Report by UWI doctoral researcher Vahid Sobhi Gollo (H2)

Project number: H2

First and last name of doctoral researcher: **Vahid Sobhi Gollo**

(Working) title of doctoral project: **Integral modelling approach for flow and reactive transport at surface water-groundwater interface**

Name of supervisors: Prof. Dr.-Ing. Reinhard Hinkelmann (TUB), PD Dr. nat. Jörg Lewandowski (IGB), Prof. Dr. rer. nat. Gunnar Nützmann (IGB)

2. Description of doctoral project and research results achieved to date:

State of the art

The hyporheic zone is the transition zone between aquifer and river [Tonina and Buffington 2007]. It is a band of permeable, saturated sediment surrounding a river, where surface water and groundwater mix; and includes riverbeds, river banks, saturated sediments under dry bars, riparian and floodplain areas [Edwards 1998]. Due to interaction of groundwater and surface water by gaining and losing fluxes, intense physical and chemical gradients occur in this zone [Stanford and Ward 1993]. Hyporheic zone is a biogeochemically active [Trauth et al. 2014] zone regarding ecological balance, transport of substances and quality of surface water and groundwater.

Biogeochemical, ecological and hydrological importance of this zone has attracted many researchers for investigating the processes occurring in this region in different scales and by using different methods.

Detailed understanding of the hyporheic zone through hydraulic and biogeochemical modelling of current and possible scenarios is being acquired considering the influence of groundwater and surface water as two main bodies affecting the exchange processes in this zone. This is being achieved with high resolution computational fluid dynamics models (CFD) for simulating surface water - hyporheic zone interactions (boundaries) [e.g. Broecker et al. 2017] as well as the use of groundwater simulations to quantify the gaining and losing (positive and negative fluxes) conditions that occur between hyporheic zone and surface. Simultaneous impacts from both groundwater and surface water are crucial in investigating hyporheic exchange processes. Thus, many modelling efforts [e.g. Tonina and Buffington 2007, Broecker et al. 2018, Trauth et al. 2014, Cardenas and Wilson 2006] are conducted to address such interactions and quantify fluxes, reactive transport, residence time of particles and purification effects. These are based on using coupling schemes of groundwater flow (using Darcy's law, Forchheimer law, etc) and surface water flow (shallow water, Navier Stokes equations with considering turbulence models) on the one hand; and integral approaches using surface flow and porous medium as phases in a single modelling approach (e.g. Oxtoby et al. 2013, Mosthaf et al. 2011) on the other hand.

Motivation and research idea

The use and further development of the integral solvers to model the hyporheic exchanges motivates this research. Using such a methodology can initially give fruitful results to understand and quantify the hydraulic exchange processes occurring in the hyporheic zone followed by conservative and reactive transport modelling to answer the open questions of reactions and chemical exchanges of this zone. It should be considered that this method as well as any other scientific action should be compared to other methodologies for its reliability, range of application through different geometries and scales and computational performance.

Therefore, the idea of the following research project is to further develop [following Broecker et al. 2018] an integral solver for high resolution modelling of hyporheic zone exchanges with groundwater and surface water. Through a step-wise procedure it is intended to compare this method to coupling methods [e.g. Trauth et al. 2014] in order to address its efficiency and functionality. Later, the idea is to test the integral solver for different geometries and scales to check its range of application and validate it based on quantitative experimental approaches [e.g. Fox et al. 2014]. Finally, with the help of field data (collaboration with other UWI project H1), functionality of the solver will be examined for conservative [and reactive] transport. In the following, the step-wise procedure will be further explained.

Scientific project relevance

Understanding of complex processes like those in the hyporheic zone requires advanced modelling approaches as well as more controlled lab and field experiments. Such a model should account for small scale processes like turbulence and should be verified, calibrated and validated regarding processes like hydraulics and reactive exchanges in this zone. Building on the existing advances in this area, this project picks up the advanced high resolution integral approach and tries to find its strengths and weaknesses, adds more details of all of the processes happening in the hyporheic zone and brings it to be realistically usable for a wide range of systems.

Research demands

To further clarify the scope of the project, the following scientific questions are designed to be answered during this project:

1) What is the application range of the integral solver? (Hydraulics)
2) What advantages and weaknesses does the integral solver have compared to other methods?
3) What methods and data can be used to validate the integral solver on different scales? What are the limitations?
4) What is the application range of the integral solver in dealing with conservative transport?
5) How can reactive transport be included in the integral solver? What methods should be used? What type of data is required for validation?

Objectives

The main objective of this project is to further develop the integral solver of Broecker et al. (2018) as a simulation tool for a wider range of applications namely a variety of stream bed geometry (scaling), conservative and reactive transport. The functionality of the solver will be examined compared to other methods and it will be validated using experimental results.

Work programme incl. proposed research methods

WP 0 *'Preparation, knowledge acquirement, course attendance'*

This work package is included for gaining the required basic knowledge about the topic as well as deepening the scientific level about the project and the bigger picture of urban water interfaces. To understand the present state of knowledge about different modelling techniques like optimal coupling methods, with and without feedbacks, a more profound literature review will be done; and as the result a table showing different methods, different softwares, running time and capability of fast iterative coupling will be presented. The time of writing this exposé is also included in the procedure as a fair amount of literature is gathered and presented in this text. Simultaneously, while finding the best simulators as well as coupling methods, the focus will also be on learning to work with the groundwater simulators and coupling schemes. As the next step of the project is going to be focused on comparison of GW-SW coupling and integral approaches, the time investment will also be shared with getting used to OpenFOAM and its pre- and post-processing tools.

The gathering of knowledge about urban water interfaces and advanced high resolution SW-GW modelling will be done by attending the core courses of UWI as well as courses of “Projekt: Einführung in Computational Fluid Dynamics (CFD)” and “Modelling Hydro- and Environmental Systems” during SoSe 2019.

WP 1 *'Comparison of the integral solver and coupled modelling approach'*

The integral solver presented by Tabea Broecker should be compared to other methods to see its range of functionality and applicability. That is why after gathering enough knowledge about other most used hyporheic zone simulation method (coupling), a comparison from different aspects will show the strengths and weaknesses of the integral solver. This work package only focuses on the hydraulic processes. The main effort in this package is implementing the best possible coupling scheme with the use of calibrated numerical solutions so the integral solver can be compared to trusted simulation results. Through personal contact with Dr. Trauth from UFZ Leipzig who has invested a lot of time and resources on hydrogeochemical modelling of hyporheic zone, it is concluded that in case the fluxes from the subsurface to the surface are low, compared to the surface water flow, a no feedback condition between GW and SW can be assumed. In his work, without using an iterative approach, he used the head pressures at the bottom of the OpenFOAM (Navier-Stokes equation) simulations (SW) and transferred them to the top of the GW-model MIN3P (Richard’s flow). To start from simpler approaches, it is intended to follow a similar path by even substituting MIN3P as a reactive transport GW modelling software with MODFLOW-USG (the software is still under consideration) to focus only on hydraulic processes. The outcome of this coupling approach will be compared to the results of Broecker et al. (2018). The cost, effort and the quality of the results will be the main factors to be compared between this coupling and the integral solver. This step is planned to be finished by the end of the first year and the results can be published pointing out the functionality range of the integral solver for hydraulic processes. Later on, to have a more realistic view on the simulation processes of the hyporheic zone, fluxes between GW to SW should be considered. Therefore, we will investigate a different coupling methodology to include feedback between GW and SW. Here, it is intended to use GW flow laws other than Darcy because in the thin layer of GW below SW, other dominating flow equations like Forchheimer’s law can be considered to model the flow velocity more realistically. There are limitations to implement this coupling approach due to technical difficulties caused by differences in operating systems and result files of OpenFOAM to many of the existing GW simulators. Thus, a technical step is also required here to see which data transferring method should be used to accelerate this iterative reading and responding between two tools. Ultimately, a fully coupled hyporheic hydraulic exchange model will be compared to the integral solver. Work package 1 will result in a full hydraulic functionality test of the integral solver, points out its weaknesses and (hopefully) promotes its advantages to other techniques. The duration of this package will be one year and will end by the end of summer 2019.

WP 2 *‘Upscaling and validation of the integral solver’*

By the end of WP 1, the integral solver is validated for application to every type of river bed morphology. In this work package the aim is to include different river bed geometries to broaden the application range of the integral solver (hydraulic). The next step is to validate the solver with an experiment which includes all the responses between GW and SW to validate the results of WP 1 and to become more realistic than the single ripple experiment of Almeida et al. (1990) which Broecker et al. (2016) used for initial investigation of the stream flow over rippled bed.

Hyporheic zone is highly under the influence of the river bed morphology. Therefore, different geometries of ripples and dunes can have a huge impact on the exchange processes between the SW and this zone. With the help of different experiment results from a variety of authors, different geometries undergo the simulation process using the integral solver. The result of pressure distributions and flow velocities will be compared with the integral solver as well as analytical solutions to verify and validate the approach for a wider range of geometries. These geometries can include different ripple shapes, heights, lengths and frequencies. Different ripple geometries will be checked for exchange rates in/out of the hyporheic zone. Results can be used in shallow water flow and transient storage models.

Another important aspect other than upscaling is checking the solver to see how precise and close to reality it can predict the hyporheic exchange processes. An independent data set or a field experiment is a perfect tool to find the relevancy of the solver to real situations. By using a well conducted experiment, the point to point data can be used to calibrate the solver. Throughout the literature, the experiments of Fox et al. (2014) seem like the most suitable ones for this procedure. As a relatively large flume tank that is under constant head circulation, includes gaining and losing conditions from groundwater and can track the movement of water in and out of the hyporheic zone (Fig.1), it has many point measurements and is a realistic flume experiment to show hyporheic exchanges (at least for the hydraulic part). Fox et al. (2014, 2016) will probably be used for validation purposes. Updates on articles are being watched so by the time of the start of this work package best experimental results can be used. The idea is to determine exchange rates between GW-SW based on high-resolution 3D simulations for different ripple geometries and other influencing parameters (e.g. discharge) and to implement them in simpler model concepts as shallow water flow or transient exchange model.

Upscaling and validation are expected to take long until the first quarter of the third doctoral thesis year. Throughout the project, uncertainties should be considered whether in calibrating and validating using the experiment results or computational capability of the approaches. Impacts of uncertainties (e.g. hydraulic conductivity fields) on the flow, transport and exchange processes will be investigated (e.g. using geostatistical models).

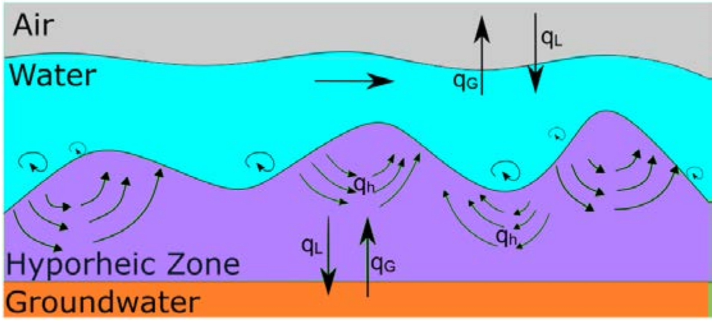

Fig.1: *Flux exchange in hyporheic zone*
q_h: *water that initially travels from the stream into the subsurface but returns after some time to the surface water.*
q_G: *gaining flux*
q_L: *losing flux*

WP 3 *‘Conservative and reactive transport modelling using the integral solver’*

By the last quarter of the 2nd doctoral thesis year, a parallel effort on including conservative/reactive transport into the integral solver will be started. This package will be the link to the 3rd cohort of UWI by opening the topic of reactive transport modelling. This work package includes conservative and reactive transport modelling as well as calibration of the reactive transport modelling.

The same procedure of using analytical solutions as well as experimental data will be used to add the details of transport modelling to the solver. As the topic is very wide, to fit a one-year package into this doctoral thesis work, the aim is to use the results of the other colleagues of UWI (e.g. project H1) who will do field experiments on the reactive transport in the hyporheic zone; and try to calibrate a 1D or 2D integral model using the fundamentals of the integral solver with adding the details of conservative/reactive transport as well as the temperature readings. This calibrated model can be used as the base for further investigations on simulating 3D integral reactive transport modelling in the hyporheic zone as the topic of the next project. One interesting aspect will be the comparison of the concept of dispersion (in porous media) with turbulent diffusion. This work package is aimed to be finished a couple of months before June 2021 (project deadline) so the remaining time can be used for the final dissertation push.

Collaboration

The main cooperation of this project is going to be conducted with the field experiment results on the project **H1** by Ms. Birgit Müller. In the following, the design of these experiments is briefly explained.

With a high frequency sampling campaign in a side channel of the River Erpe, TrOCs (Trace organic compounds) and DOC (Dissolved Organic Carbon) concentrations will be analyzed in different sediment depths, every hour over a period of 20 hours. In the same depths as the sampling points, CTD (Conductivity, Temperature, Depth) probes will measure EC (electric conductivity) to track individual water parcels using the dial EC pattern induced by the wastewater treatment plant discharges. Redox conditions in the sediment will be investigated using indicators such as nitrate, $Fe^{2+/3+}$ and $Mn^{2+/4}$. To analyze overall flow conditions, the hydraulic head at -40 cm depths in a piezometer and at the surface will be compared.

Samples will be analyzed for TrOCs as well as their transformation products (TPs, if known) and BDOC at the laboratory of the TU Berlin – Department of Environmental Technologies – Chair of Water Quality Engineering within the project **H3**. These results will be used for calibration of transport modeling.

Close collaboration is also planned with project **S2** both using the OpenFOAM model and further collaboration on the water quality modelling is intended with the projects **F2**, **F3** and **W2.**

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3. Comments on the qualification programme and supervision strategy:

Participation in the following Research Training Group events:

1. Core courses
    - Urban interface processes – fluxes, transport, interactions (3 ECTS)
    - Urban freshwater ecology (3 ECTS)
    - Modelling and measuring concepts of interface processes (3 ECTS)
2. Elective courses
    - Computational Fluid Dynamics course (6 ECTS),
    - Modelling Hydro- and Environmental Systems (6 ECTS)
    - Kolloquium Wasserwesen (3 ECTS)

Research stays or internships at other research institutions both at home and abroad:

To gain a better understanding of the integral modelling approaches of the hyporheic zone and to gather the state of the art expertise on the topic, an internship in Lawrence Berkeley National Laboratory (Berkley lab), department of geochemistry under supervision of Dr. Ilhan Özgen (former UWI kollegiate) is planned. As an alternative option, the knowledge transfer on hyporheic zone exchange and river restoration can be done through an internship in University of Idaho, center for Ecohydraulic Research under supervision of Prof. Daniele Tonina.