Integral modeling approach for flow and transport at surface water-groundwater interfaces

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Preface

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An overview of all supplementary scientific work is given in section 5.

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Abstract

Groundwater and surface waters are crucial parts of hydrological cycle which traditionally have been treated separately. Continuous interaction between these two water bodies have attracted requisite attention towards considering them as a single hydrogeochemical continuum in recent decades. Many studies have addressed these interactions on large scales such as catchments as well as local scale hyporheic zone interactions. Influenced by factors such as streambed morphology, ambient groundwater conditions, sediment heterogeneity and bioturbation, hyporheic zone is the hotspot of retention, transformation and attenuation of solutes as well as habitat of a variety of aquatic organisms. Through development of novel measurement methods and experimental techniques, investigating groundwater and surface water as a single hydrologic unit is now very well established in the scientific community. Nevertheless, numerical models as necessary tools to study wide range of scenarios and future event predictions are still based on concepts that consider groundwater and surface water separately. These so called “coupled models” result from successive execution of a surface water model and a groundwater model, oftentimes without any feedback effects. Continuous feedback across groundwater-surface water interface is a key component in successfully investigating small (local) scale intense exchange processes such as hyporheic flow and bioturbation. As opposed to coupled modeling approach, in the current study small-scale groundwater-surface water processes using a novel integral approach is discussed which allows the continuous feedback across groundwater-surface water interface. Due to high computational effort of this approach, only small-scale high-resolution scenarios in the close vicinity of the interface such as hyporheic flow through rippled streambed and bioturbation (pumping activity of tube-dwelling organisms) are investigated.

In the first step, for a case of flow and exchange across a rippled streambed the integral approach is compared to the widely used one-way sequential coupling approach. For integral modeling, porousInter solver of OpenFOAM computational fluid dynamics model is applied solving Navier-Stokes equations which are extended by resistance terms including porosity and grain size diameter parameters to account for flow in porous medium. For coupling, next to the groundwater model “PCSiWaPro®”, OpenFOAM is used for surface water modeling. The necessity of using Navier-Stokes equations-based OpenFOAM for surface water modeling is discussed next to a simpler shallow water equations model called “hms”. Integral to coupled model comparison shows that under turbulent surface water flow in the vicinity of the ripples, continuous feedback of flow between surface water and hyporheic water is simulated with the integral model leading to reduced turbulence compared to the coupled model and flow and
pressure fields near ripples are affected. Results of the two models are very similar far away from the interface in deeper sediment (> 40 cm), however, significantly differ above the interface in the surface water.

In a further step the area of application of the integral approach is expanded towards another important small-scale groundwater-surface water exchange phenomenon. Here, using the integral approach, the pumping activity of tube-dwelling macroinvertebrates in a U-shaped burrow and its impact on hydrodynamic exchange processes between porewater and overlying (surface) water are modeled and compared to experiments and coupled model (Brand et al. 2013). It was realized that unlike coupled model, by using integral model continuous feedback between burrow water and surrounding porewater resulted in modification of pressure and velocity fields in the vicinity of the burrow. As experimental approaches are not capable of direct measurement of flow and exchange processes in the burrow and its surrounding porewater, the integral approach offers a novel possibility about quantifying continuous porewater-burrow. In the first two steps, integral approach was compared to widely used coupled models. Comparison results were plausible and showed that not only integral approach can model a variety of small-scale high-resolution groundwater-surface water interaction processes, but also by allowing continuous feedback between two water bodies, could offer valuable insight towards expanding the understanding of groundwater-surface water interactions.

In the final step, the integral solver “porousInter”, which was formerly tested for transport through homogenous sediment, is further applied for tracer transport through heterogenous sediment. The solver is verified by comparing the modeled transport through heterogenous sediment to analytical solutions. It is then validated by simulating the flow and tracer transport across rippled heterogenous sediment experiments of Fox et al. (2016). Simulated tracer propagation agreed well with the experiments. The simultaneous effect of ambient groundwater conditions and sediment heterogeneity on hyporheic flow and residence times is discussed.

The main outcomes of this thesis are validation of the integral approach, discussion of its advantages in comparison to other groundwater-surface water interface modeling approaches, extension of its area of applicability in modeling small-scale groundwater-surface water interaction induced by pumping activity of tube-dwelling macroinvertebrates in a U-shaped burrow and further application for modeling tracer transport through heterogenous sediment under ambient groundwater conditions. Integral approach can be used for investigations of engineered hyporheic zones and more general for river and lake sediment ecological questions.
as well as a component in integrated water resources management. This approach can further be applied to free surface and porous media flow interaction processes such as flow through porous breakwaters and the simultaneous overtopping of and seepage through dikes and dams.
Zusammenfassung


In einem ersten Schritt wird für den Fall der Strömung und des Austauschs durch ein gerippeltes Flussbett der integrale Ansatz mit dem häufig verwendeten einseitigen sequenziellen Kopplungsansatz verglichen. Für die integrale Modellierung wird der porousInter-Löser des OpenFOAM-Modells verwendet, der die Navier-Stokes-Gleichungen löst, die um Widerstandsterme erweitert werden, die von der Porosität und dem Korngrößendurchmesser


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1. Introduction

1.1 Background

At the earth’s scale, hydraulic groundwater and surface water connection is a crucial part of hydrologic cycle. On the surface of the planet these two major water bodies are in continuous interaction through all surface water types such as streams, lakes and wetlands in many different terrains from the mountains to the oceans (Winter et al. 1998). In inland, major groundwater-surface water interaction areas are wetlands, karst, glaciers, streams, lakes, coastal areas and polar ice caps (Khan and Khan 2019). In the hydrologic continuum, groundwater and surface water are connected through groundwater-surface water interface (Sophocleous 2002, Bobba 2012). Surface water-groundwater interactions happen by groundwater lateral flow through unsaturated sediment (Sophocleous 2002) and by infiltration into or exfiltration from the saturated zones (Brunke 2001, Sophocleous 2002) hence affecting the quantity and/or quality of both systems (Bobba 2012). Although due to continuous interaction groundwater and surface water should be considered a single resource (Winter et al. 1998, Lewandowski et al. 2020), due to different characteristics and accessibilities they are generally studied separately (Brunke 2001, Lewandowski et al. 2020). In recent years the interest in understanding the importance of surface water and groundwater interactions and their integrity as a single continuum has significantly increased (Bobba 2012, Lewandowski et al. 2020). Legislative attention is as well gained towards integral consideration of groundwater and surface water bodies. Directive 2000/60/EC (34) of the European parliament states that to pursue “the purposes of environmental protection, there is a need for a greater integration of qualitative and quantitative aspects of both surface waters and groundwaters, taking into account the natural flow conditions of water within the hydrological cycle”.

1.2 Groundwater-surface water interaction measurement

Development and utilization of measurements methods and models (see section 1.5) to determine groundwater-surface water exchange processes has accentuated the significance of these processes. Next to hydraulic exchange measurements, a major focus has been given to biogeochemical processes and their significance for aquatic ecology and water quality (Rosenberry and La Baugh 2008). Many methods are being used to measure several parameters that are crucial for groundwater-surface water interaction determination. Based on the chosen method, parameters can be directly or indirectly acquired (Kalbus et al. 2006). Direct parameter measurements are conducted by performing for instance seepage meter; and temperature profile
tests to determine seepage flux; and temperature gradients, respectively. Direct oxygen concentration measurement of hyporheic water (see section 1.4) is illustrated in Figure 1-1. Small water sampling tubes (small green tubes inside the water) installed in the sediment are connected to an oxygen meter (blue device on the bridge) that directly measures oxygen concentration of the sampled water and transmits data to the laptop. Water is pumped through the tubes using syringe pumps (red devices) connected to the syringes. Indirect parameter measurements are conducted either using experimental and field methods to determine hydraulic head, hydraulic conductivity, porosity and groundwater velocity based on Darcy’s law or using tracer tests, monitoring wells and pumping tests to determine groundwater components and contaminant concentration based on mass balance approaches (Kalbus et al. 2006, Khan and Khan 2019). Spatial measurement scales of the investigated parameters with different methods vary from a single point measurement to > 1000 m (Fleckenstein et al. 2010, González-Pinzón et al. 2015, Magliozzi et al. 2018).

While direct measurements only determine parameters such as seepage flux for a 10⁻¹ m spatial measuring scale, Darcy’s law-based pumping tests as well as mass balance-based tracer tests can measure up to 10² – 10³ m sections (Kalbus et al. 2006). Seepage meter direct measurements tools follow a simple concept and are inexpensive but in practice their placement could block the streamflow and they cannot detect excessive shallow hyporheic flow (Khan and Khan
Several enhancement tools such as slow pulling of hyporheic water without disturbing the surrounding sediment using syringe pumps (Figure 1-1) were developed. Indirect measurement methods although give very good parameter characterization for measured points, however, can become challenging when dealing with large areas with high hydrogeologic complexity. Using indirect measurement for parameter characterization, a trade-off between resolution of heterogeneities and sampled subsurface volume is inevitable (Kalbus et al. 2006). Although implementing advanced measurements techniques like PIV (Particle Image Velocimetry, Blois et al. (2014), Roche et al. (2018)) has recently improved parameter characterization for laboratory experiments, generalization of acquired parameters through laboratory and especially field measurement campaigns remains challenging. Implementing different scenarios under varying hydrologic conditions to predict future events and gaining a deeper understanding of the complex dynamics of the groundwater-surface water exchange is possibly through modeling studies (Boano et al. 2009, Stonedahl et al. 2012, Brunner et al. 2017, Broecker et al. 2019). The current contribution examines the applicability of the advanced numerical models to study the groundwater-surface water exchange processes (namely the integral approach; see section 1.6). In section 1.5, various approaches to model groundwater-surface water exchange are presented. Next to the methods, it is crucial to discuss the scale of the groundwater-surface water processes.

1.3 Spatial scales of groundwater-surface water interaction

Groundwater-surface water interaction is a multiscale processes, where local scale effects aggregate and then manifest across all spatial scales. The spatial scale of a selected method has a considerable effect on the results of parameter measurement (Kalbus et al. 2006, Khan and Khan 2019). Groundwater-surface water interactions occur in a variety of spatial scales. A scale categorization done by Larkin and Sharp (1992), Brunke and Gonser (1997) and Woessner (2000) is as follows:

1) Large-scale interactions: interaction is affected by whole catchment or watershed
2) Local-scale interactions: within the streambed controlled by e.g. hyporheic flow (see section 1.4) properties
For each spatial scale, landscape diversifies physiographic and climatic settings of the area (Winter et al. 1998). Surface water types such as oceans, streams, lakes and wetlands unify perspective of the interaction of groundwater and surface water in different landscapes (Winter et al. 1998).

Figure 1-2: Groundwater-surface water exchange types: a) gaining condition, b) losing condition, c) neutral condition, after Winter et al. (1998)

For different landscapes and spatial scales, higher/lower groundwater table compared to surface water table can cause two distinctive flow patterns (Cardenas 2009, Fox et al. 2014, Fox et al. 2016). With a higher groundwater table compared to surface water table, an upwelling groundwater movement results in groundwater infiltration into the surface water. This state is referred to as “gaining condition” (Figure 1.2a). Conversely, with a lower groundwater table compared to surface water, hydraulic gradient is reversed and water exfiltrates from the surface water into the groundwater. This creates a so called “losing condition” (Figure 1.2b). In a “neutral condition” water table at the ground- and surface water are in equilibrium (Figure 1.2c; Silliman & Booth 1993, Woessner 2000).
Considering the impact of all spatial scales simultaneously is crucial in investigating regional groundwater-surface water interactions (Ellis et al. 2007; Krause et al. 2007, Mojarrad et al. 2019). Therefore, next to interactions that are triggered by groundwater-surface water table imbalances, local scale interactions like hyporheic exchange (Merill and Tonjes 2014, Mojarrad et al. 2019,) and bioturbation (Roskosch et al. 2012, Hupfer et al. 2019, Shrivastva et al. 2021) should be highlighted.

Figure 1-3: Hyporheic exchange through (1) meander, (2) dry bar, (3) pool-riffle, (4) ripple and (5) bioturbation, cross section “a” across flow direction

In local scale, large morphological features such as meanders (Figure 1-3 (1); Boano et al. 2006, Revelli et al. 2008, Gomez et al. 2012), sediment bars (Figure 1-3 (2); Tonina and Buffington 2007, Boano et al. 2010, Marzadri et al. 2010), pool-riffle (Figure 1-3 (3); Harvey & Bencala, 1993; Tonina and Buffington, 2009, Trauth et al. 2014) and ripples (Figure 1-3 (4); Cardenas & Wilson 2007a, 2007b, Bottacin-Busolin & Marion, 2010, Fox et al. 2014) trigger hyporheic flow by significantly modifying local pressure and shear stresses. Hyporheic zone and complex hydrological process occuring in this zone are further discussed in section 1.4.

Bioturbation is a generic term which is referred to a variety of activities of benthic (Kristensen et al. 2012) and hyporheic (Shrivastva et al. 2021) organisms that impact streambed/lakebed sediments. This impact is through particle reworking and burrow ventilation. By mixing the sediment, freshy settled easily degradable material is transported into deeper sediment and inorganic material from deeper sediment is introduced to the oxic sediment zones (Lewandowski et al. 2005a). Burrow ventilation of tube dwelling macroinvertebrates (Figure 1-3 (5)) such as Chironomus Plumosus (Stief et al. 2010b, Hupfer et al. 2019) results in diffusive and advective aeration of the sediment called bioirrigation (Kristensen et al. 2012) and significant loss of fixed nitrogen from shallow aquatic ecosystems (Jeppesen et al. 1998, Sondergaard et al. 2007).
Groundwater-surface water interaction spatial heterogeneities influence the fate and transport of contaminants (Conant et al. 2004, Chapman et al. 2007, Kalbus et al. 2007) and impact the ecosystem of the streams (Brunke & Gonser 1997). Water quality of both groundwater and surface water are impacted by their interaction (Stanford and Ward 1988, Edwards 1998, Fraser and Williams 1998, Hill et al. 1998, Hayashi and Rosenberry 2002, Fleckenstein et al. 2010, Mojarrad et al. 2019). Diverse biological activities and the distribution of aerobic and anaerobic conditions within groundwater as well as the fate and transport of waterborne substances such as nutrients and organic carbon (Jones and Holmes 1996, Mulholland et al. 1997, Storey et al. 1999, Stonedahl et al. 2012) are controlled by this interaction (Harvey et al. 2013, Marzadri et al. 2011, Zarnetske et al. 2011). In dealing with stream water quality issues such as spreading of industrial, agricultural and sewage contaminants, hyporheic zone, due to its self-purification effects, is an attractive hydrogeological feature. Its self-purification effect includes nutrient turnover, degradation of contaminants and the removal of trace organic compounds (Biksey and Gross 2001, Lewandowski et al. 2019).

1.4 Hyporheic zone

In terms of ecology, geochemistry and hydrogeology “Hyporheic zone” can be defined differently (Merill and Tonjes 2014, Cardenas 2009). In ecology it refers to biologically active zone near the stream where groundwater and surface water are interacting (Harvey and Bencala 1993, Harvey and Wagner 2000). Key ecosystem processes such as temperature, primary productivity, mixing and transport of dissolved oxygen, nutrient cycling, microbe and invertebrate communities and fish diversity are influenced by these interactions (Brunke and Gonser 1997, Boulton et al. 2010, Krause et al. 2011). Many freshwater organisms dwell permanently (Gibert and Deharveng 2002), temporarily, or under certain conditions in hyporheic zone. Hyporheic zone is a crucial component of the life cycle of many biota such as fishes, macroinvertebrates and amphibians (Lopez-Rodriguez et al. 2009, Resh and Rosenberg 2010, Williams et al. 2010). In presence of predators or under unfavourable surface conditions such as floods, droughts or contaminated surface water (Stubbington et al. 2011), some of organisms (hyporhoes, Boulton et al. 1998, Wood et al. 2010) use hyporheic zone as a temporary refuge. In areas where excessive deposition of fine sediment as a by-product of human development deranges the natural hyporheic zone sediment composition and hyporheos community is negatively affected (Paul and Meyer 2001, Coleman et al. 2011). Under such conditions, clogging of interstitial space between natural streambed grain blocks stream flow from downwelling into hyporheic zone (Arnon et al. 2010, Song et al. 2010) which interrupts
the dissolved oxygen supply and nutrient cycling. Fortunately, presence of (macro)invertebrates and other organisms can restore permeability in the sediment through bioturbation (Nogaro et al. 2010).


In hydrogeology, hyporheic zone is defined as sediment surrounding a river in which recent water from surface flow mixes with groundwater and soon returns to surface water (Harvey and Bencala 1993, Boano et al. 2014). Next to spatial scales heterogeneity, temporal dynamics of hyporheic zone are defined with relatively fast transport processes in surface water (Ibisch et al. 2009, Kennedy et al. 2009) and slower transport in groundwater with velocities within lower orders of magnitude (Müller 2014). This causes the dynamic exchange of water, substances and energy and circulations in the hyporheic zone (Krause et al. 2011). Water exchange at the hyporheic - surface water interface which is caused by local pressure differences and turbulence (Cardenas and Wilson 2007a) can lead to water level variations and thus pressure gradients (Elliot and Brooks 1997a, 1997b, Packman et al. 2004). Presence of features like pool-riffle or ripples in streambed (Figure 1-3) create high pressures on luv side and lower pressure on lee side of the feature thus allowing surface water infiltration from luv side and exfiltration from lee side (Elliot and Brooks 1997a, 1997b, Broecker et al. 2021). Next to that, aquifer properties (Brunke and Gonser 1997), ambient groundwater (Cardenas and Wilson 2007a) and turbulence in surface water and its propagation (Roche et al. 2018) into the sediment influence hyporheic exchange. Heterogeneity which is caused by transport and settling of sediment particles over a variety of flow conditions (Powell 1998), is the main driver in flow adjustment by redirecting flow through areas with higher hydraulic conductivities (Vaux 1968). Many studies (e.g. Freeze and Cherry 1979, Pryschlak et al. 2015) have shown that due to its major impact on hyporheic exchange processes in streams, considering heterogeneity of the streambed has as much of a priority as stream morphology and groundwater flow conditions. Therefore, the best
hydrogeological representation of hyporheic exchange processes is achieved by considering heterogeneity alongside morphology and groundwater conditions (Figure 1-4 Hydrology).

Figure 1-4: Major hyporheic drivers and processes after Lewandowski et al. (2019): (1) water-sediment interface, (2) synthetic or organic matter (dissolved or particulate) from urban areas and industry, (3) local and large scale groundwater-surface water exchange, (4) dynamic biofilm, (5) bioturbation and microbial activity, (6) macroinvertebrates, (7) protozoa, (8) labile carbon gradients, (9) anoxic microzones, (10) solute and particle transport, (11) sorption sites, (12) temperature gradients, (13) surface flow forcing, (14) hyporheic exchange flux, (15) heterogenous streambed conductivity and morphology, (16) infiltration zones and (17) exfiltration zones

Intensive material turnover and dynamic water interaction in hyporheic zone drives hydro-biogeochemical processes from many different disciplines (Figure 1-4, Lewandowski et al. 2019). An improved awareness of processes which is achieved though interdisciplinary investigations enables these processes to be considered more holistically (Lawrence et al. 2013). A combination of spatially and temporally resolved field and laboratory data with physically based numerical models is crucial in understanding dynamic processes at the groundwater-surface water interface (Tonina and Buffington 2007, Cardenas 2010, Cuthbert et al. 2010, Derx et al. 2010, Westhoff et al. 2010). In the following modeling concepts and tools to describe surface water-groundwater interactions are discussed.
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1.5 Concepts of modeling groundwater-surface water interactions

For surface water and groundwater investigations, numerical models are widely applied techniques to study hydrodynamic and hydrogeochemical processes by computational simulation of different scenarios. Understanding of these complex flow, transport and transformation processes is achieved using mathematical models that are designed to describe physical laws and equations. Compared to field and laboratory experiments, they are often less expensive and can provide information for a broader range of scenarios and future predictions and investigate parameters that are hard to measure with physical measurement methods (section 1.2). Groundwater-surface water interaction concepts were first incorporated into groundwater models in the early 1980s (e.g. Prudic 1989). Early applications were limited mostly to large scale water quantity management which resulted in coarse model resolutions in time and space (Gorelick 1986). Surface water flow processes were simplified and aquifer homogeneity was assumed (Fleckenstein et al. 2010). Later efforts to include ecological functions (Stanford and Ward 1988) and biogeochemical processes (Hill 1990) were made by presentation of transient storage models. These advances have led to the development of various advanced hydrological models that operate at the catchment (large) scale (e.g. Parflow by Ashby and Falgout 1996, Amanzi/ATS by Moulton et al. 2012, OpenGeoSys by Kolditz et al. 2012). With more focus being given to the local-scale processes (Elliot and Brooks 1997a, Packman and Brooks 2001), existing groundwater models were linked to more complex surface water models (Swain and Wexler 1993) and coupled groundwater-surface water models were presented (Kollet and Maxwell 2006, Jones et al. 2008).

Coupling of flow and transport between groundwater and surface water is achieved by either modeling of flow through pore spaces or single/two-domain strategies. Pore network models are based on modeling the flow using e.g. Navier-Stokes equations with considering the sediment matrix as well as water and air components (Figure 1-5 a). These models are used to improve the understanding of phenomena such as impact of pore geometry on microbial communities (Young and Ritz 2000), relation of pore water network to residence times (Bijeljic and Blunt 2006) and water-air interface dynamics (Hassanizadeh et al. 2002). Detailed mapping of pore spaces is often required for pore network modeling. Although recent method developments such as x-ray tomography can help in determining pore networks, they still lack the ability to differentiate between air and water phase (Van Loo et al. 2014). High computational cost along with expensive and inaccurate pore network measurements methods are the main challenges of this modeling approach.
Using superposed groundwater-surface water equations to deal with both groundwater and surface water flow is known as single-domain approach. Superposed equations are applied on a transition zone between surface and groundwater and a gradual gradient (Figure 1-5 c) of key flow parameters between them is defined. Using this approach, defining the thickness of the transition zone as well as the parameters and their gradients are very challenging (Goyeau et al. 2003, Rosenzweig and Shavit 2007).

In two-domain approach, groundwater flow is modelled with groundwater equations and surface water flow with surface water flow equations (Figure 1-5 d). The shared boundary between two models which is the surface water-groundwater interface is then used to transfer parameter information from one model to other (and back). Using this approach, there are several coupling techniques who couple surface flow velocity to groundwater flow velocity with adopting a slip coefficient. A relatively precise coupling outcome is expected through coupling with feedback effects (two-way coupling, Nützmann and May 2007) where the selected coupling parameter values from the surface water model run is fed to the groundwater model. Resulting values from groundwater model run are returned to the surface water model in an iteration step and surface water model is run again with the new value. Iteration steps continue until desired parameter convergence is achieved. Flow conditions like velocity in groundwater are orders of magnitude smaller than surface water which makes temporal coupling interval selection of both models very challenging. The most common two-domain coupling technique is one-way sequential coupling with pressure as the coupling parameter (Tonina and Buffington et al. 2009, Trauth et al. 2015). This technique is widely used and

In previous sections, it was explained how for local scale processes such as hyporheic flow and bioturbation, the surface water-groundwater interface itself was hosting crucial ecohydrological processes. Via coupling, this interface is considered as a side boundary and its continuous transition is replaced by a discontinuity. Next to other advanced numerical models such as DUMUX (Weishaupt et al. 2019) who applied the direct numerical solution of flow through a random pore-network, recently, a high-resolution integral modeling approach (Oxtoby et al. 2013) was applied to hyporheic flow and transport processes through homogenous sediment across rippled streambed by Broecker et al. (2019, 2021). This approach uses the same conceptual approach for both groundwater and surface water without adding any additional coupling parameters for the interface. To further develop this approach and its area of applicability for local groundwater-surface water exchange modeling, it is necessary to validate it in comparison to widely used coupled approaches and experiments. Local-scale high resolution modeling via this approach is done through computational fluid dynamic model OpenFOAM which is introduced in the following.

1.6 Flow and transport modeling with OpenFOAM

OpenFOAM (Open Field Operation And Manipulation) is the most widely used free, open-source computational fluid dynamics software with a vast user base across many areas of science both commercially and academically. It includes a wide range of features (libraries, solvers, utilities) for complex fluid mechanics modeling as well as fields like acoustics, solid mechanics and electromagnetics. Numerical fluid mechanics problems can be modeled via OpenFOAM in compressible/incompressible, single-/multi-phase, 1-/2-/3-dimensions forms. It is mostly based on the FVM (Finite Volume Method) in space and the FDM (Finite Difference Method) in time (Schulze and Thorenz 2014).

In pre-processing phase, structured numerical mesh is generated using the built-in utility ‘blockMesh’. Additionally, unstructured meshes from other meshing tools like ‘GMSH’ (Geuzaine and Remacle 2009) and Salome (Ribes and Caremoli 2007) can be imported. Boundaries as well as initial conditions should be selected accordantly to each other for model stability and good convergence.

The partial differential equations governing flow and transport in OpenFOAM cannot be solved directly and thus are spatially and temporally discretized as mentioned above and are transferred
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to algebraic equations. Based on computational capacity, desired outcome precision and necessary model convergence, spatio-temporal discretization, margin of error and interpolation of parameters can be defined by user; with considering limiting factors like Courant number (Schulze and Thorenz 2014).

To keep computational capacity limits of the models presented in the current study small, supercomputer cluster HPC (High Performance Computing) of the Technische Universität Berlin is used for modeling. Mathematical equations, algorithms and modeling techniques of OpenFOAM used here for modeling surface water flow as well as integral modeling of flow and exchange between groundwater and surface water are presented in the following.

1.6.1 Modeling surface water flow and transport

Most surface water flow scenarios of the present study are modeled with InterFoam solver, a component of OpenFOAM software. This widely used solver (Higuera et al. 2014, Schmitt et al. 2015, Bayon et al. 2016) allows modeling of three-dimensional Navier-Stokes equations for two (here water and air, multiphase in general) incompressible, immiscible fluids. In the current study, it is often essential to consider water level fluctuations and their effects on pressure distribution in the model as also was the case in Broecker et al. (2019). To capture the sharp water-air interfaces, the VOF (Volume of Fluid) interface locating method implemented in interFoam is applied. Fractions of air and water in partially saturated cells are defined with altering fluid properties for each fraction. Volume of fractions are detected based on their fraction indicator values ($0 \leq \alpha \leq 1$). Fluid properties include density and viscosity which must be weighted according to their fractions ($\alpha \ [-]$) and are calculated as follows:

$$\mu = \mu_w \alpha + \mu_a (1 - \alpha) \quad \text{Eq. (1.1)}$$

$$\rho = \rho_w \alpha + \rho_a (1 - \alpha) \quad \text{Eq. (1.2)}$$

where $\rho$ [kg/m$^3$] is the density of the fluids ($\rho_w =$ water density, $\rho_a =$ air density) and $\mu$ [kg/(m s)] is the dynamic viscosity ($\mu = \mu_p + \mu_t$; physical + turbulent dynamic viscosity, $\mu_w =$ water dynamic viscosity, $\mu_a =$ air dynamic viscosity).

The interface convection is described by the following equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{v}) = 0 \quad \text{Eq. (1.3)}$$

where $\vec{v}$ [m/s] is the flow velocity vector and $t$ [s] is time.

Conservation of mass (Eq. (1.4)) and momentum (Eq. (1.5)) are written as follows:
\[ \nabla \hat{v} = 0 \quad \text{Eq. (1.4)} \]

\[
\left( \frac{\partial (\rho \hat{v})}{\partial t} + \hat{v} \nabla (\rho \hat{v}) \right) = -\nabla p + \mu \nabla^2 \hat{v} + \rho g 
\]
\[ \text{Eq. (1.5)} \]

where \( p \) [Pa] is the pressure and \( g \) [m/s²] is the gravity vector acceleration.

The above equations calculate velocity in three dimensions and pressure, while pressure-velocity coupling in interFoam is done with PIMPLE algorithm which is based on the PISO (Pressure Implicit with Splitting of Operators) and SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm (Caretto et al. 1973, Issa 1986, Greenshields 2010).

To describe the transport of a conservative tracer with a concentration \( C \) [kg/m³], Broecker et al. (2018) have implemented the following advection-diffusion equation into interFoam:

\[
\frac{\partial C}{\partial t} + \nabla \cdot (\hat{v} C) + \nabla \cdot (D \nabla C) = 0 
\]
\[ \text{Eq. (1.6)} \]

\( D \) [m²/s] is diffusion coefficient which is divided into \( D_{ph} \) [m²/s] for the physical diffusivity and \( D_t \) [m²/s] for the turbulent diffusivity. Turbulent Schmidt number relates the turbulent diffusivity to the turbulent viscosity as follows:

\[
Sc_t = \frac{\mu_t}{D_t} 
\]
\[ \text{Eq. (1.7)} \]

The physical diffusivity is a fluid property, while the turbulent Schmidt number \( Sc_t \) [-] can be used for model calibration.

### 1.6.2 Turbulence models

In fluid dynamics, a fluid can either flow in parallel layers with no disruption between those layers (laminar flow) or undergo chaotic changes in pressure and flow velocity both in time and space (turbulent flow). The extent of turbulence in a flow is often characterized using Reynolds number (Re [-]) which describes the ratio of inertia to viscous forces acting on the fluid. Reynolds number is used to predict flow patterns in different flow conditions. In fully formed open channel and pipe flow with \( Re < 2300 \) flow is considered laminar and with \( Re > 2300 \) it is considered turbulent. While some modeling cases of this study have relatively low Reynolds numbers and are considered laminar (section 3), others need to be modeled with a proper turbulence model for precise high-resolution modeling outcomes (section 2 and 4). OpenFOAM offers a wide range of turbulence models. The main three types of numerical turbulence simulation methods are RANS, LES and DNS.
A simpler turbulence model compared to others in terms of computational effort is RANS (Reynolds-averaged Navier-Stokes). It consists of a variety of models such as k-\(\varepsilon\), k-\(\omega\) and k-\(\omega\) SST. k-\(\varepsilon\) is the most common RANS turbulence model to simulate mean flow characteristics for turbulent flow conditions. It is a two-equation model that consists of two transport equations to account for turbulent kinetic energy (k) and turbulent dissipation rate (\(\varepsilon\)). It is applicable for free-shear flows and small pressure gradients but not good for complex flows with strong curvatures. k-\(\omega\) (\(\omega\) is the frequency of energy dissipating eddies) is a RANS model with strength close to walls. It is a two-equation model for turbulent energy (k) and frequency (\(\omega\)) and is used mostly for low Reynolds numbers. k-\(\omega\) SST (k-\(\omega\) Shear Stress Transport) is a combination of the formerly mentioned RANS models and uses k-\(\varepsilon\) for inside of the model domain and k-\(\omega\) for the boundaries. Although computationally suitable, RANS models sometimes cannot properly capture all flow velocity fluctuations and anisotropy of eddies.

Large turbulent eddies are directly resolved with LES (Large Eddies Simulation) on relatively fine grids. Applying a user-defined low-pass filtering, the smallest length scale is put aside and its effects are modelled via subgrid algebraic models. In comparison to RANS, LES is much more computationally burdening. In DNS (Direct Numerical Solutions) all spatial and temporal eddy scales are resolved leading to extremely fine grids and extremely high computational effort. Compared to DNS, LES is computationally reasonable. In this thesis next to laminar modeling, for turbulence modeling LES is used.

1.6.3 Integral modeling of groundwater-surface water interactions

A modified version of interFoam to account for flow in porous medium was presented by Oxtoby et al. (2013). For incompressible fluids the equations averaged over region ([ ]\(f\)) for the conservation of mass (Eq. (1.4)) and momentum (Eq. (1.5)) are written as:

\[
\begin{align*}
\varphi\nabla[\bar{v}]^f & = 0 \quad \text{Eq. (1.8)} \\
\varphi \left( \frac{\partial [\rho]^f[\bar{v}]}{\partial t} + \nabla[\rho]^f[\bar{v}]^f[\bar{v}]^f \right) & = -\varphi\nabla[p]^f + \varphi[\mu]^f \nabla^2[\bar{v}]^f + \varphi[\rho]^f \cdot g + D \quad \text{Eq. (1.9)}
\end{align*}
\]

where \(\varphi\ [\cdot]\) is the effective porosity and \(D \ [\text{kg/(m}^2\text{s}^2)]\) is an additional porous drag term.

\[
D = A + B \quad \text{Eq. (1.10)}
\]

\[
A = - \left( 150 \frac{(1-\varphi)}{d_p \varphi} [\mu]^f + 1.75[\rho]^f \frac{[v]^f}{d_p} \right) \frac{(1-\varphi)}{\varphi} [v]^f \quad \text{Eq. (1.11)}
\]

\[
B = -0.34 \frac{(1-\varphi)}{\varphi} \frac{\partial [v]^f[\rho]^f}{\partial t} \quad \text{Eq. (1.12)}
\]
where \(d_p\) [m] is the effective grain size diameter.

In Eq. (1.11), the term “\(A\)” describes pressure loss due to friction of the fluid with porous medium after Ergun (1952). In porous medium, compared to free flow, more momentum is needed to accelerate a given volume of water which is called added mass. Added mass is accounted for in Eq. (1.12) (van Gent 1995).

In areas where only free flow exists, effective porosity is set to 1 which results in \(A = B = D = 0\) and ensures the use of the original Navier-Stokes equations for free water flow (Eq. (1.4) and Eq. (1.5)).

Former discussions about turbulence models apply here as well. Similar to surface water transport modeling Broecker et al. (2021) have presented “porousInterTracer” for integral modeling of conservative transport through porous zones:

\[
\frac{\partial [c]}{\partial t} + \nabla \cdot \left( \bar{v}_p \left[ c \right] f \right) + \nabla \cdot (D \nabla [c] f) = 0
\]

Eq. (1.13)

Where \(\bar{v}_p\) [m/s] is pore velocity.

In dealing with transport in porous medium, next to advection-diffusion based equations provided in “porousInterTracer”, one could consider dispersion as well. Although for the cases of this study, only diffusion was accounted for, verification of advective-diffusive-dispersive version of porousInterTracer through comparison with analytical solutions is presented in the appendix A.

### 1.7 Coupled modeling of groundwater-surface water flow

As mentioned in section 1.5 coupled models are the prevalent tools to investigate groundwater-surface water interactions and are widely applied and validated. A necessary step to discuss the advantages of the integral approach and address its area of application is to compare it to coupled approach. Due to its high validity, wide application and prominence, one-way sequential coupling with pressure as the coupling parameter is the best choice for this comparison. In this thesis, first an identical coupled model is made for comparison to integral model for the case of a rippled riverbed to inspect the full procedure of pre-processing, simulating and post-processing of both models and second, integral model is compared to an existing small-scale coupled model for the case of bioturbation. For surface water part of the coupled model, interFoam solver of the OpenFOAM is used (discussed in 1.6.1). Thereafter, to discuss the necessity of choosing a computationally expensive CFD surface water model for
1. Introduction

Shallow water equations are applicable, when the wavelength is at least 20 times larger than the water depth leading to hydrostatic pressure. These equations are derived from depth-integration of the Navier-Stokes equations and in consequence they do not include vertical components. Conservation of mass and momentum without considering sink or source terms (e.g. precipitation or infiltration) for two dimensional depth-averaged shallow water equations are written as follows:

\[
\frac{\partial h}{\partial t} + \nabla (\vec{v} \cdot \vec{h}) = 0 \tag{1.14}
\]

\[
\frac{\partial (\vec{v} \cdot \vec{h})}{\partial t} + \nabla \left( \vec{v} \cdot \frac{1}{2} gh^2 \right) - \mu_t \nabla^2 (\vec{v} \cdot \vec{h}) = -gh\nabla z_B + \frac{n^2 \rho g}{h^\frac{1}{3}} \vec{v} \cdot |\vec{v}| \tag{1.15}
\]

where \( h \) [m] is the water depth, \( z_B \) [m] is the bottom elevation, \( \mu_t \) [m²/s] is turbulent kinematic viscosity and \( n \) [s/m¹/³] is Manning’s roughness coefficient.

Java-based modelling framework \textit{hms} (hydroinformatics modeling system, Simons et al. 2014) which uses the Finite Volume Method is chosen for shallow water flow modeling.

Coupling is achieved by transferring the modeled pressures results of the shared boundary from surface water (interFoam) to groundwater model. These are then used as boundary conditions of the PCSiWaPro® groundwater model. PCSiWaPro® is a 2D Finite Element-based groundwater modeling software developed by IBGW Leipzig (Ingenieurbüro für Grundwasser GmbH Leipzig) and TU Dresden. It uses the the extended Darcy’s law (Richards equations) which is introduced in the mass conservation equation as follows:

\[
\frac{\partial \theta}{\partial t} = \nabla [K(\theta) (\nabla \psi - 1)] \tag{1.16}
\]

where \( \theta \) [m³/m³] is the volumetric water content, \( K(\theta) \) [m/s] is the hydraulic conductivity, \( \psi \) [m] is the pressure head. Further information can be found on PCSiWaPro® user guide (PCSiWaPro® Benutzerhandbuch).

1.8 Scope of this thesis

1.8.1 Current research deficits

Primarily, Broecker et al. (2019) have applied the integral approach to model flow and exchange across a rippled streambed domain. Nevertheless, a systematic comparison of this approach to prevalent coupling approach which is famously applied in groundwater-surface water interaction investigations is missing. Extensive model comparison is necessary to prove the
flexibility and applicability of the integral approach and its superiority to the coupled approach in modeling small-scale high-resolution groundwater-surface water exchange processes.

In investigating cases such as flow and ventilation in and around invertebrate-dwelled burrows, current experimental approaches only observe the overlying water flow processes and lack the ability to measure flow and exchange inside the burrow. Existing coupled models that investigate flow inside and around the burrow cannot show the connected flow system of the overlying water, burrow and the surrounding sediment. Integral approach however is potentially capable of modeling connected flow and exchange over, through and around the burrow.

Validation of the integral approach for tracking the tracer concentration along and across the groundwater-surface water interface, is the key for its application to water quality assessment and groundwater contamination modeling. Broecker et al. (2021) have validated the approach for tracer transport in homogenous sediment. However, sediment heterogeneity which strongly impacts contamination propagation by changing solute residence times in the sediment has not yet been validated for the integral approach.

1.8.2 Aim of this thesis

An integral modeling approach to describe high-resolution flow and transport processes occurring at the interface of groundwater and surface water is investigated in this thesis for local (small) scale groundwater-surface water interactions. A conclusive comparison of the approach next to the coupled approach is done for two distinctive cases and advantages of using integral approach to model local (small) scale flow near surface water-groundwater interface are discussed and area of application is determined. Thereafter, to extend the area of application to modeling tracer transport in heterogenous sediments, flow patterns and tracer propagation at heterogenous rippled streambeds with ambient groundwater flow are investigated and validated with the help of experiments.

The thesis is structured in six sections consisting of the current introduction, three peer-reviewed journal articles (one accepted, two submitted), further supplementary contributions and a synthesis. Additionally, further solver validation and complementary information are provided in two appendices.

Section 2 describes flow over and through a porous and rippled streambed. This is done through modeling flow and exchange processes with integral and coupled approaches. Integral approach uses the CFD software OpenFOAM to solve modified Navier-Stokes equations. A Richards equation-based groundwater model (PCSiWaPro®) is coupled with an interFOAM surface
water model and the necessity of using interFOAM as the surface water model is investigated against a shallow water equations-based model (hms) for the same setup. Due to integral approach being computationally slightly more expensive than coupled approach, area of application meaning distance from the groundwater-surface water interface where coupled and integral models lead to different results is analysed.

In section 3 flow induced by bioturbation activity of the macroinvertebrate Chironomus plumosus worms in a U-shaped burrow in lake sediments is modelled via integral approach and compared to similar setups modeled with coupled approach and experiments. Importance of modeling continuous surface water-groundwater flow exchanges in these burrows as hotspots of bioirrigation is emphasized in comparison to coupled approach which neglects feedback effects and to experiments which lack representing flow through sediment and are mostly conducted only for tracking flow over burrows.

By comparing the integral to coupled approach in section 2 and 3, advantages of the integral approach are revealed and its superiority to model flow and exchange in the groundwater-surface interaction space is assessed for a variety of cases.

In section 4 flow and tracer transport processes for heterogenous sediment were studied under neutral, losing and gaining groundwater flow conditions. For this purpose, the extended integral solver for modeling tracer propagation in surface water and sediment is used and further validated by performing numerical modeling of flow and tracer propagation similar to experiments of flow and tracer transport over a heterogenous rippled streambed.

An overview of the supplementary scientific work is presented in section 5. This section includes a brief introduction of two co-authored journal articles concerning flow and exchange across rippled streambed under the influence of ripple geometries, surface hydraulics and grain sizes as well as flow and transport through homogenous surface water-groundwater interface.

In section 6 the main findings of this study are conjunctively summarized and their common goal of applying, validating and extending the integral approach as a suitable modeling instrument for groundwater-surface water interface is discussed; limitations of the approach are addressed and further steps are described.

In appendix A, flow and transport integral model is validated for modeling advective-diffusive-dispersive tracer propagation with the help of analytical solutions. In appendix B, an overview of the modeled cases is given.
2. Comparison of integral approach to coupled approach for flow across rippled streambed

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This is the postprint version of the article.

The test cases setups are listed in Appendix B (B1 Seepage through a dike modelled with porousInter and PCSiWaPro®, B2 Seepage through a rectangular dam modelled with porousInter and PCSiWaPro®, B3 one-dimensional, one-phase modeling of surface water flow over rippled streambed with hms (shallow water equations), B4 Three-dimensional, two-phase modeling of surface water flow over rippled streambed with InterFoam, B5 Two-dimensional, modeling of groundwater flow in the sediment under the rippled streambed with PCSiWaPro®, B6 Three-dimensional, two-phase integral modeling of flow across rippled streambed with porousInter.
2. Comparison of integral approach to coupled approach for flow across rippled streambed

2.1 Abstract

Although both are crucial parts of the hydrological cycle, groundwater and surface water had traditionally been addressed separately. In recent decades, considering them as a single hydrological continuum in light of their continuous interaction has become well established in the scientific community through the development of numerous measurement and experimental techniques. Nevertheless, numerical models, as necessary tools to study a wide range of scenarios and future event predictions, are still based on outdated concepts that consider groundwater and surface water separately. This study compares these “coupled models” (CM), which result from the successive execution of a surface water model and a groundwater model, to a recently developed “integral model” (IM). The integral model uses a single set of equations to model both groundwater and surface water simultaneously, and can account for the continuous interaction at their interface. For comparison, we investigated small-scale flow across a rippled porous streambed. Although we applied identical model domain details and flow conditions, which resulted in very similar water tables and pressure distributions, comparing the integral and coupled models yielded very dissimilar velocity values across the groundwater–surface water interface. These differences highlight the impact of continuous exchange across the interface in the integral model, which imitates such flow processes more realistically than the coupled model. A few decimeters away from the interface, modeled velocity fields are very similar. Since the integral model and the surface water component of the coupled model are both CFD-based (computational fluid dynamics), they require very similar computational resources, namely access to cluster computers. Unfortunately, replacing the surface water component of the coupled model with the widely used shallow water equations model, which indeed would reduce the computational resources required, produces inaccuracy.

2.2 Introduction

On the surface of the planet, groundwater and surface water are in continuous interaction through all surface water types, such as streams, lakes, and wetlands, in many different terrains, from mountains to oceans (Winter et al. 1998). In the hydrologic continuum, groundwater and surface water are connected through the groundwater–surface water interface (Sophocleous 2002, Bobba 2012). Although groundwater and surface water should be considered a single resource due to their continuous interaction (Winter et al. 1998), they are generally modeled separately due to different characteristics and accessibilities (Brunke 2001). In recent years,
interest in understanding the importance of surface water and groundwater interactions and their
integrity as a single continuum has significantly increased (Bobba 2012). The development and
utilization of measurement methods and experiments to determine groundwater–surface water
exchange processes has further accentuated their significance (Kalbus et al. 2006). Groundwater–surface water interaction happens on the local spatial scale (within the
streambed) as well as on large spatial scales (affected by the whole catchment or watershed)
morphological features such as meanders (Boano et al. 2006, Revelli et al. 2008, Gomez et al.
2012), sediment bars (Tonina and Buffington 2007, Boano et al. 2010, Marzadri et al. 2010),
pool–riffle sequences (Harvey & Bencala, 1993; Tonina and Buffington, 2009, Trauth et al.
2014), and ripples (Cardenas & Wilson 2007a, 2007b, Bottacin-Busolin & Marion, 2010, Fox
et al. 2014) all trigger groundwater–surface water interaction by significantly modifying local
pressure and shear stresses. These processes occur in the hyporheic zone, where 10% of the
groundwater is induced from the surface water (Harvey & Bencala, 1993). Groundwater–
surface water interaction influences the fate and transport of contaminants (Conant et al. 2004,
Chapman et al. 2007, Kalbus et al. 2007) and impacts the ecosystem of streams (Brunke &
Gonser 1997). The water quality of both groundwater and surface water are affected by their
biological activities and the distribution of aerobic and anaerobic conditions within
groundwater as well as the fate and transport of waterborne substances such as nutrients and
organic carbon (Jones and Holmes 1996, Mulholland et al. 1997, Storey et al. 1999, Stonedahl
et al. 2012) are also controlled by these interactions (Harvey et al. 2013, Marzadri et al. 2011,
Zarnetske et al. 2011).

Compared to field and laboratory experiments, numerical models are often less computationally
demanding and can provide information for a broader range of scenarios and future predictions.
They can also investigate parameters that are hard to measure with physical measurement
methods. The first coupling of groundwater–surface water models was presented in the 1990s
(Kollet and Maxwell 2006, Jones et al. 2008) to investigate precisely this groundwater–surface
water interaction. In a coupled model, the shared boundary between the two models (a
groundwater and a surface water model), which is the surface water–groundwater interface, is
used to transfer parameter information from one model to another. The most common coupling
technique is one-way sequential coupling with pressure as the coupling parameter (Tonina and
Buffington 2009, Trauth et al. 2015). This technique is widely used and has been validated for a variety of groundwater–surface water interaction cases, including local-scale flow and exchange across streambeds (Saenger et al. 2005, Cardenas and Wilson 2007a, Jin et al. 2010, Bardini et al. 2012, Janssen et al. 2012, Trauth et al. 2013, Trauth et al. 2014, Trauth et al. 2015, Chen et al. 2018). Saenger et al. (2005) coupled shallow water equations (for surface water) with Darcy’s law (for groundwater) to model various surface water flow rates in a riffle–pool sequence. Their results showed that higher flow rates increase hyporheic exchange and reduce residence times. Cardenas and Wilson (2007a) and Janssen et al. (2012) coupled the RANS equations (Reynolds Averaged Navier-Stokes equations, for surface water) and Darcy’s law to investigate the interaction between turbulent flow and groundwater exchange. These models are capable of offering simple flow predictions. Jin et al. (2010) coupled the RANS equations with Darcy’s law to study the transport of non-sorbing solutes in a streambed with periodic bedforms. They concluded that these transport processes in the groundwater were advection-dominant. Trauth et al. (2015) investigated the exchange processes in a pool–riffle morphology by coupling the Navier-Stokes equations with the Richards equations (Richards 1931). They stated that it was necessary to use the Navier-Stokes equations to account for turbulence in the surface water. The Navier-Stokes equations are solved using CFD (Computational Fluid Dynamics) modeling software such as OpenFOAM (Open Field Operation and Manipulation; Weller et al. 1998). Open-source software such as OpenFOAM has further facilitated the development of coupling tools such as hyporheicFoam (Li et al. 2020), which allows researchers to couple the RANS equations and Darcy’s law.

When studying local groundwater–surface water interaction, the paradigm has shifted towards investigating groundwater–surface water and their interaction as a single resource. In spite of the use of novel measurement and experimental techniques, however, coupled modeling techniques still treat groundwater and surface water as two separate domains, and neglect their continuous spatiotemporal interaction. A decade ago, Oxtoby et al. (2013) presented an alternative approach to the integral modeling of surface water and groundwater flow. The integral approach allows both surface water and groundwater to be modeled using a single set of equations. Oxtoby et al. (2013) generated the porousInter solver (described in Section 2.3.3) of OpenFOAM to manage this approach. porousInter is an extension of the widely used interFoam solver, which uses the Navier-Stokes equations to model multi-phase fluid flow processes. The porousInter extension includes porosity and grain diameter as parameters over the region that characterize a porous medium in the model. Due to the high computational
requirements of the integral approach, however, its use is limited to cases at the local scale. A
local-scale physical setup by Fox et al. (2014), who used a flume experiment to investigate flow
and tracer propagation across a homogenous rippled streambed (a similar setup to the rippled
domain of this study, which is explained below) was modeled by Broecker et al. (2021) using
this integral solver. The results showed a very good agreement between Broecker et al. (2021)’s
simulations and Fox et al. (2014)’s experiments. In local-scale investigations, the integral
approach has proven to be capable of determining high-resolution continuous flow and
exchange across the groundwater–surface water interface. Although the ability of this approach
to detect continuous interaction across the groundwater–surface water interface appears to be
superior to the coupled approach, a systematic comparison between coupled and integral
approaches is still lacking. High-resolution modeling via the integral approach utilizes precise
mapping of flow and pressure; however, this is what increases its computational requirements.
Computational burden is crucial in defining the limitation of the integral approach.

In this study, we therefore aimed to model open channel flow across a rippled porous streambed
(Figure 2-1) with integral and coupled approaches to highlight the plausibility of using the
integral approach as a step towards modeling groundwater and surface water in a single
continuum. Such a study is relevant for local-scale processes, such as hyporheic exchange. For
the coupled model (CM), we chose the widely used one-way sequential coupling of
groundwater and surface water via pressure. For the groundwater component of the coupled
model (GW-CM), we used PC SiWaPro® (based on the Richards equations; see Guo et al. 2017;
PC Sickerwasserprognose (seepage flow prognosis); see Section 2.3.2). For the surface water
component of the coupled model (SW-CM), we used the interFoam OpenFOAM solver (based
on the Navier-Stokes equations; see Section 2.3.1). Throughout many local-scale coupling
studies (e.g., Saenger et al. 2005), shallow water equations have been used as the SW-CM.
While the use of the Navier-Stokes equations to account for turbulence in the surface water has
been recommended (Trauth et al. 2015), up to this point, no comparisons between the use of
shallow water equations and the Navier-Stokes equations to determine the impacts of model
simplification on model accuracy and reliability have been made. The selection of the proper
surface water modeling equations will determine the computational requirements of the CM.
This selection of equations was a major contribution to the primary objective of this study,
which was the systematic comparison of the CM and the integral model (IM). In this study, we
compared the flow fields and the computational demands of the IM and the CM to answer the
scientific questions described below.
To demonstrate the capability of the solver for the integral model (porousInter) when modeling groundwater flow, two cases (seepage through dam) have been verified by employing a comparison to PCSiWaPro® results (used as the groundwater component of the coupled model) as well as several other numerical and analytical solutions (see the appendix).

By systematically comparing an integral model and a coupled model in the flow and exchange across a rippled streambed, we aim to answer the following questions:

- How do flow fields over the entire domain appear for both models? What consequences does this have for future modeling?
- How different are flow fields in the interface region adjacent to surface water/groundwater? What causes these differences? What consequences does this have for future modeling?
- How different are the computational requirements of the two models?
- In conclusion, which approach is preferable for future modeling of the groundwater–surface water interaction?

2.3 Materials and methods

2.3.1 Surface water modeling

In this study, we first modeled the surface water flow over of the rippled streambed (SW-CM; Figure 2-1) using the interFoam solver of the OpenFOAM software (based on the Navier-Stokes equations). We also investigated the possibility of model simplification by modeling the same domain using shallow water equations.

*Navier-Stokes equations*

We used OpenFOAM version 2.4.0, an open-source computational fluid dynamics program, to simulate free surface flow over the streambed (SW-CM) as well as to simulate the IM. To model the free surface flow, we used the interFoam solver, which is applicable for multiphase fluid flows. The two-phase (water, air) solver has been widely applied in hydraulic engineering in recent years, with the air phase mainly included to account for the movement of the free water surface (Schulze and Thorenz 2014, Higuera et al. 2014, Schmitt et al. 2015, Bayon et al. 2016). Cardenas and Wilson (2007a), Tonina and Buffington (2009), and Janssen et al. (2012) recommended a Navier-Stokes equations solver when running simulations of relatively
complex geometries such as those in this study, because flow and pressure distributions are more realistically captured compared to simpler approaches.

Eq. (2-1) depicts the indicator fraction (0 [air] < α < 1 [water]) for the interface convection equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \vec{v}) = 0$$

where $\vec{v}$ [m/s] is the flow velocity vector and $t$ [s] is time.

Conservation of mass (Eq. (2-2)) and momentum (Eq. (2-3)) are thus written as follows:

$$\nabla \vec{v} = 0$$

$$\left( \frac{\partial (\rho \vec{v})}{\partial t} + \vec{v} \nabla (\rho \vec{v}) \right) = -\nabla p + \mu \nabla^2 \vec{v} + \rho g$$

where $\rho$ [kg/m$^3$] is the density of the fluids, $p$ [Pa] is the pressure, $\mu$ [m$^2$/s] is the dynamic viscosity ($\mu = \mu_p + \mu_t$; physical + turbulent viscosity), and $g$ [m/s$^2$] is the vector acceleration of gravity.

Besides laminar flow, three types of turbulence models are included in OpenFOAM. One is RANS (Reynolds-averaged Navier-Stokes) models, which include turbulence models such as $k$-$\varepsilon$, $k$-$\omega$, and $k$-$\omega$ SST. The others are LES (Large Eddy Simulations) and DNS (Direct Numerical Simulations) models. Compared to RANS models, DNS and LES are more advanced turbulence models. Here, the LES model was applied to predict turbulence within the fluid (see OpenFOAM turbulence guide documentation).

Simulating the free surface shallow water flow using solvers based on the Navier-Stokes equations such as interFoam is computationally demanding. The Navier-Stokes equations can be simplified to shallow water equations in cases where vertical flow as well as deviations from hydrostatic pressure are not important. This simplification reduces the computational time significantly and is explained in the following section.

**Shallow water equations**

Shallow water equations are widely used for river and stream flow. Shallow water equations are derived from depth-integration of the Navier-Stokes equations. As a consequence, there is no vertical velocity and the pressure distribution in the vertical direction is hydrostatic. In
addition to the Navier-Stokes equations, we also used shallow water equations to model the SW-CM.

Conservation of mass and momentum without considering sink or source terms (e.g., precipitation or infiltration) for two-dimensional depth-averaged shallow water equations are written as follows:

\[
\frac{\partial h}{\partial t} + \nabla (\vec{v} h) = 0 \\
\frac{\partial (\vec{v} h)}{\partial t} + \nabla \left( \vec{v} \cdot \vec{v} h + \frac{1}{2} gh^2 \right) - \mu_t \nabla^2 (\vec{v} h) = -gh\nabla z_B + \frac{n^2 \rho g}{h^3} \vec{v} \cdot |\vec{v}| 
\]

where \( h [\text{m}] \) is the water depth, \( z_B [\text{m}] \) is the bottom elevation, \( \mu_t [\text{m}^2/\text{s}] \) is turbulent kinematic viscosity, and \( n [\text{s/m}^{1/3}] \) is Manning’s roughness coefficient.

To model shallow water, we used the Java-based hms (hydroinformatics modeling system; compare Simons et al. 2014) modeling framework. hms makes it possible to calculate water levels and depth-averaged velocities in consideration of Manning’s roughness coefficient.

2.3.2 Groundwater modeling

The groundwater component of the coupled model (GW-CM) was simulated using PCSiWaPro®. This software is used for unsaturated and saturated groundwater flow modeling. It was developed by IBGW Leipzig (Ingenieurbüro für Grundwasser GmbH) and Technische Universität Dresden. The properties of the sediment were defined according to DIN 4220 (2008). The DIN is the well-established German National Organization for Standardization; DIN 4220 is the German standard for the identification, classification, and derivation of soil parameters. PCSiWaPro® is based on the Richards equation (Eq. (2-5)) and uses the wetting and rewetting curves from Luckner et al. (1989) to estimate unsaturated hydraulic properties.

In the following equation the extended Darcy’s law is introduced in the mass conservation equation:

\[
\frac{\partial \theta}{\partial t} = \nabla [K(\theta)(\nabla \psi - 1)] 
\]

where \( \theta [\text{m}^3/\text{m}^3] \) is the volumetric water content, \( K(\theta) [\text{m/s}] \) is the hydraulic conductivity, and \( \psi [\text{m}] \) is the pressure head.
2.3.3 Integral model

For the IM, we chose a sub-solver of interFoam called porousInter (Oxtoby et al. 2013). To account for incompressible fluids and porous mediums, the equations for the conservation of mass (Eq. (2-2)) and momentum (Eq. (2-3)) are written as modified Navier-Stokes equations; $\bar{\text{[ ]}}^\text{f}$ indicates an averaged parameter over a void region:

\[ \phi \nabla \overline{\nabla^2} = 0 \quad \text{Eq. (2-6)} \]

\[ \phi \left( \frac{\partial \rho}{\partial t} \right)[v]^f + \nabla \rho \left[ \nabla^2[v]^f \right] = -\phi \nabla \rho \left[ \nabla^2[v]^f \right] + \phi \mu \left[ \nabla^2[v]^f \right] + \phi \rho \cdot g + D \quad \text{Eq. (2-7)} \]

where $\phi$ [-] is the effective porosity and $D$ [kg/(m²s²)] is an additional porous drag term.

\[ D = A + B \quad \text{Eq. (2-8)} \]

\[ A = -\left( 150 \frac{(1-\varphi)}{d_p \varphi} \left( 1.75 [\rho]^f \left[ \nabla^2[v]^f \right] \right) \frac{(1-\varphi)}{d_p} [v]^f \right) \quad \text{Eq. (2-9)} \]

\[ B = -0.34 \frac{(1-\varphi)}{\varphi} \frac{\partial [\rho]^f [v]^f}{\partial t} \quad \text{Eq. (2-10)} \]

where $d_p$ [m] is the effective grain size diameter.

The term “A” in Eq. (2-9) describes the pressure loss of the fluid with porous medium due to friction in line with Ergun (1952). In porous medium, compared to free flow, more momentum is needed to accelerate a given volume of water, which is referred to as “added mass”; this is accounted for through “B” (van Gent 1995). In areas where only free flow exists, effective porosity is set to 1, which results in $A = B = D = 0$ and allows the use of the original Navier-Stokes equations for free water flow (Eq. (2-2) and Eq. (2-3)). Similarly, for the SW-CM, for the IM, the LES turbulence model was used.

2.3.4 Comparable hydrogeological conditions assessment

The sediment parameters $\phi$ and $d_p$ are required in porousInter when modeling a flow in a porous medium. PCSiWaPro® follows the DIN 4220 standard, which classifies sediment according to sediment type, $\theta_s$ [m³/m³] (saturated volumetric water content), $\theta_r$ [m³/m³] (the residual volumetric water content), and $K_0$ [m/s] (matching hydraulic conductivity at saturation). For consistency with natural streambed sediment (as discussed in the experiment conducted by Fox et al. (2014)), the sediment type derived from DIN 4220 (for the GW-CM) was “pure sand” with a saturated volumetric water content ($\theta_s$ or $\varphi$) equal to the porosity chosen in porousInter.
When the system is fully saturated, residual volumetric water content is not relevant. For porousInter, a particle size ($d_p$) of 2 mm and a porosity ($\phi$) of 0.25 was chosen. The saturated hydraulic conductivity ($K_0$) used in PCSiWaPro® was derived from Eq. (2-11) (following Hazen) using the same particle size chosen for porousInter:

$$K_0 = 0.00116 \, d_{10}^2$$  \hspace{1cm} \text{Eq. (2-11)}$$

where $d_{10}$ is a 10% fall-through of the sieve curve [mm].

Since porousInter is limited to a single uniform particle size, $d_{10} = 2$ mm and, with Eq. (2-11), $K_0 = 4.64 \times 10^{-3} \, \text{m/s}$ was used in this study.

### 2.3.5 Computational domain

Figure 2-1: Model setup and boundary conditions of a) the shallow water equations surface water model; b) the coupled model (CM), including the surface water component of the coupled model (SW-CM, b, top) and the groundwater component of the coupled model (GW-CM, b, bottom); c) the integral model (IM); and d) the ripple geometry.

In Figure 2-1, light blue indicates the air phase, dark blue the water phase, and light brown the sediment, including respective boundary conditions. Figure 2-1a shows the model setup of the surface water flow using hms (shallow water equations model) for single-phase flow over a
ripped streambed. We used this model to investigate if model simplification was applicable to the SW-CM (see Figure 2-1b, top). The CM is shown in Figure 2-1b, where the top depicts the SW-CM (to be modeled using interFoam; Navier-Stokes equations model) and the bottom highlights the GW-CM (to be modeled using PCSiWaPro®). Regarding the surface water and air phase, the IM shown in Figure 2-1c is identical to that of Figure 2-1b, top, and longer than the domain of the GW-CM in its sediment part. Modeling the GW-CM with a groundwater domain of the same length as the one from the IM is not necessary for our purposes. In our study, groundwater flow is only generated due to the presence of the ripple morphology (induced by surface water, which only flows in an x direction). Flow in the flat streambed of the GW-CM (“far” away from the ripples) is therefore negligible. Setting the model boundaries 2 m from both sides of the rippled area is sufficient to ensure full formation of the flow pathways on the studied area of 3 m length with 15 ripples, as shown in Figures 2-1c and 2-1d.

Model setups of the SW-CM and the IM were created in three dimensions and had a 1m width along the y axis, 15 m along the x axis, and a maximum of 1.5 m along the z axis. To be able to model turbulence using LES, we set up a 3D domain with a 1 m width on the y axis. Another reason we chose LES was its ability to better capture the formation of small eddies between the ripples in comparison with simpler and faster turbulence models such as k-ω and k-ε. A Smagorinsky sub-grid scale model with a van Driest dumping function was used to reduce the eddy viscosity in the near-wall region. This facilitates the reproduction of the characteristics of direct numerical simulations, which solve the three-dimensional Navier-Stokes equations for all eddies directly, at the near-wall region.

Coupling parameters were transferred to the GW-CM from results of pressure distribution at a y = 0.5 m cross section above the ripples of the SW-CM.

2.3.6 Meshes, initial and boundary conditions and parameters

This study utilizes unstructured meshes, which were generated using the GMSH three-dimensional finite element mesh generator (for the IM and the SW-CM). The SW-CM (Figure 2-1b, top) is meshed identically to the surface water part of the IM. The GW-CM was generated using the meshing tool in PCSiWaPro® using mesh resolutions. Cells along the interface of the surface water and pore water domain coincide for easy transfer of results. The shallow water model (Figure 2-1a) is 2D in the x-y plane. With no flow in the y direction, it is practically a 1D illustration of flow in the x direction, consisting of 15,000 cells (cell size = model resolution
The IM and the SW-CM consist of more than 430,000 and 116,000 prismatic cells, respectively. The minimum cell size (model resolution; shortest edge size) was $5 \times 10^{-3}$ m near ripples compared to a maximum size (longest edge size) of $3.5 \times 10^{-1}$ m in the air phase far above the water–air interface for both the SW-CM and the IM. The GW-CM has 15,000 cells (model resolution $5 \times 10^{-3}$ m). Model convergence was achieved using these resolutions.

Water flow with a value of 0.5 m$^3$/s was set as the boundary condition at the inlet on the left side in Figure 2-1 along the x axis for all three models. The top pressure boundary of the GW-CM (yellow line) was defined by taking the pressure distribution from the results of the steady-state run of the SW-CM; left and right boundaries (blue lines) were defined as the linear hydrostatic pressure increase according to depth. Black lines indicate no-flow boundaries with normal velocity being zero, while green lines indicate atmospheric pressure.

No sediment transport was assumed for any cases. We ran both the SW-CM and the IM with steady boundary conditions until a quasi-steady state was achieved. A full steady state would be reached when parameters such as flow velocity and pressure were constant over time. Under turbulent flow conditions, however, such a state can never be fully satisfied. For this reason, we derived initial flow and turbulence conditions after some precomputational time, as soon as the oscillations of the results were relatively small. In this study, we defined quasi-steady state conditions as the point when turbulent eddies between ripples became fully formed (although still moving) and no inconsistent changes (any irregular and unexpected jump in a variable’s value) in pressure fields, flow fields, or eddy sizes/shapes occurred. After 60 s of precomputation, these quasi-steady states for the IM and the SW-CM were reached. However, we calculated variable values as averages between 60s and 300s to account for oscillations within the adjusted range. The shallow water model achieved a full steady state after 300 s. The GW-CM was also modeled starting from a full steady state.

The IM, the SW-CM, and the shallow water model are designed to maintain a ~0.5 m water table above the streambed. We defined a 0.5 m water table above the streambed initially for all models so that it was possible to reach this condition faster. We placed a weir in all models to maintain this waterhead. The streambed was initially saturated for the GW-CM and the IM, and all the initial velocities were zero. To account for friction in the shallow water model, we set the Manning coefficient to 0.03 s/m$^{1/3}$, which is the coefficient recommended for clean and straight natural streams.
In the next section, we present the simulation results of the IM and the CM by analyzing the flow velocities in the water above and the sediment underneath the investigated 8th ripple, shown in Figure 2-1. Next, we dedicate additional attention to flow fields adjacent to the interface. These were investigated by mapping the hydrodynamic pressures and the flow fields across the interface. The next step was to consider the effects of simplifying the models by replacing the SW-CM with a shallow water model.

2.4 Results

2.4.1 IM and CM flow velocity fields in the model domain

To investigate the flow velocities in the model domain, we chose a representative slice (8th ripple in Figure 2-1; 735 cm < x < 760 cm, -50 cm < z < 50 cm in Figure 2-2) consisting of the water and the sediment parts. The air part was only simulated for precisely capturing the surface water level fluctuations; as this is not relevant here, we excluded it from the representative slice.

Figure 2-2: Graphic visualization of the ripples at the sediment–water interface and the horizontal (blue dotted lines) and the vertical (green dotted lines) cross sections used to compare flow results of the integral model (IM) and the coupled model (CM).

To compare the results, we exhibited the simulated flow velocities across several vertical and horizontal cross sections. Vertical cross sections intersect with the luv (x = 748 cm) and the lee (x = 758 cm) sides of the 8th ripple and extend through the sediment and the water parts (Figure 2-2). We placed the horizontal cross sections in the water (z = 40 cm), the sediment (z = -40 cm), and the surface water (z = 50 cm).
cm), and the interface-adjacent sediment \((z = -2 \text{ cm})\). These cross sections are slightly shifted to the left (to cover the area from the 7th ripple crest to the 8th ripple crest).

Figure 2-3: A comparison of flow velocities \(v_x\) and \(v_z\) in the x (a, c) and z (b, d) directions for vertical cross sections at \(x = 748 \text{ cm}\) (a, b) and \(x = 758 \text{ cm}\) (c, d) for the integral model (IM) and the coupled model (CM); absolute values of subtracting flow velocities have been calculated using the CM and the IM (\(|v_{CM} - v_{IM}|\)) in the x (e) and z (f) directions for both vertical cross sections.
2. Comparison of integral approach to coupled approach for flow across rippled streambed

Figure 2-3 illustrates the flow velocities of both models ($v_{CM}$ and $v_{IM}$) through vertical cross sections at $x = 748$ cm (Figures 2-3a and 2-3b) and $x = 758$ cm (Figures 2-3c and 2-3d). These are shown separately for the velocities in the x direction ($v_x$; Figures 2-3a and 2-3c) and the z direction ($v_z$; Figures 2-3b and 2-3d). CM velocities were subtracted from IM velocities for each vertical cross section and in both directions. The absolute values of these subtractions are displayed in Figures 2-3e and 2-3f. Major differences between the flow velocities of the two models in both directions ($x$ and $z$) were detected in the area close to the interface (around $z = 0$ cm). A few decimeters away from the interface (both in groundwater and surface water), however, these differences fade and reach values close to zero.

![Figure 2-3](image1)

![Figure 2-4](image2)

Figure 2-4: A comparison of flow velocities $v_x$ and $v_z$ in the x (a) and z (b) directions for the horizontal cross section at $z = -2$ cm along $735 \text{ cm} < x < 755 \text{ cm}$ for the integral model (IM) and the coupled model (CM); absolute values of subtracting flow velocities have been calculated using the CM and the IM ($|v_{CM} - v_{IM}|$) in the x (c) and z (d) directions.
To further substantiate the fact that unlike areas near the interface, differences between the flow velocities farther from the interface are negligible in the two models, we present the flow velocities across horizontal cross sections near the interface \((z = -2 \text{ cm}), \text{ Figure 2-4}\) and away from it \((z = -40 \text{ cm}, \text{ Figure 2-5}; z = 40 \text{ cm}, \text{ Figure 2-6}).

Figure 2-5: A comparison of flow velocities \(v_x\) and \(v_z\) in x (a) and z (b) directions for the horizontal cross section at \(z = -40 \text{ cm}\) along \(735 \text{ cm} < x < 755 \text{ cm}\) for the integral model (IM) and the coupled model (CM); absolute values of subtracting flow velocities have been calculated using the CM and the IM \((|v_{CM} - v_{IM}|)\) in the x (c) and z (d) directions.

Figures 2-4, 2-5, and 2-6 show the absolute value of the differences between the simulated velocities of the CM and the IM in both directions (x and z) as well. Looking at Figure 2-4 \((z = -2 \text{ cm})\), flow velocity differences between the two models reach as high as \(2 \times 10^{-3} \text{ m/s}\). For deeper groundwater \((\text{Figure 2-5}, z = -40 \text{ cm})\), these differences are almost zero in the z direction \((v_z)\) and peak at \(2.5 \times 10^{-5}\) in the x direction \((v_x)\).
2. Comparison of integral approach to coupled approach for flow across rippled streambed

Figure 2-6: A comparison of flow velocities $v_x$ and $v_z$ in the x (a) and z (b) directions for the horizontal cross section at $z = 40$ cm along $735 \text{ cm} < x < 755 \text{ cm}$ for the integral model (IM) and the coupled model (CM); absolute values of subtracting flow velocities have been calculated using the CM and the IM ($|v_{CM} - v_{IM}|$) in the x (c) and z (d) directions.

As displayed in Figure 2-6, maximum flow velocity differences between the IM and the CM (for both $v_x$ and $v_z$) for surface water at $z = 40$ cm are $7 \times 10^{-3}$ m/s. In general, flow velocities in the surface water are higher than in the groundwater. In addition, for the current case, flow in the groundwater is only induced by the surface water flow across a rippled streambed. This causes higher groundwater velocities near the interface compared to the deeper groundwater. A direct comparison of the maximum flow velocity differences between the IM and the CM over the cross sections at $z = -2$ cm, -40 cm and 40 cm would therefore be inaccurate and misleading. Instead, we divided the averaged (over the horizontal cross section) flow velocity differences ($|v_{CM} - v_{IM}|$, Table 2-1) by the averaged flow velocities of the IM and the CM ($|v_{CM}|$ and

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Comparison of integral approach to coupled approach for flow across rippled streambed

\[ |\vec{v}_{IM}| \text{, Table 2-1}. \] The results \((D_{CM}, D_{IM})\) are shown for all the horizontal cross sections and in both flow directions \((v_x \text{ and } v_z)\) in Table 2-1.

Table 2-1: \(|\vec{v}_{CM} - \vec{v}_{IM}|\), \(|\vec{v}_{IM}|\) and \(|\vec{v}_{CM}|\) velocities and \(|\vec{v}_{CM} - \vec{v}_{IM}|\) velocities over \(|\vec{v}_{IM}|\) and \(|\vec{v}_{CM}|\) velocities for \(z = -2\) cm, -40 cm and 40 cm in the \(x\) and \(z\) directions.

<table>
<thead>
<tr>
<th>(z)</th>
<th>(v_x) (m/s)</th>
<th>(v_z) (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(-2) cm</td>
<td>(4.9 \times 10^{-4})</td>
<td>(1.95 \times 10^{-5})</td>
</tr>
<tr>
<td>(-40) cm</td>
<td>(5.75 \times 10^{-5})</td>
<td>(6.02 \times 10^{-5})</td>
</tr>
<tr>
<td>(40) cm</td>
<td>(2.56 \times 10^{-5})</td>
<td>(7.97 \times 10^{-5})</td>
</tr>
</tbody>
</table>

\[ D_{CM} = \frac{|\vec{v}_{CM} - \vec{v}_{IM}|}{|\vec{v}_{CM}|} \text{ (\(-\))} \]
\[ D_{IM} = \frac{|\vec{v}_{CM} - \vec{v}_{IM}|}{|\vec{v}_{IM}|} \text{ (\(-\))} \]

\(D_{CM}\) and \(D_{IM}\) ratios demonstrate the flow velocity differences between the two models considering their deviation from the expected flow velocity simulated by each model (CM and IM). For both \(v_x\) and \(v_z\), across \(z = -2\) cm, these ratios were one to three orders of magnitude greater than those of the \(z = -40\) cm and \(z = 40\) cm cross sections. This means that CM/IM model discrepancy is higher near the interface at the \(z = -2\) cm cross section compared to other horizontal cross sections. \(D_{CM}\) and \(D_{IM}\) values at \(z = 40\) cm and \(z = -40\) cm are relatively smaller, which means that both models function more similarly a few decimeters away from the groundwater–surface water interface.

We therefore determined that major flow-velocity discrepancies exist between the two models (CM and IM) near the interface. We will further discuss the meaning of these differences in the discussion about flows across interface-adjacent surface water.
2.4.2 IM and CM pressure and velocity fields in the interface-adjacent zone

By maintaining a 0.5 m water level over the sediment in the whole domain throughout the entire simulation period, the hydrostatic pressures of both models remain equal. The surface water flow was also defined identically for the surface water component of the coupled model (SW-CM) and the surface water part of the integral model. The simulated hydrodynamic pressures (p_rgh, Figure 2-7) of the two models on the 8th ripple (see Figure 2-1 above), however, differ from each other on the ripple surface. These differences are displayed in Figure 2-7b.

Figure 2-7: a) Hydrodynamic pressure values at the surface water–groundwater interface on the investigated ripple (representative cross section, 8th ripple) for the IM and the CM; b) subtraction of the hydrodynamic pressures of the CM from that of the IM on the investigated ripple.

Another indicator of the differences between the two models near the interface is shown in Figure 2-8. Higher flow velocities and bigger turbulent eddies can be seen within the troughs between the ripples of the CM (Figure 2-8b) compared to those of the IM (Figure 2-8a). In Figure 2-8a, flow vectors are formed along and through the interface. These paths of flow display a continuous exchange between the surface water and the groundwater, and they show how surface water is transported through the sediment matrix from one side of the ripple to the other. Further information about the groundwater can be gained by looking at the groundwater component separately (Figure 2-9).
2. Comparison of integral approach to coupled approach for flow across rippled streambed

Figure 2-8: Flow velocities and directions over and through the investigated ripple (8th ripple, Figure 1) for a) the integral model and b) the coupled model. Note: red dashed line indicates the sediment–water interface; black arrows only indicate directions, and are not scaled regarding magnitude. Magnitude is shown as a color scale.

Figure 2-9: Velocity and Reynolds number (in log10 scale) distributions through the investigated ripple (8th ripple, Figure 2-1) for a) the integral model (IM) and b) the coupled model (CM). The patterns and hotspots of the flow differ when comparing the interface-adjacent flow in the groundwater (Figure 2-9). We also realized that a zone on the crest of the ripple in the IM (the
area highlighted green in Figure 2-9) has a velocity of $0.02 \text{ m/s} < v_{IM} < 0.2 \text{ m/s}$, which for this case is outside of the area where Darcy’s law would apply (Reynolds number (-) > 10).

The results emphasize that near the groundwater–surface water interface, the IM and the CM behave very differently. The fundamentals of these differences and their significance in selecting a plausible small-scale groundwater–surface water modeling approach is further discussed in Section 2.5.

2.4.3 Shallow water simplification

Figure 2-10: A comparison of the horizontal surface water flow ($v_x$) for vertical cross sections at a) $x = 748 \text{ cm}$ and b) $x = 758 \text{ cm}$ for the surface water component of the coupled model (SW-CM) and the shallow water equations in the surface water model (SW-SM).

Here we examine the plausibility of using a simpler set of equations to model the SW-CM, which could drastically decrease the computational requirements. For this purpose, we have chosen the hms solver, which solves shallow water equations. Using shallow water equations, $v_z$ is zero and $v_x$ values along a vertical cross section are constant. Nevertheless, we generated two parabolic velocity profiles (according to Bartam and Balance 1996) for vertical cross sections at $x = 748 \text{ cm}$ and $x = 758 \text{ cm}$ based on the average velocities of the shallow water equations model ($\bar{v}_x^{748\text{ cm}} = 0.803 \frac{\text{m}}{\text{s}}$, $\bar{v}_x^{758\text{ cm}} = 0.807 \frac{\text{m}}{\text{s}}$). As shown in Figure 2-10, generated $v_x$ flow profiles of the shallow water equations model ($v_{SW-SM}$) are very different compared to the SW-CM (which uses the Navier-Stokes equations). Furthermore, the $v_z = 0$ assumption in shallow water equations contradicts the $v_z$ profiles across the vertical cross sections displayed in Figure 2-3. In shallow water equations, pressure is assumed to be
hydrostatic, which conflicts with the hydrodynamic pressure results displayed in Figure 2-7 for
the SW-CM. Following the discussions of the IM and the CM flow and exchange in the next
section, we discuss the reduction of computational requirements by model simplification using
the shallow water equations model.

2.4.4 Required computational resources

Modeling the SW-CM via hms requires only 30 minutes of runtime on a PC (8 core 3.4 Ghz
AMD processors). However, to simulate the SW-CM based on the Navier-Stokes equations,
access to a computer cluster is required. Using 40 processors at the high-performance
computing cluster of Technische Universität Berlin, it takes about 24 hours for the SW-CM to
complete the simulation. Using the same resources, it takes about 70 hours for the IM to run
completely. For the GW-CM, about one hour of computing with the aforementioned PC is
sufficient.

2.5 Discussion

In the introduction, we described the coupled model studies that are most relevant to the domain
of our study (flow across a morphologically modified streambed). In these studies, groundwater
was modeled with Darcy’s law (or the Richards equations – i.e., relatively saturated Darcy’s
law equations). The surface water component of the coupled model was either simulated with
the Navier-Stokes equations or shallow water equations. By modeling the GW-CM with
Darcy’s law (Richards equations in saturated sediment are equivalent to Darcy’s law) and the
SW-CM with both the Navier-Stokes equations and shallow water equations, our coupled
model is representative of the development of previous models. Here, we discuss this
representative coupled model alongside the recently developed integral modeling approach. For
the discussion, we divide the comparison of the flow fields of the IM and the CM into two parts:

- The area a few decimeters away from the interface.
- The area near the interface.

We use the Navier-Stokes-based SW-CM for our initial discussions. In the next step, we discuss
simplifying the SW-CM approach by using shallow water equations. Then, we compare the
computational requirements of the CM to the IM.
2. Comparison of integral approach to coupled approach for flow across rippled streambed

2.5.1 Flow comparison a few decimeters away from the interface

Darcy’s law, and the Richards equation based on it (as used for the GW-CM via PCSiWaPro®), is the standard mathematical approach to determining flows in a porous medium. The IM investigated here, however, takes a different approach to determining flow in this zone. The appendix contains results showing the successful verification of the integral solver against several analytical and numerical solutions (including PCSiWaPro®) for two cases simulating seepage through a dam. Incidentally, this solver has also been validated for the case of flow triggered by bioturbation in benthic zones in comparison to a model based on Darcy’s law (Sobhi Gollo et al. 2021). Nevertheless, for flow across a morphologically modified (rippled) streambed, the current study is a further step in validating the integral approach. In Figure 2-3, we can see that when starting from the interface ($z \sim 0$), flow velocities of the models in both flow directions ($v_x$ and $v_z$) converge as depth increases. It also shows that flow velocities correspond in deep groundwater ($z = -40$ cm).

For the surface water part of the domain, both models use the same set of flow simulation equations (Navier-Stokes equations) and the meshes are identical. However, the models’ dissimilarities starting from the interface are propagated upwards. By around $z = 40$ cm, flow velocity results indicate that both models behave similarly.

Both models behave similarly a few decimeters from the groundwater–surface water interface. This shows that the mathematical solver of the IM is capable of plausibly simulating the flow processes, especially in the groundwater, where its equations are distinct from Darcy’s law. Nevertheless, the notable source of the difference between the two models – the interface-adjacent zone – requires further discussion.

2.5.2 Flow comparison near the interface

Here, we separately discuss the groundwater and surface water flow near the groundwater–surface water interface.

Interface-adjacent surface water

Looking at Figure 2-8, it is clear that velocity vectors meet the interface (body of the ripple on the luv side) at different angles. In the IM, velocity vectors are bent upon the incident, and depending on the impact angle, they either enter the groundwater or are deflected back into the surface water. The velocity of the water that enters the sediment is dampened. The deflected
flow vector (if deflected towards the foot of the lee side) creates a turbulent eddy in the trough between the ripples. In the CM, there is no path through the sediment as the interface is a no-flow boundary. As a result, the only option of the surface water flow vectors that meet the interface is to be deflected back into the surface water. Here, all the flow vectors that will be deflected and trapped in the trough between the ripples join together and create larger eddies compared to the ones in the IM. Accumulation of these larger eddies in the CM result in higher flow velocities in the interface-adjacent surface water compared to the IM. The CM (SW-CM) velocity distributions in the interface-adjacent area define the hydrodynamic pressures on the interface. In Figure 2-7, the hydrodynamic pressure of the CM is therefore greater than that of the IM.

Fox et al. (2014) and (2016) physically modeled a very similar flow across a rippled streambed setup. In these experiments, no sudden jump of flow as simulated by the SW-CM could be detected. Roche et al. (2018) studied wave propagation from the surface water into the groundwater. The absence of high-velocity zones near the interface was also confirmed by the integral model of this study.

Our results show that the assumption of a no-flow boundary at the interface leads to an overestimation of the flow at the interface adjacent to the surface water. In turn, by allowing the surface water to continuously interact with the groundwater, the IM yields more plausible results of the flow processes near the groundwater–surface water interface.

Interface-adjacent groundwater

Pressure (hydrostatic and hydrodynamic pressure) as the coupling parameter for the GW-CM was acquired from the above-mentioned SW-CM velocity distribution across the interface. The interface in the IM is included in the model domain, and therefore pressure values are constantly readjusted in light of the flow. The velocity distribution of the models across the ripple in Figure 2-9 is therefore different. The formation of one large eddy in the trough between ripples (see Figure 2-8) causes maximum hydrodynamic pressure on the foot of the ripple, where the maximum groundwater flow velocity of the GW-CM is detectable. In contrast to this, allowing continuous flow movement from the surface water into the groundwater via the IM results in an accumulation of flow hotspots in various areas across the body of the ripple. In addition, flow velocities outside of the boundaries of Darcy’s law can be seen in the IM. Due to the relatively small grain size considered in this study, these flows are limited to the top sediment (distance from the interface < 1 cm). However, for larger grain diameters, many studies (e.g.,
2. Comparison of integral approach to coupled approach for flow across rippled streambed

Blois et al. 2014, Roche et al. 2018) have shown that in a groundwater–surface water continuum, surface water turbulence can be transported into the groundwater and create areas of water velocities approaching those of surface water. Such phenomena cannot be simulated via a groundwater model based on Darcy’s law (such as the GW-CM). Distinctive numerical solvers and discretization methods of the groundwater component of the CM and the IM could potentially impact the results. However, we think that this impact is negligible in this study, as we have checked the grid convergence for both models.

Our findings demonstrate that in the area near the surface water–groundwater interface, the IM yields more plausible results compared to the CM. In the area near the interface, where the flow fields of the two models are distinctive, the advantages of the IM are particularly stark compared to the CM. Due to the similarity of the models further from this zone, however, the computational requirements should also be discussed when choosing the appropriate model.

2.5.3 SW-CM simplification using a shallow water model

When modeling the surface water using the shallow water equations model (hms), flow in the vertical direction \( v_z \) is assumed to be zero. Nevertheless, we have shown that in the presence of actual streambed morphology, multidirectional flow (by accumulation of eddies in the troughs between ripples) is generated. In addition to generating velocity in the vertical direction \( v_z \), eddies modify horizontal velocities \( v_x \) and pressure fields. A model simplification via the shallow water equations for the SW-CM is inappropriate for the following reasons:

- Exclusion of the vertical velocities;
- Oversimplification of the horizontal velocities (see Figure 2-10);
- Assumption of hydrostatic pressure.

It was essential to use a model based on the Navier-Stokes equations to model the SW-CM of this study. This corroborates the statement by Trauth et al. (2015), who claimed that due to the presence of turbulent eddies across morphologically modified streambeds, shallow water equations could not be used to model surface water flow.

2.5.4 Computational-demand comparison

Both the CM and the IM require access to computer clusters. Although the runtimes of the IM and the SW-CM differed by around 46 hours in our case, we state that the necessity to employ significant computational capacity, which is a key parameter in CFD modeling, is the same for both models.
When comparing the GW-CM to the groundwater part of the IM, it should be noted that very large domains will increase the computational requirements of the IM substantially. We have demonstrated how both models function similarly for flows far from the interface. Therefore, where the effect of the interface is negligible, a Darcy’s law groundwater model, which is computationally much less demanding than the IM, is sufficient.

2.6 Conclusions

Groundwater–surface water modeling approaches should be adjusted to reflect the current paradigm shift that conceptualizes groundwater and surface water as a single resource. Specifically, unlike current modeling approaches, the surface water–groundwater interface, which is the hotspot of biogeochemical interaction, should be accurately represented in the simulated domain. To pursue this, in our study we exhibited the plausibility of using a single set of equations (modified Navier-Stokes equations) governing small-scale flow processes in both groundwater and surface water. We achieved this by comparing our “integral approach” to the well-established approach of one-way sequential coupling via pressure in the case of flow across a rippled streambed. As a result of the integral model’s ability to reflect the continuous interaction between groundwater and surface water, it proved to represent flows close to the water–sediment interface more plausibly than the coupled model could.

Our study advocates for the use of the integral model for questions requiring a very exact simulation of local (small)-scale processes in the interface domain within a few decimeters of the interface into the surface water and the groundwater. The model domain of this study presented such an interface domain, where surface water–groundwater interaction was induced by ripples; this is one of the main drivers of hyporheic zone processes (Lewandowski et al. 2020). Furthermore, we determined that high-resolution modeling of “deep” (more than a few decimeters) groundwater is computationally too demanding when using the integral approach, and a standard groundwater model would be sufficient for these cases.

The integral approach can be applied to a wide range of scenarios, such as transient flow conditions, non-Darcy flows in porous media, and combined free and porous media flow around breakwaters and dikes.
2.7 Appendix

**porousInter verification for seepage flow**

We chose the seepage of water through a simplified rectangular dam and a dike as test cases; the results of the integral solver (porousInter), PCSiWaPro®, analytical solutions (Kobus and Keim 2001 (1D), Di Nucci 2015 (2D), Casagrande 1937 [extended Kozeny] (2D), Lattermann 2010 [Kozeny] (2D)), and other numerical solutions (Aitchison and Coulson 1972, Westbrook 1985) are compared in Figure 2-11. A particle size ($d_p$) of 2 mm ($K_0 = 4.64 \times 10^{-3}$ m/s) and porosity of 0.25 were used. The results in Figure 2-11 demonstrate very good agreement between most analytical solutions and model results, including PCSiWaPro® and the integral solver (porousInter). Only the 1D analytical solution deviates from the rest, since 1D tended to oversimplify the solution here.

![Figure 2-11: Model geometry and results of different models and analytical solutions for seepage through a rectangular dam (left) and a dike (right).](image)
3. Flow simulations in and around a ventilated U-shaped chironomid dwelled burrow using integral approach

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Flow simulations using porousInter are listed in Appendix B7 and B8 for the test cases 1 and 2 respectively.

3.1 Abstract

Tube dwelling of chironomids often dominate benthic communities in freshwater ecosystems with high population density and pumping rates which strongly enhance exchange across the sediment-water interface and impact biogeochemical processes. Such processes are investigated by tracking the flow initiated by chironomid’s pumping through and around burrows using laboratory and computer models. We used modeling and experimental results of other authors considering U-shaped burrows embedded in the sediment to improve process understanding and prove the plausibility of an integral modeling approach. In contrast to coupled models of pipe (burrow), free surface (overlying water column) and groundwater flow (surrounding sediment), we present a novel high-resolution integral formulation for the porous medium-free water domain (called porousInter as part of OpenFOAM (Open Field Operation and Manipulation)) solving extended versions of the Navier-Stokes equations which allows us
to simultaneously simulate flow in the burrow, the overlying water column and the surrounding sediment to better account for feedback effects between the sediment and free water. Using similar model setup as of a coupled approach, we performed scenarios of flow through burrow and sediment triggered by pumping in the center of the burrow. Plausible agreement of our integral model with results of a coupled model and with experimental results was obtained when comparing flow patterns around the burrows, between two burrow branches and at burrow inlet and outlet.

3.2 Introduction

Charles Darwin realized the relevance of biological reworking of soils and sediments (Darwin 1881, Meysman et al. 2006). Nowadays bioturbation is defined as “all transport processes carried out by animals that directly or indirectly affect sediment matrices. These processes include both particle reworking and burrow ventilation” (Kristensen et al. 2012). Bioturbators are considered ecosystem engineers (Meysman et al. 2006, Kristensen et al. 2012). Some bioturbators live in marine and freshwater sediment where they build open-ended or blind-ended burrows and actively pump overlying water through their burrows (ventilation) to supply themselves with oxygen and/or food. Burrow ventilation causes advective and diffusive exchange of solutes between overlying water, water in the burrows and sediment pore water called bioirrigation (Kristensen et al. 2012).

The pumping activities (ventilation) of macroinvertebrates such as *Chironomus plumosus* have severe impacts on hydrodynamic and biogeochemical processes in lake sediments as well as on exchange processes between pore water and the overlying water body (Hupfer et al. 2019; Hoelker et al. 2015, Brand et al. 2013, Roskosch et al. 2010 and 2011 and 2012, Morad et al. 2010, Lewandowski et al. 2007). Applying the 2D pore water sampler introduced by Lewandowski et al. (2002), Lewandowski et al. (2005a, 2005b, 2005c) used laboratory and field studies that systematically investigated the influence of macrozoobenthos (including *C. plumosus*) on the spatial distribution of pore water phosphorus concentrations. The results of the laboratory experiments showed that there is a change in retention of phosphorus (Lewandowski et al. 2005a, 2005b), ammonium and ferrous iron (Laskov et al. 2007, Lewandowski et al. 2007) in the sediment in the presence of macrozoobenthos. Field experiments supported the hypothesis that macrozoobenthos causes small-scale horizontal pore-water heterogeneity and regulates phosphorus exchange (Lewandowski et al. 2005c). In fact, for chironomid-dwelled burrows, there is a positive diffusive iron (II) and ammonium flux
3. Flow simulations in and around a ventilated U-shaped chironomid dwelled burrow using integral approach

from the pore water to the burrows and a reduced phosphorus release across the sediment-water interface (Lewandowski et al. 2007).

*Chironomus plumosus* larvae are known to build single U-tubes down to a sediment depth of 10 to 20 cm (Hölker et al. 2015). Roskosch et al. (2010) reported that *C. plumosus* can be found in amounts up to 10,000 individuals 1/m² in lake sediments. In Lake Müggelsee (Berlin, Germany) Roskosch et al. (2011) measured a density of 745 4th instar larvae 1/m² and reported a population pumping rate of 1.09 to 1.45 m³ m⁻² d⁻¹ depending on the assumed burrow diameter (1.6 or 2.0 mm). This value shows the impressive impact of chironomids on hydrodynamics and solute exchange in lake sediments which impacts the above-mentioned biogeochemical processes (Roskosch et al. 2010).

Although to date, there have not been any in situ flow measurements inside burrows dwelled by *Chironomus plumosus* larvae due to technical difficulties associated with the measurement in fragile, 1.6 mm diameter burrows in soft, muddy sediment (Morad et al. 2010), there are several measurements from mesocosm laboratory experiments of Roskosch et al. (2010) and Morad et al. (2010) as well as modeling approaches (e.g. Brand et al. 2013). Brand et al. (2013) used during larval pumping activity a flow velocity of 0.009 m/s in chironomid burrows in their coupled approach to model the hydrodynamic exchanges between sediment and burrow. That value is rather small compared to Morad et al. (2010) who measured a mean flow velocity of 0.0137 to 0.0154 m/s during pumping periods, Roskosch et al. (2010) determined 0.0150 m/s and Roskosch et al. (2011) reported 0.0149 m/s. There is an alternation of pumping and resting phases every few minutes. The flow velocity of pumping and resting phases can be averaged using 33 min pumping time per hour which was determined by Roskosch et al. (2011) resulting in an average flow velocity of 0.0082 m/s. They also realized that pressures initiated by water fluxes depend on burrow shape, sediment properties and ventilation activities of the macrozoobenthos. Brand et al. (2013) used an average (pumping + resting phases) flow velocity of 0.04 m/s.

Modeling of pumping activities of macrozoobenthos in U-shaped burrows started with the assumption of radially symmetric tubes. Aller (1980) set up a marine tube irrigation model assuming that the water in the burrow has the same composition as the overlying water and that a diffusive transfer mechanism transports solutes in the surrounding sediment (bioirrigation). (Chemical) mass transfer, pore water transfer, impacts of sediment type and depth of the burrow
have been discussed in later modeling studies (e.g. Furukawa et al. 2001, Koretsky et al. 2002, Meysman et al. 2006, Meile et al. 2005, Stief et al. 2010a).

Brand et al. (2013) presented a 3D coupled model (free fluid flow in burrow and porous medium flow in sediment) of the pumping activity of a *Chironomus plumosus* larvae around a U-shaped burrow. They simulated the hydrodynamics of the flow in the porous medium and applied it to the transport of an inert tracer as well as of oxygen using different sediment permeabilities. The model of Brand et al. (2013) gave insights into flow fields and flow directions as well as pressure distributions in the sediment around the burrow which could hardly be assessed using laboratory experiments. However, we think that this model like many other coupling schemes, lacks crucial aspects. In Brand et al. (2013) the overlying water above the sediment had not been considered. Their approach can be considered as one-way coupling without feedback. This limitation is due to the inability of the coupled approach to simultaneously model flow in the sediment as well as in the burrow and in the overlying water.

In this contribution we present an alternative to coupled models, an integral model for the investigation of a U-shaped burrow under the influence of pumping activities. This approach includes the groundwater-surface water interface as a crucial exchange zone directly in the model concept. It was initially developed by Oxtoby et al. (2013) who extended the InterFoam solver of OpenFOAM, which is an Open-Source solver for the Navier-Stokes equations, by a porosity and a special resistance term in the porous domain (Broecker et al. 2019). This extension called porousInter is an alternative to prevalent coupled approaches such as the one from Brand et al. (2013). PorousInter has never been applied to small scale pore water-surface water exchange processes such as invertebrate-dwelled burrows in lake sediments where there is the interaction of free flow in the burrow with the surrounding sediment and the overlying water column. Two separate models for sediment (using groundwater flow model) and free water (using e.g. Navier-Stokes equations) are coupled through the sediment-water interface as a common closed boundary. The integral approach includes the interface as well as both pore water and surface water in a single model using a modified (porosity included) version of Navier-Stokes equations resulting in a model which is very much likely to capture continuous flow exchange on the interface between surface water and groundwater in cases where it is crucial. In the present work, the same setup as of Brand et al. (2013) is used for two reasons: On the one hand as a validation case and on the other hand to discuss the differences between the two approaches. We aim to present more realistic flow and pressure fields of U-shaped
burrows under the influence of the pumping activity of *Chironomus plumosus* larvae and pupae. In addition, we include the overlying water above the sediment for plausibility tests according to the experiments of Roskosch et al. (2010) and Morad et al. (2010). A wider range of flow velocities and sediment characteristics compared to Brand et al. (2013) are employed in this study in order to satisfy the discussions on how a connected system of sediment and surface water will react to pressure/flow fields on the interface compared to a constant pressure boundary coupling scheme and to relate to results of physical experiments.

### 3.3 Materials and methods

#### 3.3.1 Computational domain

![Figure 3.1](image-url)

*Figure 3.1: Model domain (lengths are not to scale) and boundaries B1-B4 reported in Table 1; B1 is atmospheric pressure at cylinder top; B2 are cylinder walls and cylinder bottom; B3 is symmetry plane to reduce computational effort; B4 represents the pumping chironomid larvae. The left panel is a detail enlargement of the burrow shown in the right panel.*

Figure 3.1 illustrates the geometry of the computational domain. This geometry has been selected to match the one of Brand et al. (2013). The only altered lengths for some scenarios are the radius and the height of the sediment cylinder which are both 0.25 m in our study while they were both 1 m in Brand et al. (2013). The impacts of this reduction have been checked by running some test scenarios and comparing the results in the areas close to the burrow where no considerable changes have been observed. Therefore, the geometry in Figure 3.1 acts nearly
identical to the one of Brand et al. (2013). This step was necessary to reduce the considerable computational effort. Using the same number of processors, the down sized model requires only 10% of the CPU time when compared to the large model.

The water table marked yellow in Figure 3.1 shows 0.1 m overlying column of water on top of the saturated sediment. In comparison to no overlying water shown with a green line this is an alternative scenario later used for comparison to other modeling approaches and experimental results. The burrow has a tube-like shape with a diameter of 0.002 m. It goes 0.150 m into the sediment starting from the inlet, including a curved part in the lower area and is symmetrical. The pumping zone of the Chironomus plumosus is located at the bottom of the burrow (B4, marked with a short vertical red line).

### 3.3.2 Governing equations

The Open-Source computational fluid dynamics software OpenFOAM (Open Field Operation and Manipulation) version 2.4.0 is chosen to simulate flow processes in and around the U-shaped burrow using the interFoam solver which is applicable for multiphase fluid flows. It is based on the Navier-Stokes equations and is widely used in hydraulic engineering in recent years (Schulze and Thorenz 2014). In detail we have applied and extended porousInter (Oxtoby et al. 2013), a sub-branch of interFoam. Our solver has been developed for two-phase (water, air) flow in the context of groundwater-surface water interactions (Broecker et al. 2019). In the present contribution, only single phase (water) flow is investigated. In simulations of relatively complex geometries as in our case, flow and pressure distributions are realistically captured using Navier-Stokes equations (Cardenas and Wilson 2007a, Tonina and Buffington 2009, Janssen et al. 2012). For incompressible fluids and accounting for the porous medium, the equations for the conservation of mass (Eq. (3.1)) and momentum (Eq. (3.2)) are written as (is averaged parameter over void region):

\[
\varphi \mathbf{\nabla} [\mathbf{v}]^f = 0
\quad \text{Eq. (3.1)}
\]

\[
\varphi \left( \frac{\partial [p]}{\partial t} + \mathbf{V} [\rho]^f [\mathbf{v}]^f [\mathbf{v}]^f \right) = -\varphi \mathbf{\nabla} [p]^f + \varphi [\mu]^f \mathbf{\nabla}^2 [\mathbf{v}]^f + \varphi [\rho]^f \cdot \mathbf{g} + D
\quad \text{Eq. (3.2)}
\]

where \( \varphi [\cdot] \) is the effective porosity, \( \mathbf{v} \) [m/s] is the flow velocity, \( p \) [Pa] is pressure, \( \rho \) [kg/m^3] is the density of the fluids, \( t \) [s] is time, \( \mu \) [kg/(m s)] is the dynamic viscosity \( (\mu = \mu_{\text{phys}} + \mu_{\text{turb}}; \text{physical + turbulent viscosity}) \), \( \mathbf{g} \) [m/s^2] is the gravitational acceleration and \( D \)
[kg/(m²s²)] is an additional porous drag term. $D$ accounts for momentum loss by means of fluid friction with the porous medium and flow recirculation within the sediment. Porous drag term $D$ is defined with Eq. (3.3):

$$D = A + B \quad \text{Eq. (3.3)}$$

$$A = - \left(150 \left(\frac{1-\phi}{d_P\phi}\right) [\mu] + 1.75 [\rho] [v] [\nu] \right) \frac{(1-\phi)}{d_P} [v] \quad \text{Eq. (3.4)}$$

$$B = -0.34 \left(\frac{1-\phi}{\phi} \frac{\partial[v] [\rho]}{\partial t} \right) \quad \text{Eq. (3.5)}$$

where $d_P$ [m] is the effective grain size diameter.

The term “$A$” in Eq. (3.4) considers pressure loss due to friction of the fluid with porous medium after Ergun (1952). In sediment, compared to free flow, more momentum is needed to accelerate a given volume of water. This is called added mass (van Gent 1995) because the extra momentum needed suggests that a larger volume of water has to be accelerated. “$B$” in Eq. (3.5) acts to add this added mass of the fluid due to flow recirculation caused by porous medium after van Gent (1995). In areas where only free flow exists, effective porosity is set to 1 which results in $A = B = D = 0$ and ensures the use of the original Navier-Stokes equations for free water flow.

The modeling tool uses the Finite-Volume-Method in space and the Finite-Difference-Method in time and allows massively parallel computations. In order to couple pressure and velocity, a combination of the SIMPLE (Semi-Implicit Method for Pressure Linked Equations, outer-correction loop) and the PISO (Pressure-Implicit with Splitting of Operators, inner corrector loop) algorithms called PIMPLE (merged PISO and SIMPLE) for robust modeling is implemented (Rodrigues et al. 2011).

According to the definition of the Reynolds number (Eq. (3.6)) (Reynolds 1883):

$$Re = \frac{\rho v L}{\mu} \quad \text{Eq. (3.6)}$$

where $L$ [m] is a characteristic length.

and considering the highest velocity in the burrow in this study (0.097 m/s), the density of water (1000 kg/m³), the dynamic viscosity of the water (~0.001 kg/(m s)), the burrow diameter $L$ (0.002 m), the critical Reynolds number 2300 for the transition between laminar and turbulent...
flow, the highest Reynolds number here is ~200 which means that flow is always laminar and therefore, turbulence is not considered in the model.

3.3.3 Grid and boundary conditions

To set up a grid which is comparable with both, the one of Brand et al. (2013) and the experiments of Roskosch et al. (2010) and Morad et al. (2010) for the domain shown in Figure 3.1, we generated a model with 0.5 million cells which are distributed with higher resolution near and inside the burrow (cell length < 0.5 mm) and coarser resolution (cell length ~ 1 cm) in the other regions of the soil using SALOME 9.3.0. With 0.5 million cells grid convergence was obtained, i.e. the results do not change when the mesh is further refined. For this study we assumed a rigid porous medium. Movement of sediment including erosion and deposition is not considered. As initial condition, the system was fully-filled with water. We set boundaries as shown in Table 3.1. We defined the top boundary with atmospheric pressure (B1, Table 3.1). The top boundary is the sediment surface (Figure 3.1, green line) or the water surface of the 10 cm overlying water column (Figure 3.1, yellow line).

Table 3-1: Boundary locations and conditions for geometry of Figure 1 and parameter values

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Location</th>
<th>Pressure (Pa)</th>
<th>Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>cylinder top</td>
<td>atmospheric pressure</td>
<td>pressure defined velocity</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(pressureInletOutletVelocity)</td>
</tr>
<tr>
<td>B2</td>
<td>cylinder sides and bottom</td>
<td>velocity</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(fixedFluxPressure)</td>
<td></td>
</tr>
<tr>
<td>B3</td>
<td>planar surface</td>
<td>symmetry plane</td>
<td>symmetry plane</td>
</tr>
<tr>
<td>B4</td>
<td>circular patch at bottom of burrow</td>
<td>velocity</td>
<td>0.009 -0.023</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(fixedFluxPressure)</td>
<td></td>
</tr>
</tbody>
</table>

Effective grain size diameter [mm] 0.125 -0.250

Effective porosity [-] 0.39
Case 1 is set up with comparable boundary conditions as the coupling scheme of Brand et al. (2013) while Case 2 is designed to be able to track the movement of water into the burrow inlet and out of the burrow outlet. Thus, there is the opportunity of a comparison of the model with the experiments of Roskosch et al. (2010) and Morad et al. (2010).

The system is a cylindrical column with closed sides. Therefore we define no flow conditions by setting velocity to zero on the side walls and on the bottom (B2, Table 3.1). In order to reduce computational efforts, only half of the cylinder is considered (Figure 3.1). Consequently, a planar surface (B3, Table 3.1) acts as a symmetry plane to mirror the other half of the cylinder. We then defined a baffle in the bottom of the burrow (B4, Table 3.1) which is a feature in OpenFOAM allowing the user to turn internal faces into boundary faces. The use of this baffle is to mimic the pumping activity of Chironomus plumosus larvae (or pupae) in the bottom of the burrow. Like any other boundaries in OpenFOAM, velocity or/and pressure conditions can be applied to such a baffle. The defined baffle has in fact a half-circular surface perpendicular to the tubed shaped burrow. Flow is free to enter and exit a baffle from both sides. Equal to the maximum velocity value used in Brand et al. (2013), we have initially chosen 0.009 m/s as the internal pumping velocity in the baffle. Thereafter, we investigated the impact of higher pumping velocities on pressure and flow recirculation patterns in the sediment. It is applied in 0.15 m depth below the sediment surface in the center of the burrow. The difference to the boundaries of Brand et al. (2013) is that we need no inner pressure boundary between burrow and sediment as it is required and common in coupled approaches. For achieving steady state, we run each instationary model for 40 to 100 s which took about 2-3 days CPU time on 40 processors of a high performance computer (TU Berlin HPC).

3.3.4 System parameters

Previous investigations including Brand et al. (2013), Morad et al. (2010), Hupfer et al. (2019), and Roskosch et al. (2010, 2011, 2012) have all used grain size distributions found in Lake Müggelsee (Berlin, Germany) to provide insight into pumping activities of Chironomus plumosus. Brand et al. (2013) have set the range of permeabilities from $3 \times 10^{-12}$ to $1 \times 10^{-14}$ m² to cover the range of fine sandy to unconsolidated loamy fine sandy sediments.

PorousInter includes sediment in the model by using effective porosity and an additional drag term (see Eq. 3.3-3.5) which depends among other terms on the effective grain size diameter (here uniform grain size distribution) (Oxtoby et al. 2013). The relation between the intrinsic permeability $K$ [m²] and hydraulic conductivity $K_f$ [m/s] is given by Eq. (3.7):
3. Flow simulations in and around a ventilated U-shaped chironomid dwelled burrow using integral approach

\[ K_f = K \frac{\rho g}{\mu} \quad \text{Eq. (3.7)} \]

The relation can be simplified to (Hinkelmann 2005):

\[ K_f = K \cdot 10^7 \frac{c}{s} \quad \text{Eq. (3.8)} \]

if \( K_f \) is given in [m/s] and \( K \) in [m²].

Therefore, the range of hydraulic conductivities used by Brand et al. (2013) is \( 3 \times 10^{-5} \) to \( 1 \times 10^{-7} \) m/s. We used the following equation to convert hydraulic conductivity to effective grain size (after Hazen):

\[ K_f = 0.00116 a_{10}^2 \quad \text{Eq. (3.9)} \]

where \( a_{10} \) is 10 \% fall through of the sieve curve [mm].

Using Eq. (3.8) and Eq. (3.9), \( a_{10} \) ranges for the permeabilities used by Brand et al. (2013) between 0.160 and 0.009 mm. Brand et al. (2013) have chosen \( d_{50} = 0.25 \) mm. Assuming a single uniform grain size (\( d_{10} = d_{50} \)) and since the main comparison with Brand et al. (2013) is based on cases with \( K = 3 \times 10^{-12} \) m², the effective grain size is set to 0.25 mm. Scenarios with a smaller grain size diameter down to 0.125 mm are also calculated. These values are in accordance with experiments of Roskosch et al. (2010) and Morad et al. (2010).

According to DIN 4220:2008-11 (2008), the effective porosity is set to 0.39 corresponding to the porosities of different sandy soils, from pure to middle loamy sand (similar material as used by Brand et al. 2013, Roskosch et al. 2010 and Morad et al. 2010) (Table 3.1).

3.3.5 Modeling cases

Two different cases with small adjustments in model geometry are performed.

Case 1: In order to compare the integral approach to the coupled approach of Brand et al. (2013), the geometry of Figure 3.1 is used and the green line is taken as the top boundary. The advective flow was observed for uniform grain size diameter of 0.25 mm and the pumping velocity of 0.009 m/s (identical to Brand et al. 2013). The flow in and around inlet, outlet and pumping zone (B4, Figure 3.1) as well as recirculation patterns through the sediment are analysed. Furthermore, impacts of different pumping velocities and effective grain size diameters were investigated. Case 1 allows the replication of the pumping activity of chironomid larvae in the burrow systems using a standard case of a U-shaped burrow with focus on exchange processes at the interface between pore water and surface water. Added to the comparison to the coupled
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approach, this case gives insight towards the effect of pumping activity of *Chironomus plumosus* on flow characteristics by mimicking the pumping activity of the larvae using pumping velocities at B4 and a flow through a structure designed to replicate the natural upward burrow shape.

Case 2: By adding an overlying water column of 10 cm on top of the saturated system (yellow line as the top boundary in Figure 3.1, extended version: 1 m height and radius), the aim was to investigate flow patterns over burrow inlet and outlet with the intention to compare these flow patterns to experimental results of Morad et al. (2010) and Roskosch et al. (2010) and to derive a relation between velocity at inlet/outlet to pumping velocity inside the burrow triggered by *Chironomus plumosus* larvae.

### 3.4 Results and discussion

#### 3.4.1 Comparison of integral to coupled approach

*Internal pumping velocity and pressure differences at the pumping zone*

![Figure 3-2](image.png)

Figure 3-2: Pressure (left) and velocity (right) fields of Case 2 (top) and Case 1 (bottom) with pumping velocity = 0.009 m/s and $d_p$ (effective grain size) = 0.25 mm. Green and yellow lines: see Figure 3.1

Using the geometry of Figure 3.1 and sediment characteristics of Table 3.1, the goal was to test the integral approach for feasibility in ventilated U-shaped burrow case. By applying a 2400
N/m³ force, Brand et al. (2013) created a velocity equal to 0.009 m/s during pumping periods. In Brand et al. (2013), this corresponded to pressure reduction from -6 Pa right behind the pumping zone to 0 at the inlet, followed by a 6 Pa pressure right in front of the pumping zone which then reduces to 0 at the outlet. In the coupled approach of Brand et al. (2013), the burrow is assumed to be a pipe where the pressure in the burrow is imposed as boundary condition in the groundwater flow model. No feedback of the surrounding sediment on flow in the burrow is taken into account. With the integrated model this setup was modelled as Case 1 which is shown as lower panel of Figure 3.2. The lower left panel of Figure 3.2 shows the pressure distribution results for the same setup.

In Case 1, the resulting pressure difference was not only caused by the flow in the burrow (unlike the assumption of one-way pressure head boundary from Brand et al. (2013)) but also by the flow in the sediment. Therefore a range of -2.9 to +2.9 Pa was observed. In fact, with the integral approach, -6 to +6 Pa were only achieved right and left of the baffle by applying 0.023 m/s as internal boundary velocity for the pumping zone. In general, symmetric pressure and velocity fields can be seen. A velocity field similar to the one of the coupled approach is found around the burrow (Figure 3.2, bottom right, Case 1). For Case 1, absolute pressures on the left and right of the pumping zone are equal. However, they differ in sign.

![Figure 3-3: Pressure in the pumping zone (orange = left branch of the burrow, blue = right branch of the burrow) for different water depths](image)
3. Flow simulations in and around a ventilated U-shaped chironomid dwelling burrow using integral approach

Figure 3.2 top shows a similar setup for Case 2. Compared to Case 1, under the same velocity conditions Case 2 experiences a larger total pressure ($P_{total} = P_{pumping} + P_{atm} + P_{ρgh}$) in the pumping zone with $P_{pumping}$ - pumping pressure, $P_{atm}$ - atmospheric pressure and $P_{ρgh}$ - hydrostatic pressure which increases linearly with depth below the water surface. due to added pressure ($P_{ρgh}$) of the overlying water column (Figure 3.2). To investigate the impact of overlying water height on total pressure at pumping zone, we ran case 1 with an altering overlying column of water as an addition to the top boundary (top boundary B1 = atmospheric pressure + pressure caused by a column of water). Figure 3.3 shows the relation between lake bed depth to pressure at the pumping zone for a range of lake bed depths with $U = 0.009$ m/s and $d_p = 0.25$ mm. A linear trend is observed.

The pumping pressure distribution in the sediment depends on the effective grain size. With growing effective grain size, water eases more to flow through sediment and thus the pressure drops. With smaller grain sizes, the system will look more like pipe flow. Flow is more concentrated in the burrow and less distributed in the sediment. The relation between pressure $P$ at the pumping zone and the ratio of the maximum velocity $U$ at the pumping zone to the effective grain size diameter $d_p$ is shown in Figure 3.4. Using 10 different cases with varying velocities and grain sizes a linear approximation between pressure and $U/d_p$ ratio is obtained. It shows that higher pumping velocities ($U$) and smaller grain sizes ($d_p$) result in a higher absolute value of the pressure at the pumping zone.

![Figure 3-4: Maximum/minimum pressure at the pumping zone for 10 different cases of $U/d_p$; $U$ is the maximum velocity at the pumping zone and $d_p$ is the effective grain size diameter; blue](image-url)
stands for the right side of the baffle where pressure is positive and orange stands for the left side of the baffle where pressure is negative

*Pressure and flow fields*

The velocity in a porous medium is generally orders of magnitude smaller than in free flow (surface water or pipe flow). In a burrow embedded in fine sediment, the flow is similar as in a pipe where a fully developed semi-circular velocity profile occurs between the walls. To see if OpenFOAM can handle smooth transitions of the maximum flow in the center of the pipe to its ‘walls’ where velocity is nearly zero, the flow in the burrow was investigated. Such a plausibility test has not been published so far to our knowledge. Figure 3.5 shows the flow profile inside the inlet and outlet branches of the burrow in a cross section at \( z = -0.05 \) m in which a semi-circular flow profile can be seen. The formation of this semi-circular flow profile provides a good basis for investigations of interactions between free and porewater flow. The flow in the sediment is not only influenced by the effective porosity and grain size, but also by the velocity and pressure field in the interacing burrow. In Brand et al. (2013) the mass exchange between burrow and sediment is driven by a pressure boundary condition, while in our approach such a forcing is not required as the pressure along the burrow wall, the mass exchange and feedback effects between burrow and sediment are directly included in the model concept. Therefore, we think our approach is more realistic when compared to Brand et al. (2013).

Figure 3-5: Velocity and pressure profiles at \( z = -0.05 \) m through inlet and outlet branches of the burrow for \( d_p \) (effective grain size) = 0.25 mm, Case 1
Another noticeable aspect is the distribution of pressure between two branches of the burrow. The pressure difference of these two branches is caused by the pumping activity at the bottom of the burrow. Figure 3.5 shows the pressure distribution along the cross section at \( z = -0.05 \) m which is point-symmetrical with zero pressure at \( x = 0 \) m. The highest and the lowest pressures occur in the burrows. This induces (1) flow in the burrows and (2) flow through the sediment from the burrow branch with high pressure (outlet) to the burrow branch with low pressure (inlet). The pressure differences are zero at the sediment surface and gradually increase with depth.

Figure 3.6 shows flow directions in the domain (Figure 3.6a), close to pumping zone (Figure 3.6b) and between two branches (Figure 3.6c) for pumping velocity = 0.009 m/s and \( d_p = 0.25 \) mm. Overall, flow directions and magnitudes show a very good agreement with the results of Brand et al. (2013) with the exception of areas near the burrow where flow exchange is considered differently in the integral approach.

![Figure 3-6: Velocity magnitudes (colors) and flow directions (arrows) a) in the entire domain, b) around pumping zone and c) between inlet and outlet branches](image)

```
Figure 3.6 shows that there is a flow recirculation between inlet and outlet branch of the chironomid burrow caused by the pressure distribution shown in Figure 3.4. This recirculation is more intense close to the pumping zone (Figure 3.6b) and less intense further away from it. Compared to Brand et al. (2013), lower pressures (e.g. ± 2.9 compared to ± 6 Pa in Brand et al. (2013) at pumping zone) are observed in areas close to the burrow and velocities larger than $10^{-4}$ or $10^{-5}$ m/s, respectively, occur in smaller areas compared to results of Brand et al. (2013).

![Figure 3.6](image)

Figure 3-7: Dominant flow directions (white arrows) on $z = -0.05$ m plane, looking from a) top b, c) lateral sides; blue plane is the cross section of a half cylinder

To make a comparison to the coupled approach of Brand et al. (2013), lateral velocities and directions for $z = -0.05$ m are shown in Figure 3.7. We found out that dominant flow from outlet to inlet branch (Figure 3.6b and 3.6c) is similar to the one shown in Brand et al. (2013). However, a circular flow field occurs (Figure 3.7a and 3.7b). Water leaving the outlet burrow branch is transported from the right side of the outlet branch to the left side of the inlet branch and enters the burrow again. For $d_p = 0.25$ mm and pumping velocity $U = 0.01$ m/s there is a difference between the percentage of water leaving the burrow in different areas.
3.4.2 Comparison of flow patterns to experiment results

A further step towards better understanding the hydraulics of ventilated U-shaped burrows as well as proof of plausibility of the integral approach is achieved by focusing on flow above burrow inlet and burrow outlet. Using Case 2, the modelled results are compared to flow patterns of experiments of Roskosch et al. (2010) and Morad et al. (2010). Velocity vector fields shown by Morad et al. (2010) map flow magnitudes and directions. Higher magnitudes occur close to inlet/outlet. Figure 3.8 shows a comparison of modeling results and results of Morad et al. (2010) for flow directions and flow fields above inlet and outlet. Values obtained in the modeling effort (≤ 38 mm/s over inlet/outlet) are among the range of Morad et al. (2010) (~35 mm/s over inlet/outlet). It can be seen that the model has successfully simulated the outward (outlet) and inward (inlet) flows at thresholds.

Figure 3-8: Comparison of the modeled flow pattern (left) above inlet (top row) and outlet (bottom row) with results of Morad et al. (2010) (right); dashed lines in modeled images mark the sediment surface; note: values differ due to unidentical burrow lengths and pumping velocities. Images based on the same measurements/raw data as images shown in Morad et al. (2010)/Roskosch et al. (2010)
We tested the integral approach (Case 1, $d_p$ (effective grain size) = 0.25 mm) and related the maximum inlet/outlet velocity (1.23 mm/s) to the triggering pumping velocity of 7.98 mm/s. Using a wider range of pumping velocities (5 to 25 mm/s, Figure 3.9), we tried to find a relationship where we could predict pumping velocity for given inlet/outlet velocities for this geometry. Figure 3.9 displays the relation between flow at inlet/outlet to pumping velocity. Throughout all scenarios, pumping velocity is \( \approx 6.5 \) times bigger than the inlet/outlet velocity. This ratio depends on the burrow geometry, i.e. its depth. It can be generally said that having a shallower burrow will also reduce the difference between the velocity at inlet/outlet and the velocity at the pumping zone for identical pumping velocities.

![Figure 3-9: Velocity at pumping zone to velocity at inlet/outlet (measured at outlet) for 5 different scenarios; $d_p$ (effective grain size) = 0.25 mm](image)

An important point that Roskosch et al. (2010) have addressed is the accumulation of advective flow as the result of pumping activity (mentioned as bioirrigation in their paper, also shown in Morad et al. 2010). With the integral approach, this was observed in a setup which allows good mass exchange between burrow and sediment. There is a slight difference between flow velocity at inlet and outlet imminent overlying water reported by Roskosch et al. (2010) and illustrated by Morad et al. (2010). Similar patterns where velocity at outlet is slightly (<1%) higher than the one at inlet were seen. Velocity patterns over inlet and outlet branches agree with observations of Morad et al. (2010).
3.5 Conclusion

This study aimed at gaining a better understanding of flow and exchange processes in, above and around U-shaped chironomid-dwelled burrows and to present an innovative method in dealing with such ecohydraulic topics. For that purpose the integral solver of Oxtoby et al. (2013) was applied and compared to experiments and other modeling approaches. In the integral approach mass exchange and feedback effects between burrow and sediment as well as sediment and overlying water column are directly included in the model concept, while in coupled approaches they are forced by ‘internal’ boundary conditions and therefore cannot account for feedback effects.

Plausible results were obtained for advective flow in the burrow (Roskosch et al. 2010). Sensivity analysis on pressure, effective grain size and pumping velocity resulted in a linear relation between pressure at the pumping zone and the ratio of pumping velocity to effective grain size. Using the identical setup as a prevalent coupled approach (Brand et al. 2013), flow pattern and magnitudes qualitatively agreed. Further, the formation of the semi-circular flow between the burrow branches was investigated.

Considering the overlying water, the missing link between the experiments of Roskosch et al. (2010) and the modeling of Brand et al. (2013) was filled. Roskosch et al. (2010) focused on areas above inlet and outlet and Brand et al. (2013) on flow in the sediment surrounding the burrows, while we could do both investigations together with the integral approach. The pumping activities of the Chironomus plumosus larvae control directly the flow in the burrows and in the surround sediment as investigated in the present study. This alters not only the local biogeochemistry in the sediment by oxygen supply (Lewandowski et al. 2007), particle reworking (Kristensen et al. 2012) and long-term fixation of phosphate (Hupfer et al. 2019) but also the water body above the sediment and thus, has severe impacts on the entire lake ecosystem including the food web (Hölker et al. 2015). Our approach seems to be interesting in quantifying the biogeochemical relevance of burrows for surface water quality. On the other hand one has to take into account that the computational effort is huge. The drag term of the integral solver has been derived for coarse and sandy soils. its application to very fine material such as clay is hardly recommended. A more realistic comparison of the formation of advective flow using this approach to bioturbation of animals which dwell in sandy sediment like Nereis diversicolor or Arenicola marina (Kristensen et al. 2012) is expected.
4. Flow and transport modeling in heterogeneous sediments using integral approach

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The test cases’ setups are listed in Appendix B (B9 one-dimensional tracer transport in heterogenous groundwater, B10 transport simulations for heterogenous groundwater-surface water interactions at rippled streambeds).
4. Flow and transport modeling in heterogeneous sediments using integral approach

4.1 Abstract

An integral approach which can simultaneously model turbulent flow and transport at the sediment-water interface has been recently developed and validated for homogeneous sediment which was achieved by comparing numerical results to flume experiments on flow and transport over a rippled streambed and through the sediment for neutral, gaining and losing conditions. In the present study we validated the approach for heterogeneous conditions by comparing numerical simulations of flow and transport in heterogeneous sediment to analytical solutions as well as flume experiments on flow and transport through rippled streambed consisting of heterogeneous sediment. For this complex setup, simulation and experimental results agree well showing that flow and tracer transport prefer paths through areas with bigger grain diameters and higher porosities. The effect of flow redirections under losing and gaining conditions on hyporheic flow and residence times is discussed.

4.2 Introduction

In the hyporheic zone, which is the transition zone between aquifer and river, groundwater and surface water are closely coupled (Cardenas 2009, Boano et al. 2014, Pryschlak et al. 2015, Lewandowski et al. 2019). This zone includes riverbeds, riverbanks, saturated sediments under dry bars and riparian areas (Edwards 1998). A multi-directional, multi-scale flow exchange between groundwater and surface water occurs and is controlled by factors such as stream morphology, ambient groundwater and sediment heterogeneity (Buffington and Tonina 2009, Cardenas 2009, Pryschlak et al. 2015). Hyporheic exchange transports contaminants (McKnight et al. 2001, Medina et al. 2002, Feris et al. 2003), organic carbon and nutrients (Valett et al. 1996, Hill and Cardaci 2004) from the surface water to the streambed. The streambed is populated by microbial biomass (Stonedahl et al. 2012). Biomass, hyporheic exchange fluxes and residence times in sediments are crucial factors in determining geochemistry of stream ecosystems (Arnon et al. 2013, Trauth et al. 2015, Fox et al. 2016).

Transport, settling and remobilization of sediment particles under different flow conditions result in heterogeneous sediment composition (Powell 1998). Compared to a homogeneous sediment, heterogeneity modifies flow paths, exchange fluxes, solute transport and residence times (Cardenas et al. 2004, Salehin et al. 2004, Singha et al. 2008, Sawyer and Cardenas 2009, Stonedahl et al. 2018). The influence of morphology on hyporheic exchanges has been addressed through many physical and numerical setups, by using different bedforms and structures (e.g. Elliot and Brooks 1997, Stonedahl et al. 2010, Broecker et al. 2019). Due to its
major impact on hyporheic exchange processes in streams, heterogeneity should be given high priority in presence of morphology (Freeze and Cherry 1979, Pryschlak et al. 2015). In studying hyporheic flow through morphological structures such as bed forms, heterogeneity adjusts flow by redirecting it through areas with higher hydraulic conductivities (Vaux 1968). Other major factors which affect hyporheic exchange flows are groundwater down- and upwelling. The effects of losing and gaining groundwater conditions have been physically (Fox et al. 2014, Gomez-Velez et al. 2014, Fox et al. 2016) and numerically modelled (Broecker et al. 2021).

Fig. 4-1 shows a cross section through the hyporheic zone with potential subsurface flow paths. Representation of hyporheic exchange flows is best achieved by considering stream morphology, sediment heterogeneity and ambient groundwater simultaneously. Field investigation addressing these aspects simultaneously require setups which are extremely challenging (Fox et al. 2016). Instead, a combination of flume experiments which consider the above-mentioned factors with a modeling tool which can be calibrated using the experiment and can be used to track flow and transport of solutes offers valuable insight in hyporheic exchange flows.

![Figure 4-1: Schematic view of hyporheic zone.](image)

To visualize flow and solute exchange in hyporheic zones, Fox et al. (2014) investigated the propagation of a tracer into a rippled streambed with a unidirectional surface water flow over bedforms. The flume consisted of a homogeneous streambed (including bedform morphology) with overlying flowing water. At the flume bottom gaining or losing conditions were simulated. Broecker et al. (2021) have modelled the flume experiment of Fox et al. (2014) with a newly developed integral approach which has advantages compared to coupled approaches (e.g. Saenger et al. 2005, Chen et al. 2018). Instead of using the interface between stream and groundwater as the transitional zone where results of surface water modeling are applied as
4. Flow and transport modeling in heterogeneous sediments using integral approach

Pressure boundary condition to a groundwater model (as is common with one-way coupling), integral approach allows the continuous exchange between two zones by using a modified form of Navier-Stokes equations which can include the porous zone directly in the flow model. Sobhi Gollo et al. (2021 and 2022) have shown that compared to prevalent coupled approaches, the integral approach allows capturing flow and pressure distributions at the interface between groundwater and surface water more realistically.

Transport across a homogenous rippled streambed has been investigated by flume experiments of Fox et al. (2014) and simulations of Broecker et al. (2021). Fox et al. (2016) used a setup very similar to the one of Fox et al. (2014) and included heterogeneity. They generated a random field with three sediment types and tracked flow and transport through the heterogeneous sediment.

The aim of the present study is to validate the integral approach of Broecker et al. (2021) for tracking flow and transport in a heterogeneous hyporheic zone using the experiments of Fox et al. (2016). To do so, we first compare the model results to a one-dimensional analytical solution to check if the transport of a tracer in different porous zones can be captured correctly. We then reproduce the exact sediment system presented in Fox et al. (2016). Next, we investigate flow through the heterogeneous sediment and introduce tracer accordingly for flow and transport validation.

4.3 Materials and methods

4.3.1 Computational domain

The numerical model geometry is based on the circulating flume experiments of Fox et al. (2016). Via obtaining reasonable anisotropy values and meeting ergodicity requirements, conditions close to natural streambed are imitated in the geometry of Fox et al. (2016) experiment which makes it a representative bed texture to study the effect of streambed heterogeneity on the hyporheic exchange fluxes. To reduce the computational effort, the numerical model is smaller (2.375 m) in length compared to the original experimental setup (6.4 m). The model width (in y-direction, see Fig. 4-2) is 0.29 m for both numerical and experimental setups. The inflow from the inlet enters a ramp before flowing over the rippled streambed (as done in Fox et al. 2016). The ramp slope starts at the base of the inlet and ends at the height of 0.2 m and is 0.93 m long in x-direction (Fig. 4-2). The height of the water from ripple crests is set to 7 cm. Identical to Fox et al. (2016), the sediment is packed with 20 layers
of heterogeneous sediment with 1 cm spatial resolution in z-direction. The ripples (dune-shaped forms) are each 20 cm long and 2 cm high. The ripple crest is positioned 15 cm from the left and 5 cm from the right foot of the ripple.

A mesh was generated using GMSH (Geuzaine and Remacle 2009) using different element types. To enable mapping the heterogeneity in the sediment, the sediment part (ripples excluded) is meshed with cuboid elements. Surface water and ripples are meshed with unstructured elements. The model consists of 72000 elements in total. To account for the steep gradients at the surface water-groundwater interface, mesh elements are finer on the interface with minimum cell size of $1 \times 10^{-3}$ m$^2$ compared to maximum of $8 \times 10^{-3}$ m$^2$ in some distance above the interface. In x-z plane, each 1 cm $\times$ 1 cm $\times$ sediment cell from Fox et al. (2016) is represented in the numerical grid by four 0.5 cm $\times$ 0.5 cm $\times$ cells.

![Figure 4-2: Model setup and geometry for modeling flow and transport in heterogenous sediment based on Fox et al. (2016); sediment heterogeneity is explained in Fig. 4-3.](image)

### 4.3.2 Boundary and initial conditions

The system is initially saturated with water and remains so during the modeling process for neutral, gaining and losing conditions. The heterogeneous structure is generated using Fox et al. (2016) who used three different sediments (fine, intermediate and coarse sand) with porosity values of 0.33, 0.44 and 0.44 and mean grain diameters of 0.38, 1.3 and 2.3 mm, respectively. Fig. 4-3 shows the generated patterns according to the sediment pattern plan acquired through personal contact with the authors of Fox et al. (2016).

An overview of the boundary conditions is illustrated in Fig. 4-4. Fox et al. (2016) defined a constant velocity of 0.15 m/s over the bedforms for a mean water level of 0.07 m and a flume width of 0.29 m which, for this setup, accounts for a fixed inlet volumetric flow rate of 0.003045 m$^3$/s and inlet velocity of 0.0362 m/s. Slip conditions are defined for the top boundary. Ramp surface as well as left and right side of the sediment are defined with no slip wall conditions.
The outflow at the flow outlet boundary equals the inflow at the flow inlet for neutral conditions. Under losing and gaining conditions, outflow equals inlet inflow plus/minus gaining/losing flow. The sediment bottom is defined as a no-flow boundary for neutral conditions. For gaining ($q_G$) and losing ($q_L$) conditions a 100 cm/d flow is defined in analogy to Fox et al. (2016). This value corresponds to a fixed inlet/outlet volumetric flow rate of $4.85 \times 10^{-6}$ m$^3$/s in ±z-direction. Pressure is fixed to 0 Pa at the outlet. To adjust the pressure gradient according to boundary fluxes for losing and gaining conditions, a special boundary condition (called fixedFluxPressure in OpenFOAM) is applied to sediment bottom.

In all cases pre-runs of 5 minutes with initial surface water flow of 0.15 m/s in x-direction are carried out in order to reach quasi steady state. For losing and gaining cases, $q_L$ and $q_G$ are applied as well. Results of these pre-runs are then used as initial conditions and then an inert constant tracer with a concentration of 1 mg/l and a molecular diffusion coefficient of $10^{-9}$ m$^2$/s enters the system through the inlet boundary.

4.3.3 Governing equations and computational tool

Figure 4-3: (top) Grain diameters and (bottom) porosities.

Figure 4-4: Model boundary conditions.
Simulations were carried out with OpenFOAM (Open-source Operation and Manipulation) software version 2.4.0. The porousInter solver, which is based on the InterFOAM solver, was developed by Oxtoby et al. (2013) and was used here to model the simultaneous flow in surface water and sediment. In this study, the sediment is fully saturated. Being based on an extended version of the Navier-Stokes equations, porousInter, considers porosity and grain diameter of the sediment as additional resistance terms. The equations for the conservation of mass and momentum are written as ([ ] the averaged parameter over void region):

\[ \varphi \nabla [v]^f = 0 \] (4-1)

\[ \varphi \left( \frac{\partial [\rho] [v]}{\partial t} + \nabla [\rho] [v] [v] [v] \right) = -\varphi \nabla [p]^f + \varphi [\mu] \nabla^2 [v]^f + \varphi [\rho] [v] \cdot g + \alpha \] (4-2)

where \( v \) [m/s] is the flow velocity, \( t \) [s] is time, \( p \) [Pa] is pressure, \( \rho \) [kg/m\(^3\)] is the density of the fluids, \( \mu \) [kg/(m s)] is the dynamic viscosity \( \mu = \mu_{\text{ph}} + \mu_t \) physical + turbulent viscosity, \( g \) [m/s\(^2\)] is the gravitational acceleration, \( \varphi \) [-] is the effective porosity and \( \alpha \) [kg/(m\(^2\)s\(^2\))] is an additional porous drag term. \( \alpha \) accounts for momentum loss by means of fluid friction with the porous medium and flow recirculation within the sediment. Porous drag term \( \alpha \) is defined with Eq. (3):

\[ \alpha = A + B \] (4-3)

\[ A = -\left( 150 \frac{(1-\varphi)}{d_p \varphi} [\mu] [v] + 1.75 [\rho] [v] [v] \right) \frac{(1-\varphi)}{d_p} [v] \] (4-4)

\[ B = -0.34 \frac{(1-\varphi)}{\varphi} \frac{\partial [v] [\rho]}{\partial t} \] (4-5)

where \( d_p \) [m] is the effective grain diameter.

Eq. (4-4) defines pressure loss due to fluid friction with sediment after Ergun (1952). In sediment, compared to surface water flow, more momentum is needed to accelerate a given volume of water. This so-called added mass (van Gent 1995) provides extra momentum needed for a larger volume of water to be accelerated. Eq. (4-5) considers this extra momentum due to flow recirculation by porous medium, after van Gent (1995). Where there is only surface water flow, effective porosity is set to 1 and therefore \( A = B = \alpha = 0 \). This means that for areas without sediment, the standard Navier-Stokes equations are used. To apply the set of equations to the flow domain, OpenFOAM uses the semi-discrete FVM (Finite Volume Method) discretization scheme and for time it uses FDM (Finite Difference Method). The interface between water and air phase is captured via the VoF (Volume of Fluid) method. In OpenFOAM,
velocity is discretized using sparse linear solver (smoothSolver, smoother: symGaussSeidel). Pressure is calculated by using GAMG (geometric agglomerated algebraic multigrid preconditioner) solver. Coupling of velocity and pressure is done via the PIMPLE algorithm. PIMPLE (combined PISO and SIMPLE) is a semi-implicit method for pressure-velocity coupling that accounts for transient flow conditions.

For modeling transport processes, we use the extension of porousInter called porousInterTracer developed by Broecker et al. (2021). They have implemented the following advection-diffusion equation for transport using diffusion coefficient \( D \) [m\(^2\)/s]:

\[
\frac{\partial [C]}{\partial t} + \nabla \cdot \left( \overline{v_p} [C] \right) + \nabla \cdot (D \nabla [C]) = 0 \tag{4-6}
\]

Where \( \overline{v_p} \) [m/s] is pore velocity, \( C \) is tracer concentration in [mg/l] and \( D \) [m\(^2\)/s] is diffusion coefficient. In OpenFOAM, tracer concentration is discretized with BICCG (bioconjugate gradient) solver which is used for asymmetric matrices and has good parallel scaling.

For the present study, we initially used a simple and computationally efficient RANS turbulence model (k-\( \varepsilon \); \( k \) = turbulent kinetic energy, \( \varepsilon \) = dissipation rate of turbulent kinetic energy). RANS was not capable of capturing flow velocity and pressure fluctuations in the model. Therefore, we then chose the LES turbulence model (Large Eddy Simulation; Smagorinsky 1963) which is more robust than the more commonly used RANS model for this study. Modeling the setup of Fig. 4-2 by using 96 parallel processors of the North-German Supercomputing Alliance (HLRN) and applying LES turbulence model takes 24 days (15 days for k-\( \varepsilon \)) for a 60-minute study of tracer propagation. Tracer expansion modelling with this turbulence model led to comparable results as in laboratory experiment serving as a justification for this approach.

### 4.4 Results and discussion

#### 4.4.1 Validation of flow and transport in heterogenous sediment with a 1D analytical solution

A one-dimensional 10 m long domain which is separated into two 5 m long sections with porosities of 0.44 and 0.3 (compliant with Fox et al. 2016) is shown in Fig. 4-5. An inert tracer with a diffusion coefficient of \( 10^{-9} \) m\(^2\)/s is continuously injected from the left side of the domain. Fig. 4-5 shows the tracer progression under constant velocity of 0.01 m/s. Simulation results
are compared to one-dimensional continuous injection analytical solutions of Kinzelbach (1992). A very good agreement between analytical solution results and simulations can be seen in Fig. 4-5 for different timesteps.

Figure 4-5: Comparison of integral model to analytical solutions for a continuous tracer injection in a simple 1D model domain: Model domain and porosities (left top), tracer fronts modelled with integral model after t=400 and 600 s (left bottom) and comparison of tracer concentrations for different timesteps for the integral model and the analytical solution.

4.4.2 Comparison of numerical to experimental results for tracer transport

Figure 4-6: Tracer propagation for the investigated 6th ripple after 10, 40 and 60 min. Results shown for both the lab experiment (a) and the integral model (b; purple). For 40 min, tracer fronts simulated via MIN3P groundwater model (from Fox et al. 2016) are as well illustrated.
The ripples of the lab experiments deviated slightly from the shape at the start of the experiment because of minor sediment movement during previous experiments.

In this section, for the transport of a tracer into heterogeneous sediment the lab observations of Fox et al. (2016) are compared to the results of the integral model. Simulated tracer propagation is compared to experiment in Fig. 4-6 under the 6th ripple. Numerical results of an alternative model (MIN3P, Mayer et al. 2002; modelled by Fox et al. 2016) after 40 min tracer propagation are also shown in Fig. 4-6 and compared to the integral model in Table 4-2.

Fig. 4-6 shows that the tracer first spreads around the green zone in the upper left with its small hydraulic conductivity (smallest grain size diameter; Fig. 4-6, neutral 10 and 40 min, losing 10 min, gaining 10, 40 and 60 min). Compared to the integral modelling, basically the same behavior is observed in experimental runs. The tracer propagates fastest under losing conditions and slowest under gaining conditions and prefers higher grain size diameter pathways under all conditions.

As suggested by Fox et al. (2016), to model sharp tracer fronts of the experiment, we assumed advection-diffusion dominant tracer propagation. By calculating the Peclet number, we have shown the contribution of advection and diffusion to transport in Fig. 4-7 for tracer propagation at 60 minutes. We have displayed that the fastest tracer propagation occurs under losing conditions where advective transport is dominant. Tracer propagation is slower under neutral conditions and smallest under gaining conditions. Under these two conditions, diffusive transport is dominant (Fig. 4-7).
Figure 4-8 shows how minor differences in dyed areas between experimental runs and modelled simulations are probably caused by inaccurate implementations of the sediment geometry and pattern in the experiment. Although such inaccuracies can be considered negligible for an experimental setup, in comparison to modelled tracer fronts in heterogeneous sediments they can be important. In Fig. 4-8 it is displayed how the original sediment setup and ripple geometry (as suggested by Fox et al. (2016) and applied for integral model) changed during sediment packing and experiment. Local changes of sediment pattern \( e_t \) compared to the original setup are illustrated for the investigated zone as an example. Throughout the experiment, these small changes are very important in opening and blocking pathways of flow and tracer propagation. Although compared to the original plan the generally heterogeneous sediment pattern is
relatively intact (except $e_l$), a small bedform migration ($e_{a1-5}$) and deformation ($e_{b1-6}$) of the bedforms can be detected. Presumably, these changes of the sediment surface cause a formation of a thin layer right underneath the bedform. This unidentified (thickness unknown) sediment layer ($e_u$) is also displayed in Fig. 4-8. As local and bedform geometry changes cannot be quantified exactly, original bedform geometry and sediment composition are used for modeling. The experimental sediment composition and bedform morphometry deviates only slightly from this plan as shown in Fig. 4-8.

Table 4-1: Tracer propagation comparison with time between integral model and experiment under neutral, losing and gaining conditions.

<table>
<thead>
<tr>
<th></th>
<th>Dyed area [cm$^2$]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Neutral</td>
</tr>
<tr>
<td></td>
<td>Experiment Simulation</td>
</tr>
<tr>
<td>10 min</td>
<td>45.726</td>
</tr>
<tr>
<td>40 min</td>
<td>92.620</td>
</tr>
<tr>
<td>60 min</td>
<td>101.042</td>
</tr>
<tr>
<td>RMSE</td>
<td>9.55</td>
</tr>
<tr>
<td>N-RMSE</td>
<td>0.17</td>
</tr>
</tbody>
</table>

To compare results of experimental runs and simulations quantitively, they are compared through photographs of tracer fronts at 10, 40 and 60 min. Applying “ImageJ” which is used for scientific image analysis, a comparison of the dyed areas of experiment and simulation is shown in Table 4-1. Tracers are most quickly propagating under losing conditions and slowest under gaining conditions. For gaining conditions the propagation rate drastically decreases with time and results show very little further tracer propagation between 40 and 60 min (Table 4-1, Fig. 4-9). RMSE (root mean square error) and N-RMSE (normalized RMSE; $0 < N$-RMSE $< 1$; $N$-RMSE closer to 0 than 1 shows plausible fitting) values show that model and experiment agree best for losing conditions followed by gaining and neutral conditions. This indicates that less unexpected ripple geometry deformations throughout the experiment under losing conditions result in less discrepancy between simulation and experiment. Considering
undefined experimental setup modifications, they fairly match experimental tracer propagation trends both qualitatively (Fig. 4-6) and quantitively (Table 4-1). If experimental setup modifications could be definable in the model or could be eliminated from the experiment, a perfect match between simulation and experiment is to be expected.

Table 4-2: Tracer propagation comparison after 40 minutes between the MIN3P and the integral model (porousInter) under neutral, losing and gaining conditions.

<table>
<thead>
<tr>
<th>Dyed area [cm²]</th>
<th>MIN3P Neutral</th>
<th>porousInter Neutral</th>
<th>MIN3P Losing</th>
<th>porousInter Losing</th>
<th>MIN3P Gaining</th>
<th>porousInter Gaining</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIN3P</td>
<td>84.873</td>
<td>porousInter</td>
<td>84.713</td>
<td>136.030</td>
<td>136.145</td>
<td>56.007</td>
</tr>
</tbody>
</table>

Comparing the integral model results at 40 minutes to an alternative groundwater model (MIN3P; Fig 4-6; obtained from Fox et al. 2016) in Table 4-2 shows that the integral solver simulates the tracer propagation for all the conditions very similar to a widely used groundwater model like MIN3P.

By observing a good match between experimental and integral model results (as well as comparison to MIN3P), next, we will describe the modelled pressure distribution and velocity fields in the heterogenous sediment.

### 4.4.3 Pressure and flow distribution in heterogenous sediment

**Hydrodynamic pressure**

Hydrodynamic pressure distributions under neutral, losing and gaining conditions on 4th, 5th and 6th ripples are shown in Fig. 4-9. These ripples are sufficiently far away from the inlet and potential impacts of the flume inlet. Neutral conditions are defined by setting zero velocity to the lower boundary of the sediment bed. For losing conditions an outflux of $4.85 \times 10^{-6}$ m³/s is set for the bottom of the flume in analogy to Fox et al. (2016). For gaining conditions an influx of $4.85 \times 10^{-6}$ m³/s through the bottom of the flume is applied equal to the flux used in Fox et al. (2016).
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Figure 4-9: Hydrodynamic pressure distribution under neutral, losing and gaining conditions and the location of a horizontal cross section (z = 0.195 m, white line) as well as grain diameter maps at 4th, 5th and 6th ripples.

Figure 4-10: Hydrodynamic pressures under neutral, losing and gaining conditions for a horizontal cross section through the sediment bed in the depth marked in Fig. 4-9 as white line.

Hydrodynamic pressure results from subtracting total pressure from hydrostatic pressure. In the present study, hydrodynamic pressures are higher on the luv (upstream) side of the ripple as shown in Fig. 4-9. Compared to losing conditions, gaining and neutral conditions show lower hydrodynamic pressure. Hydrodynamic pressure values for a horizontal section underneath the ripples (z = 0.195 m) of Fig. 4-9 are displayed in Fig. 4-10. The 60 cm long horizontal cross section (1.575 m < x < 2.175 m, z = 0.195 m) which cuts through several sediment types with different grain diameters is located 2.5 cm under the ripple crests. Looking at Fig. 4-10,
hydrodynamic pressure patterns are affected by changes in grain size diameters and porosity. However, a general periodicity of the hydrodynamic pressure distribution due to the presence of bedforms can also be seen in all three flow environments. Hydrodynamic pressures fluctuate under neutral conditions between 0.2 Pa and 0.9 Pa, under losing conditions between 3 Pa and 8 Pa and under gaining conditions between 0.3 Pa and 0.8 Pa. Generally, hydrodynamic pressure peaks under the mid part of the luv sides of the ripples and reaches minimum beneath the troughs between the ripples.

Under neutral, gaining and losing conditions, differences between hydrodynamic pressures and local pressure oscillations result from different ambient groundwater flow conditions as well as from sediment heterogeneity. To investigate these effects more precisely, flow velocities resulting from hydrodynamic pressures are illustrated for different grain size diameters in the next section.

Flow patterns

Different hyporheic flow vectors result from the hydrodynamic pressure distribution. Looking at the flow patterns shows the effects of gaining/losing conditions for different porosities and grain size diameters. Fig. 4-11 displays groundwater flow velocities greater than $1 \times 10^{-3}$ m/s, $1 \times 10^{-4}$ m/s and $1 \times 10^{-5}$ m/s and their directions for neutral, gaining and losing conditions. These are superimposed on grain diameters map in the sediment underneath ripples 4, 5 and 6. Higher velocity in a zone is an indicator that it is a zone of preferred flow. Unlike neutral and gaining conditions, with $v > 1 \times 10^{-3}$ m/s, a slight downward flow across ripple surfaces is detected under losing conditions which indicates that under such conditions larger volumes of water enter the sediment compared to gaining and neutral conditions. Looking at $v > 1 \times 10^{-4}$ m/s, some hyporheic flow occurs under neutral and gaining conditions. Gaining conditions display slight upward flow through the hyporheic sediment. In this velocity class and for losing conditions, not only strong hyporheic flow occurs but also intense downward flow. Through downward pulling of water, hyporheic zone becomes deeper in losing conditions compared to neutral and gaining conditions. Even with velocities as low as $1 \times 10^{-5}$ m/s, there is not much flow through the sediment under neutral conditions and the hyporheic flow is limited to the top 5-6 cm sediment. Ambient flow conditions on the other hand cover the entire sediment at these flow velocities.

In Fig. 4-11, the effect of sediment heterogeneity on flow under different conditions can be investigated by tracking the flow over grain size diameters and porosities (see also Fig. 4-3).
Under neutral conditions, where no upward/downward ambient groundwater flow exists, water majorly enters the streambed from the luv side of the ripples and leaves the streambed from the lee (downstream) side of the ripples. The extent in which this flow can enter the sediment is controlled by the grain size diameter distribution in the sediment. For \( v > 1 \times 10^{-4} \) m/s, the hyporheic flow of the 4th ripple is allowed to enter deeper into the sediment compared to the 5th and the 6th ripple. This is due to the flow being blocked by the blue stretch of lower grain size diameter (as well as lower porosity) under the 5th and the 6th ripple. At less intense (\( v > 1 \times 10^{-5} \) m/s) flow under neutral conditions, a blue block underneath the 5th ripple and partly the 6th ripple has limited hyporheic flow to the upper 5-6 cm as opposed to the 4th ripple in which flow can enter deeper into the sediment. Under the 4th ripple, hyporheic flow which reaches deeper sediment is deflected by the less porous/smaller grain size diameter areas and instead of flowing back to the surface water, partly continues downward flow. Therefore, as opposed to the conditions in 5th and 6th ripples, for hyporheic flow through the 4th ripple longer residence times occur.

![Figure 4-11: Flow vectors (dimensionless) mapped over grain size diameters of the sediment underneath 4th, 5th and 6th ripples for v > 1 \times 10^{-3} \) m/s, v > 1 \times 10^{-4} \) m/s and v > 1 \times 10^{-5} \) m/s for neutral, losing and gaining conditions.](image)

As was previously mentioned, hyporheic zone is thicker under losing conditions compared to gaining and neutral conditions. Under losing conditions and at higher flow rates (\( v > 1 \times 10^{-4} \) m/s), deflected hyporheic flow under the 4th ripple is being pulled down by the downwelling groundwater flow. By entering deeper groundwater, the flow meets new heterogeneous zones and is further deflected causing residence times to increase drastically. The hyporheic flow
beneath the 5th and 6th ripple is being pulled down left (under 5th ripple) and right (under 6th ripple) of the blue block (Fig. 4-11). The low grain size diameter/low porosity blue block under the 5th ripple causes the hyporheic flow to partly take a long path of entering the sediment from its left side. A part of the flow takes the shorter path across the blue block. As the result, a portion of the flow resides longer in the sediment compared to the other portion that leaves immediately by flowing towards the lee side of the ripple. Under gaining conditions and at high velocities ($v > 1 \times 10^{-4} \text{ m/s}$), water enters the streambed sediment less deep and behaves similar to neutral conditions. At less intense flow ($v > 1 \times 10^{-5} \text{ m/s}$), upwelling groundwater flow that finds its way up through higher grain size diameters/higher porosity zones, opposes the inflowing hyporheic water in some areas and pushes the outflowing hyporheic flow towards the lee sides of the ripples. A better connectivity of the upwelling flow towards the 4th ripple due to higher grain size diameter/higher porosity underneath this ripple, results in more impact of gaining conditions on the hyporheic flow compared to the 5th ripple. Investigating the flow across rippled heterogeneous streambeds under different ambient groundwater flow conditions shows that a base hyporheic zone generated under neutral conditions becomes deeper by downwelling groundwater flow (losing conditions). Under upwelling groundwater flow (gaining conditions), the depth in which hyporheic flow occurs is decreased. Sediment heterogeneity strongly affects flow under all conditions, i.e. neutral, gaining and losing. Compared to neutral conditions, under losing and gaining conditions the impact is stronger and more complex as the ambient groundwater flow prefers zones of higher grain size diameter/higher porosity. This impact is stronger under losing conditions compared to gaining conditions as downward pulling of flow entraps the hyporheic water in deeper heterogeneous zones. This entrapment which happens by the deflection of flow through complex heterogeneous zones can occur to a lesser extent under neutral and gaining conditions as well. If occurring near the sediment-water interface, flow reflection decreases hyporheic flow path length by redirecting flow towards surface water. Therefore, depending on the base hyporheic flow rates (generated under neutral conditions), sediment heterogeneity and ambient groundwater flow conditions hyporheic flow residence times can be modified. For investigating such complex phenomenon, the integral solver which can detect flow redirections for heterogeneous sediment under different ambient flow conditions seems very competent.
4.5 Conclusion

An integral solver was further developed to model tracer transport through heterogeneous rippled streambeds and thereby gain deep insights into hyporheic flow processes in the sediments. For this purpose, an integral model was compared with the results measured on a physical model, i.e. a laboratory flume. Even in the presence of groundwater flow and with complex streambed heterogeneity, the modelled tracer propagation agrees well with the experiment. This confirms the applicability of the model. A look at the resulting flow fields suggests that hyporheic zone thickens under losing conditions more than under neutral and gaining conditions. Sediment heterogeneity can increase the hyporheic flow domain volume. Consequently, with velocity in the stream channel being constant, increased sediment heterogeneity in the porous medium (resulting in thicker hyporheic flow domain) causes higher residence time of the water when comparing flow through sediment underneath ripples. In zones with higher porosity/larger grain size diameter, stronger water flow occurs than in zones with lower porosity/smaller grain size diameter. Different sediment types lead to complex flow patterns and deflect the flow, also towards deeper sediment layers. In part, water is also trapped in low flow zones, which further increases residence times in the hyporheic zone. Small-scale, high-resolution integral modeling of hyporheic flow through heterogeneous sediment provides the necessary information on changes in residence times and flow pathways that are crucial for determining the purification effect and fate of contaminants in the hyporheic zone. In this case, the application of the integral approach should be preferred over the prevailing coupling schemes which neglect the mutual, continuous feedback between groundwater and surface water (Sobhi Gollo et al. 2022).

The integral solver has already been validated to account for streambed morphology (Broecker et al. 2019) and transport through homogeneous sediment under ambient groundwater conditions (Broecker et al. 2021). Transport through heterogeneous sediment under ambient groundwater conditions has now been discussed and validated in the present study. The integral approach has so far proven to be very powerful in modeling flow and transport processes across groundwater-surface water interface. Further development of the integral solver by including a wider range of scenarios, transient flow conditions, reactive transport and sediment transport are highly recommended.
5. Supplementary contributions

5.1 Integral Flow simulations for groundwater-surface water interactions at rippled streambeds

This study was published in Water as:


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This is the abstract of the article (postprint).

Abstract

Exchange processes of surface and groundwater are important for the management of water quantity and quality as well as for the ecological functioning. In contrast to most numerical simulations using coupled models to investigate these processes, we present a novel integral formulation for the sediment-water-interface. The computational fluid dynamics (CFD) model OpenFOAM was used to solve an extended version of the three-dimensional Navier–Stokes equations which is also applicable in non-Darcy-flow layers. Simulations were conducted to determine the influence of ripple morphologies and surface hydraulics on the flow processes within the hyporheic zone for a sandy and for a gravel sediment. In- and outflowing exchange fluxes along a ripple were determined for each case. The results indicate that larger grain size diameters, as well as ripple distances, increased hyporheic exchange fluxes significantly. For higher ripple dimensions, no clear relationship to hyporheic exchange was found. Larger ripple
lengths decreased the hyporheic exchange fluxes due to less turbulence between the ripples. For all cases with sand, non-Darcy-flow was observed at an upper layer of the ripple, whereas for gravel non-Darcy-flow was recognized nearly down to the bottom boundary. Moreover, the sediment grain sizes influenced also the surface water flow significantly.

5.2 Transport simulations for groundwater-surface water interactions under neutral, losing and gaining flow conditions for homogenous streambed

This study was published in Groundwater as:


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This is the abstract of the article (postprint).

Abstract

Transport processes that lead to exchange of mass between surface water and groundwater play a significant role for the ecological functioning of aquatic systems, for hydrological processes and for biogeochemical transformations. In this study, we present a novel integral modeling approach for flow and transport at the sediment-water interface. The model allows us to simultaneously simulate turbulent surface and subsurface flow and transport with the same conceptual approach. For this purpose, a conservative transport equation was implemented to an existing approach that uses an extended version of the Navier-Stokes equations. Based on previous flume studies which investigated the spreading of a dye tracer under neutral, losing
and gaining flow conditions the new solver is validated. Tracer distributions of the experiments are in close agreement with the simulations. The simulated flow paths are significantly affected by in- and outflowing groundwater flow. The highest velocities within the sediment are found for losing condition, which leads to shorter residence times compared to neutral and gaining conditions. The largest extent of the hyporheic exchange flow is observed under neutral condition. The new solver can be used for further examinations of cases that are not suitable for the conventional coupled models, for example, if Reynolds numbers are larger than 10. Moreover, results gained with the integral solver provide high resolution information on pressure and velocity distributions at the rippled streambed, which can be used to improve flow predictions. This includes the extent of hyporheic exchange under varying ambient groundwater flow conditions.
6. Synthesis

6.1 Summary and conclusions

Due to a recent shift of perception towards considering groundwater and surface water as a single resource, many field and laboratory techniques utilizing advanced measurement methods are developed. Nevertheless, numerical models are not keeping pace with these developments and look upon groundwater and surface water separately. The present thesis is an endeavor to introduce, validate, apply and further develop an integral approach to capture continuous transport and exchange between groundwater and surface water. For that matter, using a single set of mathematical equations (modified three-dimensional Navier-Stokes equations), groundwater and surface water are modeled in one domain. Simulations are based on CFD software OpenFOAM. The benefit of utilizing this software is spatiotemporally high-resolution modeling of groundwater-surface water exchange processes which however limits the spatial scale due to its high computational effort.

6.1.1 General outcomes

Prior to detailed description of the outcomes of model comparison as well as validation and further development of the integral approach, a general summary of this thesis is put forward. In sections 2 and 3, integral approach is compared to coupled approach for two cases: flow and exchange across rippled streambed and ventilation in U-shaped burrows:

- For both cases, steep velocity gradients and pressure variations occur at the immediate interface between groundwater and surface water. The comparison of flow and pressure results indicate that:
  - In the case of flow across rippled streambed, by defining identical overlying surface water flow velocity and water table for coupled and integral models, identical total pressure fields in surface water are achieved. However, it is displayed that integral approach shows smaller velocities and hydrodynamic pressures in the vicinity of the ripples.
  - In the case of ventilation through U-shaped burrow, by defining a fully saturated sediment and burrow, identical hydrostatic pressure fields in the domain are achieved. In the pumping zone however, identical hydrodynamic pressures were only obtained when applying a higher flow velocity in the integral model compared to coupled model. On the other hand, if identical flow velocities were exhibited,
integral model’s hydrodynamic pressure was smaller than the one of the coupled model.

- In the immediate interface between groundwater and surface water, a continuous exchange of flow occurs. Therefore, considering feedback between groundwater and surface water is crucial:
  - In the flow across rippled streambed case, surface water entering the rippled area can continuously flow in from one side of the ripple and flow out at the other side using the integral model. On the contrary, using coupled approach, the effect of flow over the ripple is translated into pressure distributions to be transferred into the groundwater model.
  - In the case of ventilation through U-shaped burrow, unlike coupled model, a continuous flow from inlet to outlet branch through the sediment is captured via integral model.

- Very high spatiotemporal resolution of the integral approach authorizes its application for small scale groundwater-surface water interface phenomena. Its high computational burden should however be considered:
  - In the flow across rippled streambed case, on account of a comparison with a simpler shallow water equation model, the use of a CFD Navier-Stokes model for modeling the surface water part of the coupled model is proved essential. Therefore, computational resources required for the coupled and integral models are in fact similar as they both require high performance computing clusters.
  - In the ventilation through U-shaped burrow case, due to symmetric geometry of the burrow, in the coupled model Navier-Stokes equations are applied for the flow through the burrow without using a CFD model. Consequently, computational burden of the integral model is relatively higher than the coupled model.

In section 4, the integral approach which was formerly validated for transport through homogenous sediment by Broecker et al. (2021) is validated for modeling tracer transport through heterogenous sediment. Through comparison with analytical solutions and experimental results, it is demonstrated that:

- Complex hydraulics of flow and tracer propagation through a heterogenous sediment can be plausibly captured using the integral approach.

This study was embedded in the collaborative research common topic group of “Interface Hyporheic zones” of the 2nd cohort of the Urban Water Interfaces Research Training Group (UWI). Next to the model development provided in this study, a series of field and laboratory
experiments which examined different biogeochemical processes of the hyporheic zone and bank filtration processes are provided in other projects.

6.1.2 Outcomes of comparing integral to coupled approach for flow across rippled streambed

For the case of flow across a rippled streambed, an integral model (using modified Navier-Stokes equations and LES turbulence model) to model flow and exchange processes in groundwater, surface water and groundwater-surface water interface is compared to a coupled model of groundwater (using Richards equation model) and surface water (using Navier-Stokes equations and LES turbulence model) flow. Furthermore, a shallow water equations model is used to model flow in surface water. For accurate compatibility of the integral model to the coupled model, next to using identical model domain details like model length, mesh resolution, weir placement and ripple geometry in surface water part of both models, same flow conditions are applied which result in very similar water tables and pressure distributions. However, allowing continuous exchange near interface in integral model yields velocity distributions very dissimilar to coupled model. Near the interface in surface water, velocity vectors meet the ripple with different impact angles. In coupled model, these vectors are deflected as they cannot enter the rigid bottom boundary of the surface water model causing turbulent eddies to form. In integral model however, the interface is connected to the porewater and depending on the sediment porosity, a portion of the flow enters the sediment causing considerably less deflection and formation of less turbulence near the interface in surface water. In groundwater, coupled model is bound to flow velocities within Darcy’s law. Contrarily, integral model can detect areas where flow as the result of close contact to surface water has velocities outside of the range defined by Darcy’s law. As continuous flow across interface in connected groundwater-surface water streams constantly occurs, results of integral model for flow and exchange processes in this zone are more plausible compared to coupled model and application of coupled models on the interface results in overestimation of flow fields in interface region. The extent of discrepancies between integral and coupled models can depend on factors like stream flow velocity, streambed morphology, sediment characteristics and its heterogeneity.

Next to more plausible estimation of flow fields near interface, the use of the modified Navier-Stokes equations for modeling groundwater-surface water exchange has further advantages. Under proper hydrogeologic conditions (such as surface water flow, sediment porosity, streambed morphology) surface water eddies are to some extent transferred into the sediment close to the interface. Unlike coupled model, the equations governing the integral model can
detect these eddies. Nevertheless, the extent of turbulence penetration in relation to the hydrogeological conditions needs to be further verified for the mathematical model of the integral approach.

The residence time of the hyporheic water is a crucial topic in investigations on water quality and purification potential of the hyporheic zone. The integral model continuously traces the hyporheic water flow conditions and its pathways as it enters and leaves the hyporheic zone. Such capability is far more superior to coupled models which only function by transferring the resulting pressure distributions over the common boundaries from one model to the other.

By comparing surface water model outcomes of Navier-Stokes equations-based model to shallow water equations-based model, application of the Navier-Stokes equations-based model is proven necessary. Consequently, for modeling flow across rippled streambed, applying computationally expensive CFD models is necessary for both approaches. Although run time of the integral model is a few hours higher than of the surface water part of the coupled model, both need access to supercomputers. Concurrently, modeling results are very similar a few decimetres away from the interface. Although the difference in computational requirement is not significant in this study, the outcomes suggest that if investigations for deeper groundwater are intended, coupled model is computationally more efficient compared to integral model. Detailed information of this study can be found in section 2.

### 6.1.3 Outcomes of comparing integral to coupled approach for ventilation through U-shaped burrow

In the next step, by examining a distinctive case, application area of the integral approach is extended and further advantages to coupled approach are discussed. Here, a case of flow initiated by pumping activities inside a U-shaped burrow (by bioturbation of the tube-dwelling invertebrates) that generates flow and exchange across surrounding sediment (porewater)-burrow (surface water) interface is modelled with integral solver and compared to an existing identical coupled model. For accurate compatibility of the integral model to the coupled model, identical model domain details like burrow geometry, sediment characteristics and flow source placement (at the pumping zone) are carefully implemented. It was however realized that to generate the same pressure conditions at the pumping zone in the integral model, higher velocities compared to coupled model should be deployed. Similar to rippled streambed case, here allowing continuous exchange of flow between burrow and surrounding sediment by using integral model results in unequal pressure-velocity fields in the pumping zone compared to coupled model. In coupled model, the generated pressure (resulting from solving Navier-Stokes
equation for surface water flow) in the burrow which is used as coupling parameter is independent from the sediment characteristics. By continuous burrow-porewater exchange in the integral model, sediment characteristics participate in determining flow and pressure conditions. Integral modeling of burrow ventilation processes with different flow velocities and grain diameters show that higher velocities and smaller grain diameters result in higher pressures in the pumping zone (which then spreads to the whole domain).

Next to plausible modeling of flow and pressure fields, integral model allows continuous investigation of the transport of flow through the sediment, burrow and on the overlying water and their interactions. As biochemical composition of water in the sediment, in the overlying water and on the burrow branches are often different, monitoring their interactions gives insight to better understanding the hydro-biogeochemical processes across tube-dwelling invertebrates habitat.

Although required computational capacity of the integral model is higher than of the coupled model in this case, negligence of important hydrogeological parameters in determining velocity-pressure fields using the coupled model points towards the absolute necessity of using integral model for plausible results acquirement. It should be noted that the velocity values used in both coupled and integral numerical simulations are limited to the averages over pumping and resting periods and do not mimic the actual generated velocities during burrow ventilation. Detailed information of this study can be found in section 3.

6.1.4 Outcomes of transport modeling for heterogenous groundwater-surface water-interactions

After gathering significant evidence of superiority of the integral approach to prevalent methods for modeling groundwater-surface water interactions and pointing out its ability to track flow across the interface, it is very beneficial to extend the solver for modeling transport processes that it can step into the vast topic of contamination remediation, nutrient transformation and water quality modification. The initial validation step for transport across homogenous streambed (now backed by profound flow and exchange model validation and comparison carried out in this thesis) has been taken as stated in section 5.2. Next to streambed morphology (studied in 5.1), ambient groundwater conditions and sediment heterogeneity are decisive factors in tracking transport in the sediment. Throughout this step, the integral solver, formerly validated for transport through homogenous sediment by Broecker et al. (2021), was extended for advective-diffusive transport in heterogenous sediment and under ambient groundwater conditions. The mathematical model was initially validated next to analytical solutions. A flume
experiment conducted to track the tracer propagation through heterogenous sediment was modeled via integral approach. Velocity and hydrodynamic pressure results indicated that under losing condition more water is transported through the sediment compared to neutral and gaining conditions resulting in an extended hyporheic zone. The transported water is deflected in various areas as it reaches stretches with varying porosities and grain diameters resulting in very different residence times. The collective impact of sediment heterogeneity and ambient groundwater conditions is higher for losing condition as water meets more layers of heterogeneity while entering the sediment. These findings were validated by comparing tracer propagation in the model to the experiment. Plausible comparison of results authorizes the use of the integral solver for transport modeling in heterogenous sediment and determining the effect of sediment heterogeneity under ambient groundwater conditions on flow intensity, direction and residence times. Detailed information of this study can be found in section 4.

6.1.5 Recommendations for modeling and data processing

Qualitative advantages of the integral approach compared to coupled approach should be investigated next to comparing velocity-pressure and intrinsic computational effort differences of the models. This study carries out pre-processing, processing and post-processing of two methodically distinctive models. Here a few additional notes for model selection are presented:

- Groundwater models that resolve seepage flow in x-z axis and are capable of meshing complex structures like ripples are usually not freely available. For this study, a commercial groundwater model was licenced through scientific collaborations.
- Utilizing a coupled model requires a very good knowledge in modeling both groundwater and surface water processes as well as coupling techniques.
- Groundwater and surface water models used in coupled approach oftentimes use different pre- and post-processing tools. For instance, generating a numerical mesh with identical mesh nodes on the boundaries is sometimes challenging. Applying the resulted pressure distribution from the surface water model to the groundwater model is very dependent of precise placement of nodes.
- In comparing necessary time to run coupled and integral models that essentially use the same computational resource (inevitability to access supercomputers), the coupling step is often neglected. Depending on the models used for coupling, this step can be time-consuming.

All the discussions above indicate that integral approach is a very powerful method and should be prioritized to coupled approach in addressing small-scale high-resolution groundwater-
6. Synthesis

Surface water interaction processes. This approach is now capable of modeling flow and transport of tracers from the surface water to heterogeneous groundwater. As it was formerly mentioned, the advantages of the integral approach vanish in modeling very deep groundwater and its use is only recommended where the effects of groundwater-surface water interaction are present. By comparing k-ε and LES turbulence models for the case of transport in the heterogeneous sediment, it was realized that the use of LES turbulence model for accurate modeling of such complex case is necessary. For simpler cases like homogenous sediment (see case in section 5.2), computational effort can decrease by choosing k-ε as the turbulence model. With the use of 96 processors of the HLRN supercomputer, each 1 minute of model run for the heterogenous streambed case took ~8 hours. With bigger domain and by including other factors like overlying air, higher run times are expected. It is therefore advised to limit model dimensions to be as small as possible, while still representative, and consider modeling options such as symmetry planes (as used in U-shaped burrow case) that can noticeably reduce computational effort.

Although many cases and aspects have been studied in this thesis, there are cases such as breakwater structure flow and aspects such as sediment transport and reactive transport that can draw the next steps of model application and development. These are explained in the next section.

6.2 Outlook

To apply the integral approach to a wider range of scenarios, modeling of wave intensity reduction through shoreline breakwater structures is recommended. This can be done by investigating wave and turbulence penetration under different hydrogeological conditions. Validation of wave and turbulence penetration can be done by comparing model results to experiments of Roche et al. (2018) and Blois et al. (2014) who investigated the depth in which turbulence can penetrate sediment with relatively large grain size. As for this case flow fluctuations are a decisive factor, transient flow conditions (unlike what was assumed in the previous studies) can be applied. The integral solver is currently embedded in OpenFOAM 2.4.0 version. A wider and more efficient range of libraries, boundary conditions and tools are available in the newer versions of OpenFOAM which can be very useful in modeling wave impact on breakwater structures. The integral solver has been recently validated which opens up the potential to use the extended libraries and boundary conditions of the newest OpenFOAM version.
Using integral solver in section 2 and under assumption of no bedform movement, a small area of very high Reynolds number has been detected. Depending on sediment coherency, at a certain Reynolds number in the sediment (under increasing surface water flow velocities), bedform can presumably move. For sandy sediment, it is very beneficial to use the integral solver to **realize the maximum Reynolds numbers where sediment transport starts**. This can be done by sediment characteristics sensitivity analysis and modeling sediment transport experiment setups. As long as the realized maximum Reynolds numbers are exceeded for a cell in the model, sediment transport equations can be applied to them. As a basis “SedFoam” (Chauchat et al. 2017) can be used to include sediment transport processes into the integral solver.

To this date, advective-diffusive tracer propagation for heterogenous sediment and under ambient groundwater condition has been verified and validated for the integral solver. The next step in developing the solver is to include and validate it for advective-diffusive-dispersive transport. In Appendix A, the solver is mathematically verified for 2D advective-diffusive-dispersive transport next to analytical solutions of Kinzelbach (1992). For validation, a comparison to experiments which include dispersion into their transport investigations is recommended. Thereafter, reactive components of transport across groundwater-surface water interface like phosphorus, nitrogen, dissolved oxygen and organic carbon can be included. As a basis “BioChemFOAM” (Hernandez Murcia 2014) can be used to include reactive transport processes into the integral solver.

Further development and validation of the integral solver through using experimental results via **collaborative research in the 3rd cohort of UWI** is strongly advised. A detailed model of flow and transport processes benefits field and laboratory experiment by providing indication of flow rates and pathways which are crucial in determining biogeochemical processes.
Appendix A: Validation of porousInter for dispersive transport

This study was partly presented in Groundwater Quality 2019 conference as:


This is the extended version of the presented study.

The study in section 4 as well as Broecker et al. (2021) who have modeled transport of tracer through homogenous sediment, have both neglected dispersion. In addition, validation in section 6 as well as in Broecker et al. (2021) has been done by using a 1D analytical solution. Here, by implementing the general balance equation for transport of tracer with initial concentration of “C” into the porousInter solver, we validate the solver for a 2D dispersive tracer by a comparison to 2D analytical solutions of Kinzelbach (1992) for further use in future cases. The general balance equation is written as follows:

$$\frac{\partial (\varphi \rho_w C)}{\partial t} + \nabla \cdot [v C - \varphi D_{hyd} \nabla (\rho_w C)] = q_C$$

Eq. (A-1)

Where $\rho_w$ [kg/m$^3$] is density of water, $q_C$ [kg/(m$^3$s)] is sink or source of concentration and $D_{hyd}$ [m$^2$/s] is the hydrodynamical dispersion tensor and is written as follows:

$$D_{hyd} = D_{mot} + D_{mech} = D_{mot} \mathbb{I} + D_{mech} = \begin{bmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{bmatrix}$$

Eq. (A-2)

$D_{mech}$[m$^2$/s] is mechanical dispersion tensor and $\mathbb{I}$ is the unit tensor. The components of the dispersion tensor on the right side of Eq. (A-2) are written as follows:

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_T \frac{v_x v_y}{|v|} + D_{mot}$$

$$D_{yy} = \alpha_T \frac{v_y^2}{|v|} + \alpha_L \frac{v_y v_x}{|v|} + D_{mot}$$

Eq. (A-3)

$$D_{xy} = \frac{D_{yx}}{\alpha_T} (\alpha_L - \alpha_T \frac{v_x v_y}{|v|})$$
Appendix A: Validation of porousInter for dispersive transport

In Eq. (A-3) $\alpha_L$ [m] is longitudinal and $\alpha_T$ [m] is transversal dispersion length. These two parameters are defined using $D_L$ [m$^2$/s] (longitudinal dispersion coefficient) and $D_T$ [m$^2$/s] (transversal dispersion coefficient):

$$\alpha_L = \frac{D_L}{v}, \quad \alpha_T = \frac{D_T}{v}$$

Eq. (A-4)

Figure A-1: Model domain of 2D dispersive transport validation. Small red square centered at $x = 1$ m and $y = 5$ m shows the location of initial pulse injection with $C = 1$ mg/l. Flow is 1D in x-direction.

Figure A-2: Model of dispersive pulse tracer transport progression using porousInter after 1 s, 50 s and 100 s.
Appendix A: Validation of porousInter for dispersive transport

A two-dimensional 10×10 m² domain which is filled with a sediment with porosity of 0.3 is shown in Figure A-1. A tracer with diffusion coefficient of 10⁻⁹ m²/s, longitudinal dispersion length of 0.3 m and transversal dispersion length of 0.03 m is injected over the area of 1 m ≤ x ≤ 1.1 m and 4.95 m ≤ y ≤ 5.05 m. We display the simulated tracer propagation after 1, 50 and 100 s in Fig. A-2. As the tracer progresses forward with the flow, dispersion results in the extension of the affected area. Higher longitudinal than transversal dispersion results in wider tracer propagation in the x direction. For each timestep, in Fig. A-3, we compare the simulation results (left) to the analytical solutions (right).

Figure A-3: Simulated (left) and analytical (right) tracer concentrations after 1, 50 and 100 s over the model domain. Tracer concentration is displayed in the vertical axis.
Furthermore, we calculate the correlation between the simulated and analytical tracer propagations by looking at the tracer concentrations across several cross sections (Fig. A-3). These cross sections are highlighted with the dotted red lines in Fig. A-3. For all three timesteps, cross-sections are located at $y = 5\, \text{m}$. Perpendicular to these cross sections, for $t = 1\, \text{s}$, 50 s and 100 s respectively, cross-sections are located at $x = 1\, \text{m}$, 6 m and 10 m. Both cross sections intercept at the maximum tracer concentration in each timestep.

![Graphs showing simulated and analytical tracer propagations at different times and locations](image)

Figure A-4: Comparison of the simulated and analytical tracer propagation after 1, 50 and 100 s for cross sections in $x$ and $y$ directions. These cross-sections are highlighted as red dotted lines in Fig. A-3.

In Fig. A-4, we used root mean squared error (RMSE) and normalized-root mean squared error (N-RMSE) as correlation variables to verify the likeness of our simulations to the Kinzelbach (1992) analytical solutions. Both variable values are very low (RMSE $\ll$ tracer concentration ranges; N-RMSE $\ll 1$) for all the cross-sections confirming a very good agreement between the simulations and analytical solutions. Therefore, the extended mathematical code of the integral approach is affirmed to be capable of plausibly simulating the dispersion of a tracer in the porous medium.
Appendix B: Test case overview

### B1 Seepage through a dike modeled with porousInter and PCSiWaPro®

Table B 1: Model setup for test case B1 (seepage through a dike modeled with porousInter and PCSiWaPro®)

<table>
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</tr>
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<td>Broecker et al. (2019), Sobhi Gollo et al. (2022a)</td>
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<td></td>
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**Domain discretization**

| Dimensions                  | 1*) two-dimensional (length: 120 m/1.2 m, height: 25 m/2.5 m), 2*) two-dimensional (length: 8.7 m, height: 2.2 m) |
| Mesh generator              | 1) blockMesh, 2) PCSiWaPro mesh generator                            |
| Number of cells             | 1) 75000, rectangular, 2) 27728, triangular                          |

**Turbulence model**

| 1) laminar, 2) -            |                                                                      |

**Hydrodynamic simulations**

| Solver                      | 1) porousInter, 2) PCSiWaPro® (Richards equations)                   |
| Time step                   | 1) variable, 2) min: 0.0001 s, max: 1 s                             |
| Simulation time             | 1) 9000 s, 2) 3 h                                                   |

**Transport simulations**

| Not performed               |                                                                      |

*1 = porousInter, 2 = PCSiWaPro®
Table B 2: Boundary conditions for test case B1 - porousInter

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<th>p_rgh (kg/(ms²))</th>
<th>U (m/s)</th>
<th>effPackingRadius (m)</th>
<th>porosity (-)</th>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>value: uniform 0</td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>outlet</strong></td>
<td>zeroGradient</td>
<td>totalPressure</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td>p0: uniform 0</td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>atmosphere</strong></td>
<td>inletOutlet</td>
<td>totalPressure</td>
<td>pressureInletOutletVelocity</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td>inletValue: uniform 0</td>
<td>p0: uniform 0</td>
<td>value: uniform 0</td>
<td>(0 0 0)</td>
<td>zeroGradient</td>
</tr>
<tr>
<td><strong>ground</strong></td>
<td>zeroGradient</td>
<td>fixedFluxPressure</td>
<td>fixedValue</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td>value uniform 0</td>
<td>value: uniform (0 0 0)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>sidewalls</strong></td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
</tr>
<tr>
<td><strong>initial conditions</strong></td>
<td>uniform 0</td>
<td>define initial water level of 19 m/1.9 m the first 100 m/10 m using boxToCell in setFields (volScalarFieldValue alpha.water 1)</td>
<td>uniform (0 0 0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>uniform 0</td>
<td>define initial water level of 19 m/1.9 m the first 100 m/10 m using boxToCell in setFields (volScalarFieldValue p_rgh 186390/18639)</td>
<td>uniform (0 0 0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>uniform 0.0159/0.002</td>
<td></td>
<td>uniform 0.0159/0.002</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>uniform 1</td>
<td>in the sediment 0.25 defined by setFields</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table B 3: Boundary conditions for test case B1 – PCSiWaPro®.

<table>
<thead>
<tr>
<th></th>
<th>Linear pressure head distribution to account for constant water level of 1.9 m</th>
</tr>
</thead>
<tbody>
<tr>
<td>left</td>
<td>Free drainage</td>
</tr>
<tr>
<td>right</td>
<td>Free drainage</td>
</tr>
<tr>
<td>top</td>
<td>Free drainage</td>
</tr>
<tr>
<td>bottom</td>
<td>No flow</td>
</tr>
<tr>
<td>initial conditions</td>
<td>Dam fully saturated (water content = 0.25), material: DIN 4220 pure sand, porosity is manually set to 0.25</td>
</tr>
</tbody>
</table>
Appendix B: Test case overview

B2 Seepage through a rectangular dam modeled with porousInter and PCSiWaPro®

Table B 4: Model setup for test case B2 (Seepage through a rectangular dam modeled with porousInter and PCSiWaPro®).

<table>
<thead>
<tr>
<th>General</th>
<th>2.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Published in</td>
<td>Broecker et al. (2019), Sobhi Gollo et al. (2022a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th>1*) two-dimensional (length: 250 m, height: 48 m), 2*) two-dimensional (length: 16 m, height: 24 m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh generator</td>
<td>1) blockMesh, 2) PCSiWaPro mesh generator</td>
</tr>
<tr>
<td>Number of cells</td>
<td>1) 191744, 2) 14266</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Turbulence model</th>
<th>1) laminar, 2) -</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th>1) porousInter, 2) PCSiWaPro® (Richards equations)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>1) variable, 2) min: 0.0001 s, max: 1 s</td>
</tr>
<tr>
<td>Time step</td>
<td>1) 9000 s, 2) 3 h</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transport simulations</th>
<th>Not performed</th>
</tr>
</thead>
</table>

*1 = porousInter, 2 = PCSiWaPro®
<table>
<thead>
<tr>
<th>Section</th>
<th>Boundary Conditions</th>
</tr>
</thead>
</table>
| **inlet_water** | inletOutlet  
value: uniform 1  
value: uniform 1 |
| **inlet_air** | inletOutlet  
value: uniform 0  
value: uniform 0 |
| **outlet** | zeroGradient |
| **atmosphere** | inletOutlet  
value: uniform 0  
value: uniform 0 |
| **ground** | zeroGradient  
value: uniform 0 |
| **sidewalls** | empty |
| **initial conditions** | uniform 0  
define initial water level of 24 m at the left side of the dam, to 4 m at the right side and stepwise from 24 to 4 m inside the dam using boxToCell in setFields (volScalarFieldValue alpha.water 1) |

**Table B 5: Boundary conditions for test case B2 - porousInter**

<table>
<thead>
<tr>
<th>Section</th>
<th>Boundary Conditions</th>
</tr>
</thead>
</table>
| **inlet_water** | inletOutlet  
value: uniform 1  
value: uniform 1 |
| **inlet_air** | inletOutlet  
value: uniform 0  
value: uniform 0 |
| **outlet** | zeroGradient |
| **atmosphere** | inletOutlet  
value: uniform 0  
value: uniform 0 |
| **ground** | zeroGradient  
value: uniform 0 |
| **sidewalls** | empty |
| **initial conditions** | uniform 0  
define initial water level of 24 m at the left side of the dam, to 4 m at the right side and stepwise from 24 to 4 m inside the dam using boxToCell in setFields (volScalarFieldValue alpha.water 1) |
### Table B 6: Boundary conditions for test case B2 – PCSiWaPro®

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>left</td>
<td>Linear pressure head distribution to account for constant water level of 24 m</td>
</tr>
<tr>
<td>right</td>
<td>Linear pressure head distribution to account for constant water level of 4 m</td>
</tr>
<tr>
<td>top</td>
<td>Free drainage</td>
</tr>
<tr>
<td>bottom</td>
<td>No flow</td>
</tr>
<tr>
<td>initial conditions</td>
<td>Dam fully saturated (water content = 0.25), material: DIN 4220 pure sand, porosity is manually set to 0.25</td>
</tr>
</tbody>
</table>
Appendix B: Test case overview

B3 One-dimensional one-phase modeling of surface water flow over rippled streambed with hms (shallow water equations)

Table B 7: Model setup for test case B3 (surface water flow over ripples using hms)

<table>
<thead>
<tr>
<th>General</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>2.3.5</td>
<td></td>
</tr>
<tr>
<td>References</td>
<td>Broecker et al. (2019)</td>
<td></td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2022a)</td>
<td></td>
</tr>
<tr>
<td>Domain discretization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dimensions</td>
<td>one-dimensional (length: 15 m)</td>
<td></td>
</tr>
<tr>
<td>Mesh generator</td>
<td>hms</td>
<td></td>
</tr>
<tr>
<td>Number of cells</td>
<td>1500</td>
<td></td>
</tr>
<tr>
<td>Turbulence model</td>
<td>laminar</td>
<td></td>
</tr>
<tr>
<td>Hydrodynamic simulations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solver</td>
<td>hms (shallow water equations)</td>
<td></td>
</tr>
<tr>
<td>Time step</td>
<td>forward_Euler, 10 s (max)</td>
<td></td>
</tr>
<tr>
<td>Simulation time</td>
<td>1200 s</td>
<td></td>
</tr>
<tr>
<td>Transport simulations</td>
<td>Not performed</td>
<td></td>
</tr>
</tbody>
</table>

Table B 8: Boundary conditions for test case B3 – PCSiWaPro®.

| Inlet (left) | HSurfaceFlowOrthogonalUnitDischargeValues: Volumetric inflow rate: 0.5 m³/s | |
| Outlet (right) | HSurfaceFlowFreeOutflowValues: free outflow | |
| bottom | HSurfaceFlowNoFlowValues: No flow | |
| initial conditions | 0.5 m water table for the entire domain, Manning coefficient: 0.03 s/m³/³ to account for clean and straight natural streams | |
Appendix B: Test case overview

B4 Three-dimensional two-phase modeling of surface water flow over rippled streambed with interFoam

Table B 9: Model setup for test case B4 (surface water flow over ripples using interFoam)

<table>
<thead>
<tr>
<th>General</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>2.3.5</td>
</tr>
<tr>
<td>References</td>
<td>Broecker et al. (2019)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2022a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>three-dimensional (length: 15 m, height: 1 m, depth: 1 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>gmsh</td>
</tr>
<tr>
<td>Number of cells</td>
<td>1160900</td>
</tr>
</tbody>
</table>

| Turbulence model         | LES              |

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>interFoam</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>60 s</td>
</tr>
</tbody>
</table>

| Transport simulations    | Not performed    |
Table B 10: Boundary conditions for test case B4

<table>
<thead>
<tr>
<th></th>
<th>alpha.water [-]</th>
<th>p_rgh [kg/(ms²)]</th>
<th>U [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>inlet_water</td>
<td>inletOutlet</td>
<td>fixedFluxPressure</td>
<td>flowRateInletVelocity</td>
</tr>
<tr>
<td></td>
<td>inletValue: uniform 1</td>
<td>value: uniform 0</td>
<td>volumetricFlowRate 0.5 [m³/s]</td>
</tr>
<tr>
<td></td>
<td>value: uniform 1</td>
<td>value: uniform 0</td>
<td>value: uniform (0 0 0)</td>
</tr>
<tr>
<td>inlet_air</td>
<td>inletOutlet</td>
<td>totalPressure</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td>inletValue: uniform 0</td>
<td>p0: uniform 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>value: uniform 0</td>
<td>value: uniform 0</td>
<td></td>
</tr>
<tr>
<td>outlet</td>
<td>zeroGradient</td>
<td>totalPressure</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td></td>
<td>p0: uniform 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
</tr>
<tr>
<td>atmosphere</td>
<td>inletOutlet</td>
<td>totalPressure</td>
<td>pressureInletOutletVelocity</td>
</tr>
<tr>
<td></td>
<td>inletValue: uniform 0</td>
<td>p0: uniform 0</td>
<td>value: uniform (0 0 0)</td>
</tr>
<tr>
<td></td>
<td>value: uniform 0</td>
<td>value: uniform 0</td>
<td></td>
</tr>
<tr>
<td>walls</td>
<td>zeroGradient</td>
<td>fixedFluxPressure</td>
<td>fixedValue</td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td>value: uniform (0 0 0)</td>
</tr>
<tr>
<td>initial conditions</td>
<td>uniform 0</td>
<td>uniform 0</td>
<td>uniform (0 0 0)</td>
</tr>
<tr>
<td></td>
<td>define initial water level of 0.5 m</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>using boxToCell in setFields (volScalarFieldValue alpha.water 1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix B: Test case overview

**B5 Two-dimensional modeling of groundwater flow in sediment under rippled streambed with PCSiWaPro®**

Table B 11: Model setup for test case B5 (surface water flow over ripples using PCSiWaPro®)

<table>
<thead>
<tr>
<th>General</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>2.3.5</td>
</tr>
<tr>
<td>References</td>
<td>Broecker et al. (2019) (for ripple geometry)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2022a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>two-dimensional (length: 7 m, height: 0.556 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>PCSiWaPro mesh generator</td>
</tr>
<tr>
<td>Number of cells</td>
<td>15524</td>
</tr>
</tbody>
</table>

| Turbulence model | - |
| Hydrodynamic simulations | - |
| Solver | PCSiWaPro® (Richards equations) |
| Time step | min: 0.0001 s, max: 1 s |
| Simulation time | steady state |

| Transport simulations | Not performed |

Table B 12: Boundary conditions for test case B5

<table>
<thead>
<tr>
<th>left</th>
<th>Linear pressure head distribution to account for constant water level of 0.495 m over the top node</th>
</tr>
</thead>
<tbody>
<tr>
<td>right</td>
<td>Linear pressure head distribution to account for constant water level of 0.487 m over the top node</td>
</tr>
<tr>
<td>top</td>
<td>Pressure head distribution from bottom wall modeling results of case B4 – applied node to node</td>
</tr>
<tr>
<td>bottom</td>
<td>No flow</td>
</tr>
<tr>
<td>initial conditions</td>
<td>Domain fully saturated (water content = 0.25), material: DIN 4220 pure sand, porosity is manually set to 0.25, hydraulic conductivity is set to $4.64 \times 10^{-3}$ m/s</td>
</tr>
</tbody>
</table>
# Appendix B: Test case overview

## B6 Three-dimensional two-phase integral modeling of flow across rippled streambed with porousInter

Table B 13: Model setup for test case B 6 (Integral modeling of groundwater-surface water interactions across rippled streambeds using porousInter)

<table>
<thead>
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</tr>
</thead>
<tbody>
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<td>2.3.5</td>
</tr>
<tr>
<td>References</td>
<td>Broecker et al. (2019)</td>
</tr>
<tr>
<td>Published in</td>
<td>Broecker et al. (2019), Sobhi Gollo et al. (2022a)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>three-dimensional (length: 15 m, height: 1.5 m (max), depth: 1 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>gmsh</td>
</tr>
<tr>
<td>Number of cells</td>
<td>1806450</td>
</tr>
</tbody>
</table>

| Turbulence model         | LES             |

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInter</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>300 s</td>
</tr>
</tbody>
</table>

| Transport simulations    | Not performed    |
### Table B 14: Boundary conditions for test case B6

<table>
<thead>
<tr>
<th></th>
<th>alpha.water [-]</th>
<th>p_rgh [kg/(ms²)]</th>
<th>U [m/s]</th>
<th>effPackingRadius [m]</th>
<th>Porosity [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>inlet_water</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>inlet_value</td>
<td>inletOutlet</td>
<td>fixedFluxPressure</td>
<td></td>
<td>flowRateInletVelocity</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td>volumetricFlowRate 0.5 m³/s</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td>value: uniform (1 0 0)/(0.5 0 0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>fixedFluxPressure</td>
<td></td>
<td>zeroGradient</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td>zeroGradient</td>
<td></td>
</tr>
<tr>
<td>inlet_air</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>inlet_value</td>
<td>inletOutlet</td>
<td>totalPressure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>p0: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>fixedFluxPressure</td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
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<td></td>
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</tr>
<tr>
<td>outlet</td>
<td>zeroGradient</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>totalPressure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>p0: uniform 0</td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>atmosphere</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>inlet_value</td>
<td>inletOutlet</td>
<td>totalPressure</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>p0: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>pressureInletOutletVelocity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform (0 0 0)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>walls</td>
<td>zeroGradient</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>fixedFluxPressure</td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
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<td></td>
</tr>
<tr>
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<td>fixedValue</td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>value uniform (0 0 0)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>side</td>
<td>slip</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>slip</td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td></td>
<td>slip</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>slip</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>initial</td>
<td>uniform 0</td>
<td></td>
<td></td>
<td>uniform 0</td>
<td></td>
</tr>
<tr>
<td>conditions</td>
<td></td>
<td>define initial water level from x = 0 m to x = 12 m and y = -0.5 m to 0.5 m and z = 0 m to z = 1 m using boxToCell in setFields (volScalarFieldValue alpha.water 1)</td>
<td>uniform 0</td>
<td>uniform 0.002</td>
<td>uniform 1 in the sediment 0.25 defined by setFields</td>
</tr>
</tbody>
</table>
Appendix B: Test case overview

B7 Three-dimensional flow simulation in and around a ventilated U-shaped burrow using porousInter – case 1

Table B.15: Model setup for test case B7 (Integral modeling of U-shaped burrow ventilation using porousInter - case 1)

<table>
<thead>
<tr>
<th>General</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>3.3.1</td>
</tr>
<tr>
<td>References</td>
<td>Brand et al. (2013)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2021)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>three-dimensional (half-cylinder: height: 0.25 m, radius: 0.25 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>Salome 9.3.0</td>
</tr>
<tr>
<td>Number of cells</td>
<td>450399</td>
</tr>
</tbody>
</table>

| Turbulence model | laminar |

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInter</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>100 s</td>
</tr>
</tbody>
</table>

| Transport simulations | Not performed |
### Table B.16: Boundary conditions for test case B7

<table>
<thead>
<tr>
<th></th>
<th>porosity [-]</th>
<th>e/packingRadius [m]</th>
<th>p_rgh [kg/(ms²)]</th>
<th>U [m/s]</th>
<th>( \alpha_{\text{water}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>top</strong></td>
<td>zeroGradient</td>
<td>symmetryPlane</td>
<td>fixedValue</td>
<td>uniform 0</td>
<td>uniform 0</td>
</tr>
<tr>
<td><strong>Walls</strong></td>
<td>zeroGradient</td>
<td>symmetryPlane</td>
<td>fixedValue</td>
<td>(0 0 0)</td>
<td>(0 0 0)</td>
</tr>
<tr>
<td><strong>baffle</strong></td>
<td>zeroGradient</td>
<td>fixedFluxPressureGradient: uniform 0</td>
<td>fixedValue</td>
<td>uniform (0.005 0 0) up to (0.025 0 0)</td>
<td></td>
</tr>
<tr>
<td><strong>initial conditions</strong></td>
<td>uniform 0</td>
<td>uniform 1</td>
<td>uniform 0</td>
<td>uniform 0</td>
<td>uniform 0.000125 to 0.00025</td>
</tr>
</tbody>
</table>

Defined 1 for U-shaped burrow and SurfaceToCell in setFields

Defined 0.000125 to 0.00025 in the sediment 0.39 using SurfaceToCell in setFields
B8 Three-dimensional flow simulation in and around a ventilated U-shaped burrow using porousInter – case 2

Table B 17: Model setup for test case B8 (Integral modeling of U-shaped burrow ventilation using porousInter - case 2)

<table>
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<tr>
<th>General</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>3.4.2</td>
</tr>
<tr>
<td>References</td>
<td>Morad et al. (2010), Roskosch et al. (2010)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2021)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>three-dimensional (half-cylinder: height: 1.1 m, radius: 1 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>Salome 9.3.0</td>
</tr>
<tr>
<td>Number of cells</td>
<td>399531</td>
</tr>
</tbody>
</table>

| Turbulence model      | laminar                  |

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInter</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>40 s</td>
</tr>
</tbody>
</table>

<p>| Transport simulations   | Not performed            |</p>
<table>
<thead>
<tr>
<th>Condition</th>
<th>Boundary Condition</th>
<th>Total Pressure</th>
<th>Pressure Inlet/Outlet Velocity</th>
<th>Effective Packing Radius</th>
<th>Porosity [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>top</td>
<td>slip</td>
<td>p0: uniform 0</td>
<td>value: uniform 0</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>symmetry</td>
<td>symmetryPlane</td>
<td>symmetryPlane</td>
<td>symmetryPlane</td>
<td>symmetryPlane</td>
<td>symmetryPlane</td>
</tr>
<tr>
<td>Walls (including bottom)</td>
<td>zeroGradient</td>
<td>fixedFluxPressure gradient: uniform 0</td>
<td>fixedValue</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>baffle</td>
<td>fixedValue</td>
<td>fixedFluxPressure gradient: uniform 0</td>
<td>fixedValue</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>initial conditions</td>
<td>uniform 1</td>
<td>uniform 0</td>
<td>uniform (0 0 0)</td>
<td>uniform 0.00025</td>
<td>Defined 1 for U-shaped burrow and overlying water, in the sediment 0.39 using SurfaceToCell in setFields</td>
</tr>
</tbody>
</table>
**Appendix B: Test case overview**

**B9 One-dimensional tracer transport in heterogeneous groundwater with porousInterTracer**

Table B 19: Model setup for test case B9 (One-dimensional tracer transport in groundwater with two porosities)

<table>
<thead>
<tr>
<th>General</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>4.4.1</td>
</tr>
<tr>
<td>References</td>
<td>Kinzelbach (1992)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi et al. (2022b)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>one-dimensional (length: 10 m, width: 1 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>blockMesh</td>
</tr>
<tr>
<td>Number of cells</td>
<td>10000</td>
</tr>
</tbody>
</table>

| Turbulence model                     | laminar       |

| Hydrodynamic simulations             | Not performed |

<table>
<thead>
<tr>
<th>Transport simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInterTracer</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>700 s</td>
</tr>
<tr>
<td>Tracer diffusivity</td>
<td>$10^{-9}$ m$^2$/s</td>
</tr>
</tbody>
</table>
Table B 20: Boundary conditions for test case B9.

<table>
<thead>
<tr>
<th></th>
<th>alpha.water (-)</th>
<th>p_rgh (kg/(ms²))</th>
<th>U (m/s)</th>
<th>C (kg/m³)</th>
<th>effPackingRadius (m)</th>
<th>porosity (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>inlet</td>
<td>inletOutlet</td>
<td>zeroGradient</td>
<td>FIXED</td>
<td>FIXED</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td>inletValue:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>uniform 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>value: uniform 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>outlet</td>
<td>zeroGradient</td>
<td>fixedValue</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td></td>
<td>zeroGradient</td>
</tr>
<tr>
<td></td>
<td></td>
<td>value: uniform 0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Upper,</td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
<td>empty</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>lower and</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>sidewalls</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>initial</td>
<td>uniform 1</td>
<td>uniform 0</td>
<td>uniform 0</td>
<td>uniform 01</td>
<td></td>
<td></td>
</tr>
<tr>
<td>conditions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Define sediment porosity 0.44 from x = 0 m to x = 5 m and 0.33 for x = 5 m to x = 10 m through y = 0 m to 1 m and z = 0 m to z = 1 m using boxToCell in setFields (volScalarFieldValue)
### B10 Transport simulations for groundwater-surface water interactions at heterogenous rippled streambeds

Table B 21: Model setup for test case B10 (Transport simulations for groundwater-surface water interactions at heterogenous rippled streambeds).

<table>
<thead>
<tr>
<th>General</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Referred to in section</td>
<td>4.3.1, 4.3.2</td>
</tr>
<tr>
<td>References</td>
<td>Fox et al. (2016)</td>
</tr>
<tr>
<td>Published in</td>
<td>Sobhi Gollo et al. (2022b)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Domain discretization</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions</td>
<td>three-dimensional (length: 2.375 m, height: 0.29 m, width: 0.29 m)</td>
</tr>
<tr>
<td>Mesh generator</td>
<td>gmsh</td>
</tr>
<tr>
<td>Number of cells</td>
<td>hexahedra: 17110, prisms: 55014</td>
</tr>
</tbody>
</table>

| Turbulence model      | LES              |

<table>
<thead>
<tr>
<th>Hydrodynamic simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInterTracer</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>300 + 3600 s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transport simulations</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solver</td>
<td>porousInterTracer</td>
</tr>
<tr>
<td>Time step</td>
<td>variable</td>
</tr>
<tr>
<td>Simulation time</td>
<td>3600 s</td>
</tr>
<tr>
<td>Tracer diffusivity</td>
<td>$10^{-9}$ m²/s</td>
</tr>
</tbody>
</table>
Table B 22: Boundary conditions for test case B10.

<table>
<thead>
<tr>
<th></th>
<th>alpha.water (-)</th>
<th>p_rgh (kg/(ms²))</th>
<th>U (m/s)</th>
<th>C (kg/m³)</th>
<th>effPackingRadius (m)</th>
<th>porosity (-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>inlet</td>
<td>fixedValue value: uniform 1</td>
<td>zeroGradient</td>
<td>flowRateInletVelocity volumetricFlowRate 0.003045 value: uniform (0.0362069 0 0)</td>
<td>inletOutlet inletValue: uniform 1 value: uniform 1</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>outlet</td>
<td>inletOutlet inletValue: uniform 1 value: uniform 1</td>
<td>fixedValue value: uniform 0</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>atmosphere</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
<td>uniform (0 0 0)</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>lower walls</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>fixedValue value: uniform (0 0 0)</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
<td>zeroGradient</td>
</tr>
<tr>
<td>sidewalls</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
<td>slip</td>
</tr>
</tbody>
</table>
### Appendix B: Test case overview

<table>
<thead>
<tr>
<th>groundwater inflow (for gaining and losing conditions)</th>
<th>fixedValue value: uniform 1</th>
<th>fixedFluxPressure</th>
<th>flowRateInletVelocity volumetricFlowRate $\pm 4.85 \times 10^{-6} \text{m}^3/\text{s}$ value: uniform $(0 \pm 1.15738 \times 10^{-5})$</th>
<th>inletOutlet inletValue: uniform 1 value: uniform 1</th>
<th>zeroGradient</th>
<th>zeroGradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>initial conditions</td>
<td>uniform 1</td>
<td>uniform 0</td>
<td>for surface water: uniform $(0.15 \ 0 \ 0)$, for the sediment: uniform $(0 \ 0 \ 0)$ for neutral conditions, uniform $(0 \pm 1.15738 \times 10^{-5})$ for gaining and losing conditions defined by setFields</td>
<td>uniform 0</td>
<td>nonuniform, in the sediment, a combination of $0.00038$, $0.0013$ and $0.0023$ defined by setFields (surfaceTo Cell)</td>
<td>uniform 1, in the sediment, a combination of $0.33$ and $0.44$ uniform $0.33$ defined by setFields (surfaceTo Cell)</td>
</tr>
</tbody>
</table>
Bibliography


Darwin, C. 1881. The formation of vegetable mould through the action of worms with observation of their habits. *John Murray*.


Bibliography


Bibliography


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