Report by UWI doctoral researcher Tabea Broecker (N7)

Project number: N7
First and last name of doctoral researcher: **Tabea Broecker**
(Working) title of doctoral project: **Integral modelling approach for flow and reactive transport in groundwater - surface water interaction space**
Name of supervisors: Prof. Dr.-Ing. Reinhard Hinkelmann (TUB), Prof. Dr. rer. nat. Gunnar Nützmann (IGB)

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

Motivation

Groundwater and stream water are important resources for the extraction of fresh water [1]. But especially urban water systems are heavily affected by human influences which can lead to a decrease of biodiversity or an increase of human health risks due to harmful solutes [2] [3]. An important zone for the retention, attenuation and transformation of substances is the transition zone between groundwater and surface water – the hyporheic zone [4] [5]. Unevenness in streambeds enhance the exchange of water at the sediment-water interface and lead to an increase of the processes in this zone, indicated by the hyporheic exchange [6] [7]. Investigations of hyporheic exchange processes like transportation and transformation are therefore important for understanding the prevailing processes and to predict consequences of changing situations which influence the management of water quantity as well as the water quality. With respect to the complexity of the hyporheic exchange processes including the turbulent flow through three-dimensional bedforms, numerical simulations offer a leading potential for understanding the mechanisms of flow dynamics and biogeochemical reactions.

For an accurate description of surface water flow, the full Navier-Stokes-equations are used. To investigate the flow from the surface to the subsurface or vice versa, surface water simulations are usually coupled to a second model that describes the flow in the porous medium [8] [9] [10] [11]. Compared to stream water, groundwater shows immense variances in spatial and temporal dimensions leading to different partial differential equations that result in coupled models for surface water-groundwater interactions.

The objective of this dissertation project is to investigate the usage of an integral model approach for both systems including advantages and disadvantages compared to coupled models. First examinations consider flow and transport processes at the upper part of the hyporheic zone. A surface water model is extended to investigate conservative transport along different bedforms. For groundwater-surface water interactions, a modified solver of the open source software OpenFOAM is applied and tested for the application within the hyporheic zone. The existing integral solver, developed by [12] was tested for a porous dam break and was not used so far for the examination of hyporheic exchange processes. The integral model solves the three-dimensional Navier-Stokes equations, considering also soil properties like porosity and medium grain size diameter. Within this project, the integral solver is validated for the use of the hyporheic zone. Afterwards examinations of flow processes influenced by different bed forms in the hyporheic zone are executed. Turbulences around various streambed structures based on different flow scenarios are considered using a complex turbulence model. For the investigation of transport processes, the solver will be extended and validated for conservative transport resulting in a three-dimensional integral modelling approach for the transport of substances in the surface water groundwater interaction space.

Model Concepts

For investigations of flow processes in the surface water, the two-phase flow solver interFoam is used. A two-phase model is necessary to depict water level fluctuations which affect pressure distributions in the domain. InterFoam solves the Navier-Stokes equations and is based on a volume of fluid approach that considers the water and air phases as one fluid with rapidly changing fluid properties. An additional transport equation considers the volume fraction of a phase. The governing equations can be found in [13]. Various turbulence models (three Reynolds Averaged Navier Stokes turbulence models and a Large-Eddy-Simulation) are applied to consider turbulence. The transport of a passive tracer is examined with an advection-diffusion equation that has to be implemented into the interFoam solver. For the investigation of surface water and groundwater flow, a solver called porousInter is used. This solver was developed by [12] and extends the interFoam solver by soil porosity and median grain size within an additional drag term. The drag term considers pressure loss as well as flow recirculation. For transport processes within the hyporheic zone an advection-diffusion equation has to be implemented into this solver.

Current State of Work

A first study considers free-surface flow and tracer retention over streambeds with varying ripple morphologies and surface hydraulics. The three-dimensional Navier-Stokes equations were used in combination with an implemented transport equation to investigate the transport of a passive tracer pulse from surface water to surface dead zone. To account for hyporheic exchange, pressure gradients were examined at the streambed (upper boundary of the hyporheic zone), assuming flow from high pressure to low pressure areas. Flow velocities and ripple morphologies affected the pressure gradients and the tracer transport significantly. Most of the tracer pulse from surface water was transported above the ripples (Figure 1). The tracer mass which entered the space between the ripples was retained due to low velocities and recirculation. The recirculation zones between the ripples (Figure 2) were shown to depend on the ripple height to length ratio. This has a large influence on the residence time of the tracer. Moreover, the retention is mainly influenced by flow velocities, the ripple size and the spacing between the ripples: low flow velocities and increasing ripple sizes lead to higher retention. Higher spaces between the ripples lead to temporarily higher tracer concentrations, but also lower tracer retention. The results of this study are important for understanding substance movement, exchange and transformation within the hyporheic zone and were published in [14].

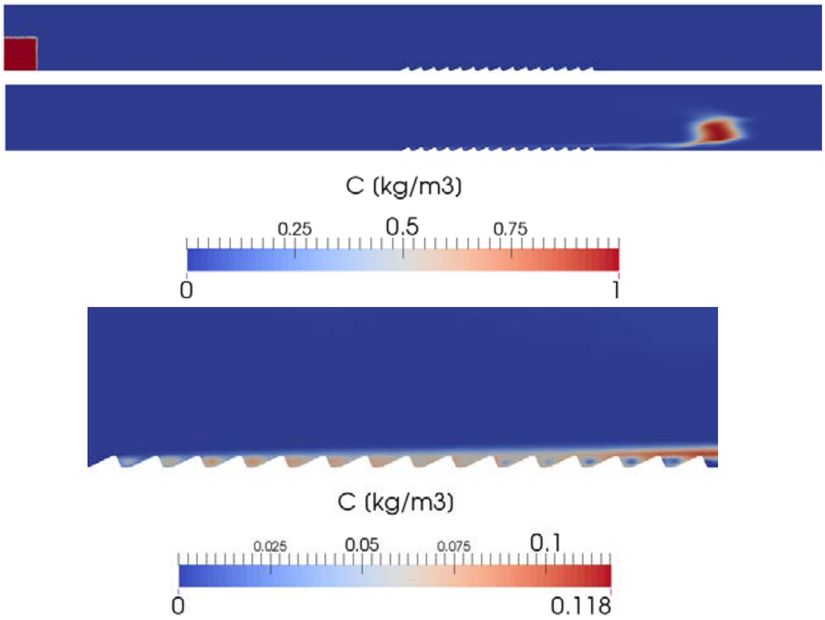

Figure 1: Tracer distribution at t = 0 s (top) and, t = 10 s from section x = 0 m to x = 12 m (center) and for the rippled area (section from x = 6 m to x = 9 m, bottom) for the reference case.

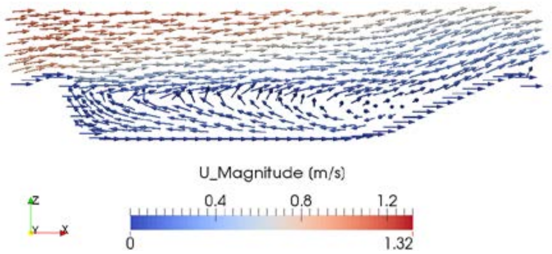

Figure 2: Velocity vectors for case 5 (ripple spacing)

In a next step, the river bed (porous medium) is included and the integral solver is applied. To our knowledge, this modelling approach was never used for the hyporheic zone so far. Consequently, it was first validated based on two test cases describing seepages through homogeneous dams with gravel material. The results of the integral solver were compared with analytical and numerical solutions and a good agreement was achieved for both cases (Figure 3 and 4).

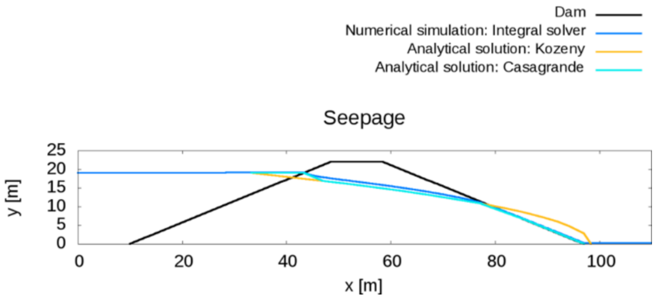

Figure 3: Dam geometry and seepages through a dam for the integral solver and two analytical solutions

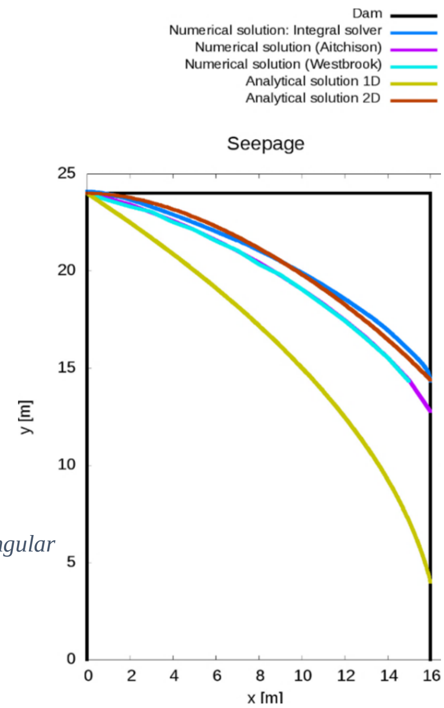

Figure 4: Dam geometry and seepages through a rectangular dam for numerical and analytical solutions

The integral solver was further examined concerning the drag term by the variation of the porosity and the grain size diameter which affected the hydraulics as well as the computational times significantly.
The test cases demonstrated that the integral solver showed good results and therefore further studies are examined in the hyporheic zone with the help of the integral solver. The ripple morphologies of the first study (see [14]) are retained and a part of the river bed soil is added to investigate flow processes within the surface water-groundwater interaction space. The results of this study will be published in a further journal paper and can help project N6 to understand measured retentions of chemical compounds in urban hyporheic zones (e.g. river Erpe).

Future Work planned

The integral solver will be extended by an additional transport equation. Experimental data by [15] will be used to analyse the capability to describe transport processes within the hyporheic zone. Photos from dye spreading within a rippled streambed as a result of the experiment will be compared with numerical results gained with the integral modelling approach and will be subject to the third journal paper.

Collaboration

Modelling issues are discussed in close collaboration with research project T3 (Katharina Teuber) where the same modelling tools are used. Opportunities and challenges of the used software for each interface were presented in [16]. This research project is part of the common topic group “Modelling”. Facing general modelling issues, this group could be addressed, but also the kollegiate Dr. Ilhan Oezgen supported with helpful hints. The joint research of the COMMON topic group “Surface water – groundwater interactions” was presented in [17]. Experimental data for the validation of the transport processes were provided by Aryeh Fox from the Ben-Gurion University of the NegevSede Boqer, Israel. A first test of the solver was executed by Federica Capannelli, a visiting student researcher from the Università degli Studi Roma Tre, Italy.

References

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3. Comments on the qualification programme and supervision strategy:

The collaborative research of natural scientist as well as of engineers helped to get different perspectives and enhanced the exchange of various disciplines. The core courses – especially in the field of natural sciences – broadened my horizons and helped me to get a deeper understanding of the work of my colleagues. Arising questions could be discussed in a small circle of people (e.g. with the supervisors, with other UWI students or kollegiates) or in larger circles like the student meetings, summer schools or interim meetings with many experts which always advised in scientific questions. For the personal development (self-positioning, organisation and negotiation), the women only courses helped to advance the personal progress, but also inspired to think about personal goals.

The Research Training Group offered an excellent support to balance family and work. It was possible for me to attend a course in Copenhagen with my small child. Flexible time management and working at home office allowed me to work most efficiently. After the birth of my second child I look forward to the family-friendly work with UWI.

The programme was always well structured and organized. The professional independence as well as the transfer of knowledge, the exchange through discussions and collaborative working were always encouraged.

Participation in the following Research Training Group events:

1. Core courses
   - I – Urban interface processes – fluxes, transport, interactions (3 ECTS)
   - II – Modelling and measuring concepts of interface processes (3 ECTS)
   - III – Urban freshwater ecology (3 ECTS)
2. Elective courses
   - CFDe (Introduction to OpenFOAM) (5 ECTS)
   - HypoBASICS (Summer School on Hyporheic Zone Processes at the IGB) (3 ECTS)
   - Surface-ground water interaction: From watershed processes to hyporheic exchange (Ph.D. course, University of Copenhagen, Denmark) (2 ECTS)
3. Gender courses
   - Time is honey – the new approach to time, self and workload organization
   - Self positioning
   - Negotiation
   - Project management
4. Other UWI events
   - Orientation Seminar and UWI Opening Ceremony (08. – 09.09.2015)
   - Exposé Talks (08.12.2015)
   - Summer School (13. – 14.09.2016)
   - Kollegiate Seminar (22.09.2016)
   - Interim Meeting (19.05.2017)
   - Student Research Council (17. – 18.03.2017)
   - Summer School (18.-20.09.2018)

Participation in conferences, congresses, etc., at home and abroad:

2017:

- Wasser Berlin International (28. – 31.03.2017, Berlin, Germany)
- SimHydro (14. –16.6.2017, Sophia Antipolis - Nice, France)
- 37th IAHR World Congress (13. – 18.08.2017, Kuala Lumpur, Malaysia)

2018:

- European Geosciences Union General Assembly (8. – 13.04.2018, Vienna, Austria)

4. Individual publications:

I. Articles:

- Broecker,T., Elsesser,W., Teuber,K., Özgen,I., Nützmann,G. & Hinkelmann,R. (2018): High-resolution simulation of free-surface flow and tracer transport over streambeds with ripples. *Limnologica* 68: 46-68
- Teuber,K., Broecker,T., Bayón,A., Nützmann,G. & Hinkelmann,R. (2018): CFD-modelling of free-surface flows in closed conduits. *Progress in Computational Fluid Dynamics*, accepted

II. Conference, poster presentations etc.:

- Broecker,T., Teuber,K., Elsesser,W. & Hinkelmann,R. (2017a): Multiphase Modeling of Hydrosystems using OpenFOAM. *Proceedings of SimHydro* (14. –16.6.2017, Sophia Antipolis - Nice, France), reviewed paper and oral presentation
- Broecker,T., Schaper,J., El-Athman,F., Gillefalk,M., Hilt,S. & Hinkelmann,R. (2017b): Surface water – groundwater interactions. *Proceedings of the 37th IAHR (International Association for Hydro-Environment Engineering and Research) World Congress* (13. – 18.08.2017, Kuala Lumpur, Malaysia), reviewed paper and oral presentation
- Broecker,T., Teuber,K., Ladwig,R. & Hinkelmann,R. (2018): Impact of small-scale riverbed topography on stream flow and surface detention of a tracer. *European Geosciences Union General Assembly* (8.-13.04.2018, Vienna, Austria), abstract and oral presentation
- Teuber,K., Broecker,T., Barjenbruch,M. & Hinkelmann,R. (2016a): High-resolution numerical analysis of flow over a ground sill using OpenFOAM. *Proceedings of the 12th International Conference on Hydroscience & Engineering (ICHE)* (6. – 10.11.2016, Tainan, Taiwan), reviewed paper and oral presentation
- Teuber,K., Broecker,T., Elsesser,W., Agaoglu,B. & Hinkelmann,R. (2016b): Investigation of flow around a ground sill using OpenFOAM. *XXI International Conference Computational Methods in Water Resources (CMWR)* (20. – 24.06.2016, Toronto, Canada), abstract and oral presentation
- Teuber,K., Broecker,T., Elsesser,W. & Hinkelmann,R. (2017): Beyond shallow water flow: Navier-Stokes simulations with OpenFOAM, *BIMoS-Day Shallow water flow Simulations* (22.05.2017, Berlin, Germany), abstract and oral presentation