poulten & Graf, Werheim, Germany); peristaltic pump Ecoline; ISMATEC, Glattbrugg, Switzerland) filled with sediment and placed in a water bath at constant temperature (15ºC) and in darkness (F38-EH; Julabo, Seelbach, Germany). Sediment of different permeability and grain size was used: gravel (8–4mm) and sand (0.8–0.4mm), and pre-incubated (3 days, 20ºC in darkness) in a sediment community solution from the experimental catchment Chicken Creek [9]. Each measurement consisted of three replicates of uniform sediment (gravel and sand) and three replicates of heterogeneous arrangement of sand and gravel (Figure 1). All microcosms remained saturated throughout the measurement. The experimental set-up was allowed to run for 5 days and regular measurements were taken for the pumping-rate of water and for the dissolved oxygen concentrations (Microx TX3; PreSens, Regensburg, Germany) at the inlet and outlet of the microcosms, used to calculate respiration rate as a proxy Hz heterotrophic metabolism,. Oxygen concentrations were well above substrate saturation constant for aerobic respiration. Therefore, respiration rate was independent of oxygen concentrations [13].

3. Coupled simulation model

A coupled subsurface-flow and Hz metabolism model was used for reproducing the results obtained from the laboratory experiments described in section 2. The two models were set up using parameters that were measured in the laboratory. The exchange of physical state variables between the two models takes place with the aid of a prototype of a software framework for model coupling which is responsible for communication between the model and adaptation of information according to the model requirements.

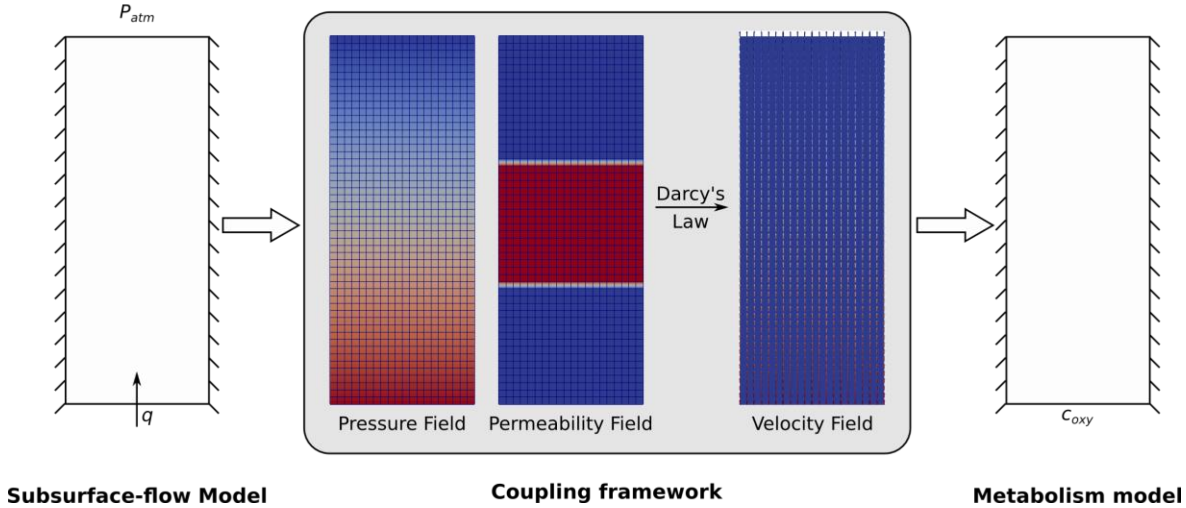

Figure 2: Schematic diagram of the coupled subsurface-flow and Hz metabolism model with the software framework for coupling models acting as the coupling broker.

For reproducing the results obtained from the laboratory experiment, a subsurface-flow model was coupled with the Hz metabolism model using a prototype of a software framework for coupling models (Figure 2). The subsurface-flow model is used to compute the pressure-field in the microcosm and the Hz metabolism model makes use of this velocity field to simulate the metabolic activity of the sediment community. A coupling framework is responsible for the communication and information exchange between the models and for transforming information from the models as required e.g. interpolation, transforming the pressure-field to a velocity field, etc. The dimensions and other parameters for both the models are set from the laboratory model.

3.1. Subsurface-flow model

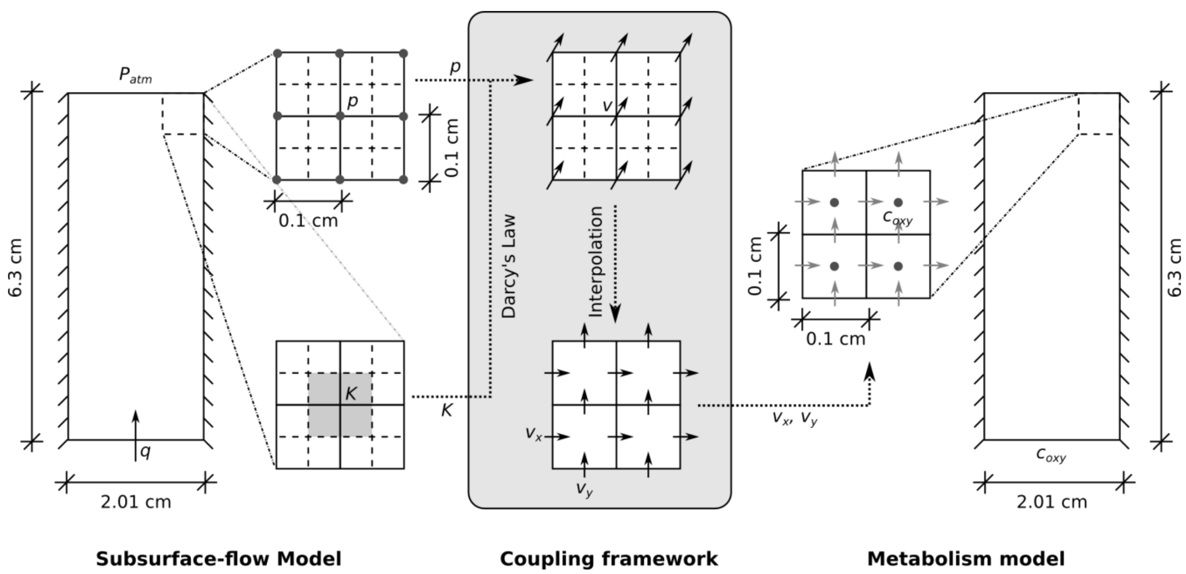

Figure 3: Dimensions and space discretisation of the subsurface-flow and Hz metabolism model.

DuMu^X stands for DUNE for Multi-{Phase, Component, Scale, Physics ...} flow and transport in porous media and it is a free and open-source simulator for flow and transport processes in porous media [8]. Since the soil in the laboratory model remains saturated throughout the experiment, a two-dimensional fully-implicit single-phase model is employed for simulating the subsurface flow. The governing equations in this case are the transport equation (equation 1) for the conservation of mass and the Darcy's law (equation 2) for the conservation of momentum:

$$f \frac{\partial r_w}{\partial t} + \underline{\nabla} \cdot \underline{v} = q_w \tag{1}$$

$$\underline{v} = -\frac{\underline{\underline{K}}}{\mu}\left(\underline{\nabla} p - \rho_w \underline{g}\right) \tag{2}$$

Here, μ is the viscosity of water, ϕ is the porosity of the soil, ρ_w is the density of water, g is the acceleration due to gravity, K is the permeability of the soil, p is the pressure and v is the flow velocity, q_w is the source term for water and t is the time.

The dimensions of the subsurface-flow model are set from the laboratory model to 2.01cm × 6.3cm (Figure 3). The space-discretisation is in the form of vertex-centred finite-volume scheme having a regular structured grid with square cells that are 0.1 cm in length. Time-discretisation is in the form of implicit Euler method with adaptive time-step size. For the boundary conditions, the pumping rate of 0.043mL/min, as measured in the laboratory, is set as the Neumann boundary condition at the bottom and atmospheric pressure (patm) as the Dirichlet boundary condition at the upper edge of the model (Figure 3). The lateral edges are treated as closed (no-flow) boundary conditions.

3.2. Hz metabolism model

A Hz metabolism model for simulating the metabolic activities of the microorganisms has been developed for this work. Like in the case of the subsurface flow model, the Hz metabolism model computes the distribution of oxygen in the domain using the transport equation (equation 3).

$$\frac{\partial r_o}{\partial t} + \underline{\nabla} \cdot \underline{v} = q_o \tag{3}$$

Here, ρ_o stands for the density of oxygen and q_o stands for the source term for oxygen. Since oxygen is modelled as a solute, the velocity v is provided by the subsurface-flow model.

Like for the subsurface-flow model, the metabolism model has the dimensions of 2.01cm × 6.3cm (Figure 3), set from the laboratory model. The space discretisation is in the form of a cell-centred finite-volume scheme with each cell having the dimensions of 0.1cm × 0.1cm. Time discretisation is in the form of explicit Euler method with a constant time-step size of 100s. The metabolism model is a two-dimensional model with the measured concentrations of oxygen used as the Dirichlet boundary conditions at the lower edge of the model and the lateral boundaries being modelled as closed boundaries. The upper boundary is treated as an open boundary and the oxygen concentrations computed at the outlet are used for validation against the laboratory measurements and for calculating the average respiration rates in the microcosms.

3.3. Coupling mechanism

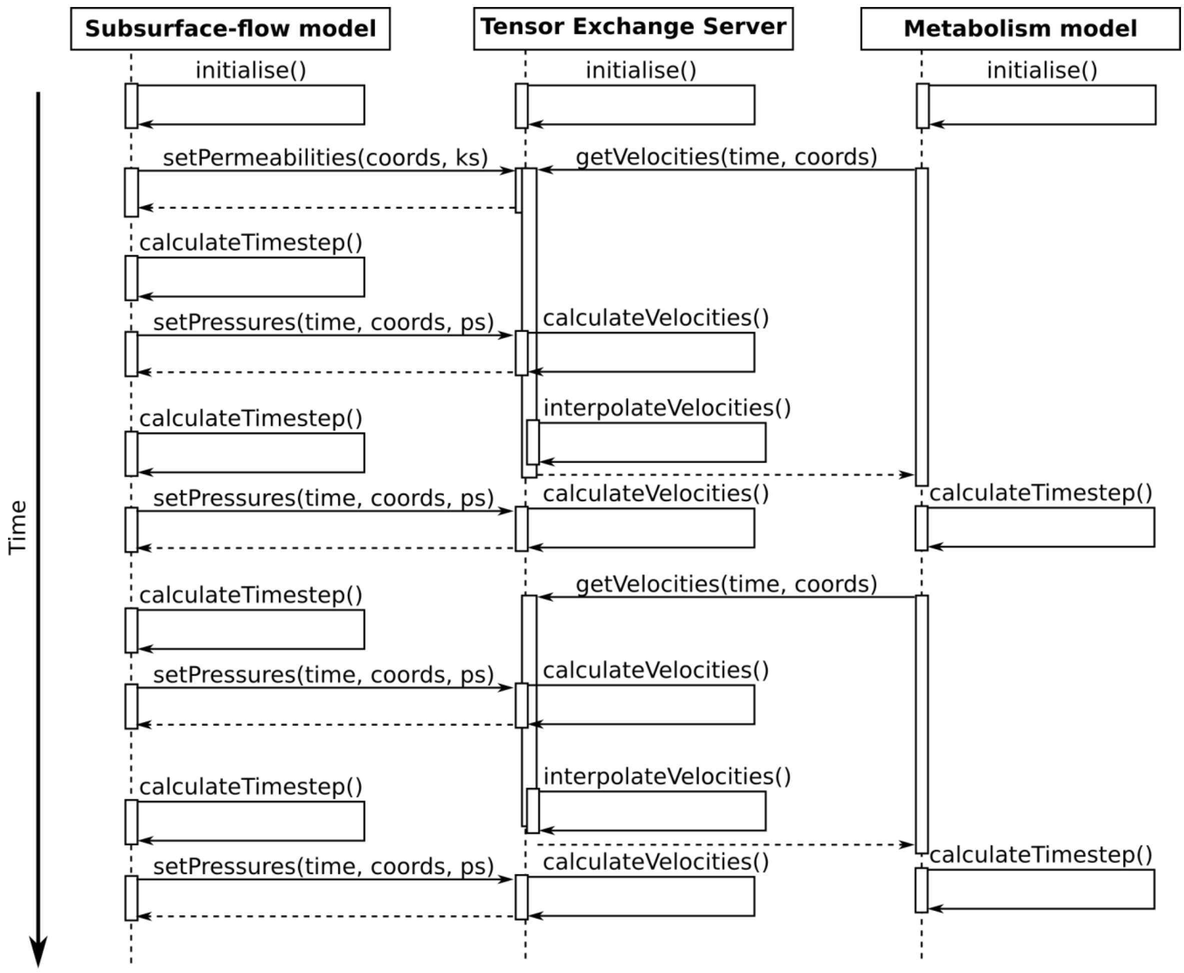

Figure 4: Coupling mechanism

To make the task of coupling the subsurface-flow model with the metabolism model easier, a prototype of a framework for coupling of models based on Tensor objects is used [12]. This is shown as the 'Tensor Exchange Server' in Figure 4. The Tensor Exchange Server acts as a broker between the coupled models and is responsible for:

- Providing a generalised and comprehensive representation of physical state variables i.e. the permeability, pressure and velocity fields
- Providing a channel of communication between the coupled models through the use of web-services making use of the XML-RPC standard [14]
- Adapting the information from the subsurface flow model to the requirements of the metabolism model. This includes applying Darcy's Law for converting the permeability and pressure fields from the subsurface flow model to the velocity field required by the Hz metabolism model.
- Performing bicubic interpolation in space for estimating flow-velocities at the centres of the cell-faces of the metabolism model from the results of the subsurface-flow model
- Performing linear interpolation in time of the velocity field for the metabolism model.
- Regulating the coupling process e.g. by making the coupled models wait until the values requested by them from the other model are available

Figure 4 shows a UML representation of the sequence of calls that take place between the coupling framework and the coupled models. In this particular case, the information flows only in one direction. As a result, the complexity involved in coupling of models is relatively simpler when compared to bidirectional flow of information and the models don't necessarily need to run concurrently. The sequence of events involved in the coupling can be summarised as follows:

- The Tensor Exchange Server (TES) and the coupled models start up.
- The subsurface-flow model sends the permeability field to the TES at the beginning of its computation. The permeability field is later used for calculating the velocity field by the TES.
- The subsurface-flow model carries out its calculation and at the end of every time-step sends the computed pressure field to the TES. The TES computes the velocity field from the pressure and the permeability fields using Darcy's law.
- The metabolism model requests the velocity values from the TES.
- The TES waits for pressure values from the subsurface-flow model for computing the velocity field, if they are not already available. The TES interpolates, as required, the velocities calculated in the previous step in time and space, and returns the interpolated velocities to the metabolism model.
- The metabolism model computes the next time step using the values it receives from the TES. At the beginning of the next time-step, it again requests the velocity field from the TES for that time-step.

Compared to other model coupling approaches such as OpenMI [10] where models are coupled with each other directly and the responsibility for understanding, adapting and transforming the information received from the coupled models lies on the models themselves, the use of TES as the coupling broker reduces the effort required in coupling by doing such adaptations and transformations on behalf of the coupled models.

4. Results

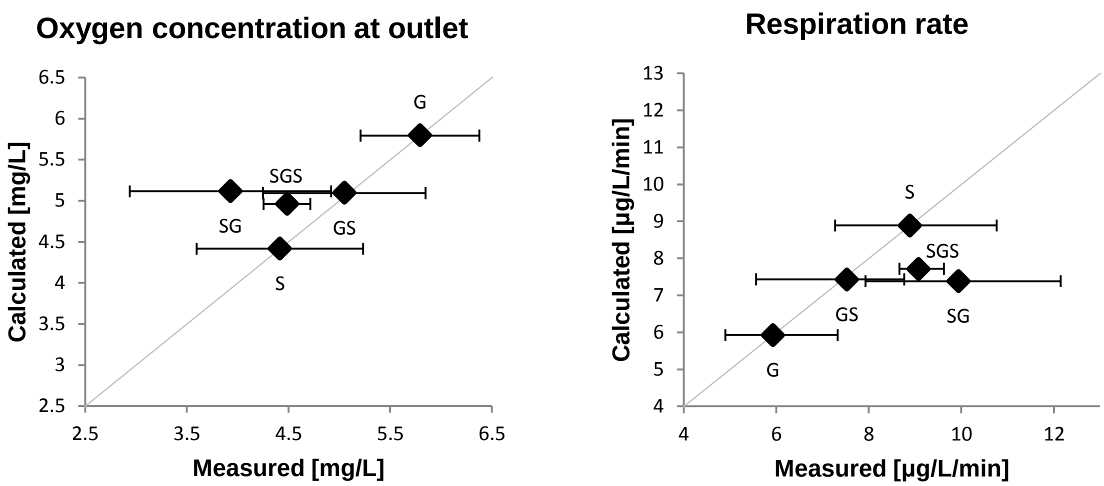

Figure 5: Comparison of the measured oxygen concentration at the outlet of the microcosm (left) and the average respiration rate in the microcosm (right) (measured values mean ± min/max values, n = 3) with the calculated values (single simulation). Diagonal lines indicates 1:1 ratio. S = Sand, G = Gravel.

Figure 5 shows the comparison of the results of the coupled numerical simulation to the values measured in the laboratory model. These figures demonstrate that the coupled model is able to simulate very accurately the homogeneous set-ups, while more complex set-ups such as sand-gravel-sand are underestimated as a result of handling heterogeneity in permeability.

As expected in our initial hypotheses, even with our simple heterogeneous set-ups, respiration of the microcosms varied. It is interesting to note that even when used in similar proportions, different respiration rates are observed for the different arrangements of the sediments. Since the metabolism model is based simply on the principle of conservation of mass (section 3.2 above) similar proportions of sediment result in similar values for oxygen concentration being computed at the outlet of the microcosm, irrespective of the order of the sediments. As a result, the simulation model is not able to reflect the heterogeneities observed in the laboratory and further investigations are required to find the impact, if any, of the order of the sediments on the respiration rates and how the simulation model might be able to model these effects.

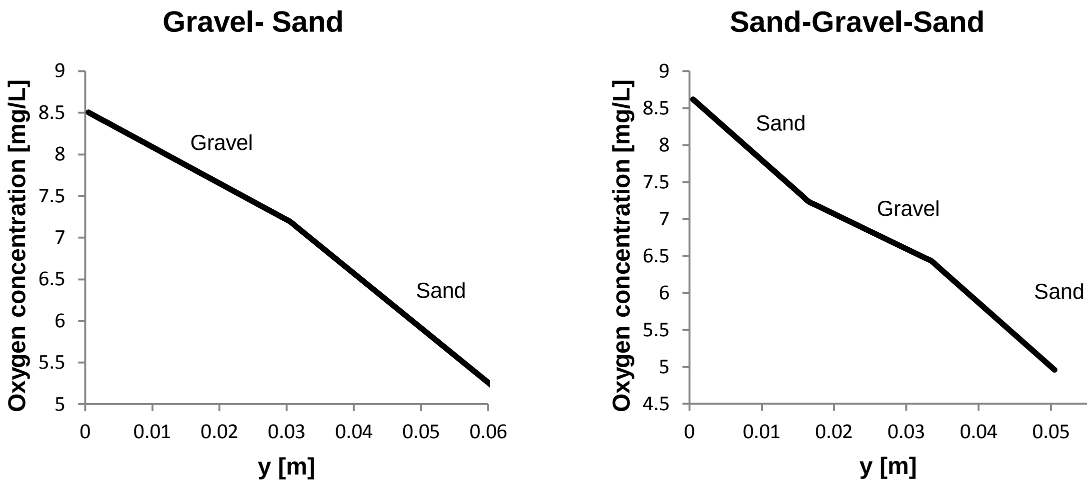

Figure 6: Longitudinal profile of oxygen concentration through the centre of the microcosms.

Figure 6 shows the longitudinal profile of the oxygen concentration through the middle of the microcosm as computed by the metabolism model. As expected, the heterogeneities in permeability affect the distribution of oxygen with the oxygen concentration falling more rapidly in the downstream direction in sand than in gravel.

5. Summary and Outlook

A coupled subsurface-flow and Hz metabolism model demonstrates that a coupling framework based on Tensor objects facilitates the task of coupling by providing functionality such as a com-munication mechanism between the coupled models, adaptation of information based on the re-quirements of the coupled models through mathematical operations, etc.

- As shown by the results, even with such a simple set-ups, heterogeneity in respiration reflects heterogeneity in the sediments as proposed. Thus our coupled model is feasible for investigating the role that heterogeneities in the Hz play on the solute fluxes and metabolism.
- At our small scale, differences in respiration among sediment combinations might be of low relevance for ecosystem metabolism, however the observed differences point out that when at bigger scale more complex set-ups and other metabolic processes are considered relevant differences for ecosystem metabolism will arise. Therefore, in agreement with [11], it is likely that the understanding of hyporheic flow processes will mature by addressing, rather than bypassing, hyporheic dynamics and heterogeneity

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