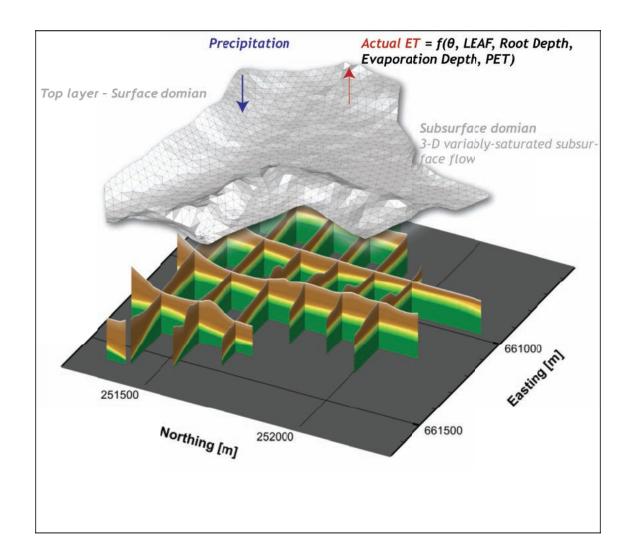
## 3<sup>rd</sup> International

## HydroGeoSphere User Conference 2013



 ${
m April} \ 3^{
m rd} - 5^{
m th}, \ 2013$  CHYN, University of Neuchâtel

Switzerland

https://www2.unine.ch/HGS-NEUCH2013

Program with Abstracts

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#### 1 Welcome

Dear HydroGeoSphere Users,

Building upon the success of the first and second HydroGeoSphere meeting in Liège and Hannover, the third HydroGeoSphere meeting is held at the University of Neuchâtel (Switzerland) from the  $3^{\rm rd}$  –  $5^{\rm th}$  of April 2013.

The objectives of the meeting are similar to those in previous years:

- Meet with the HGS developers, and get informed on the latest changes and future directions
- Present research activities related to HydroGeoSphere
- Exchange ideas and coordinate future research
- Increase the communication between users and developers strengthen the HGS community

For questions please contact:

Prof. Philip Brunner

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Phone: +41 32 718 26 74

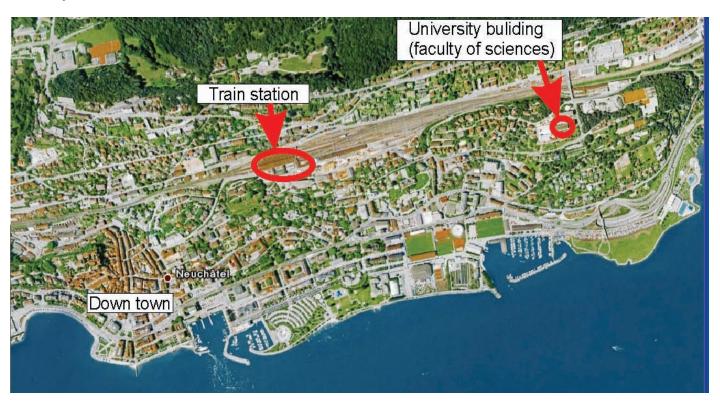
Fax:  $+41\ 32\ 718\ 26\ 03$ 

 $Conference\ email:\ HGS.Conf@unine.ch$ 

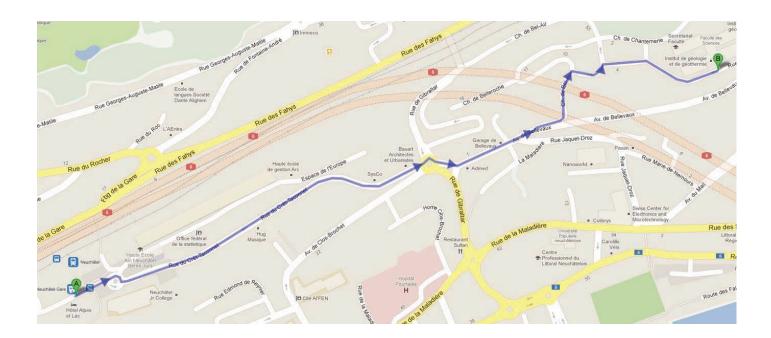


#### 2 Conference Venue

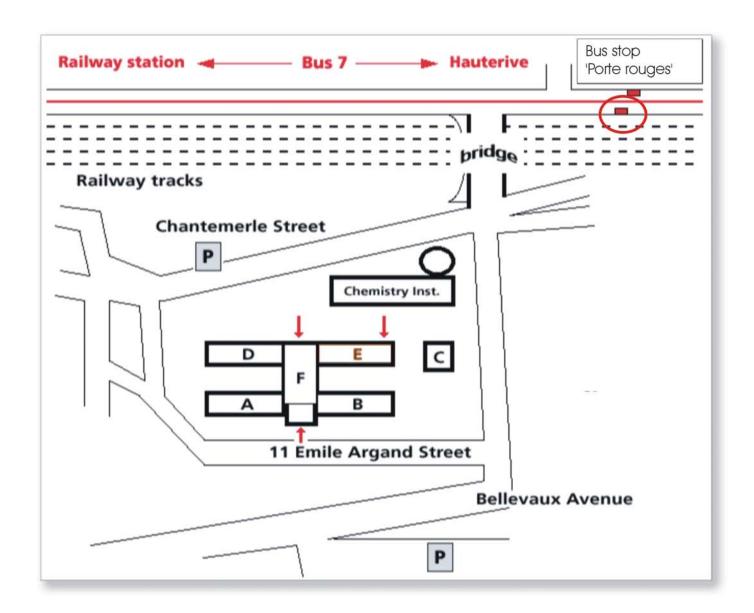
This years conference will be held in the city of Neuchâtel, located on a hillside overlooking lake Neuchâtel and the Swiss mountain panorama. The conference will be hosted by the Centre for Hydrogeology and Geothermics (CHYN) of the University of Neuchâtel.



You can walk in 20 min from the Neuchâtel train station (A) to the venue (B) at Rue Emile-Argand 11:



The conference takes place in the Aula of the UniMail building. The Aula is in Building F, basement level. You can enter building as indicated by the red arrows.

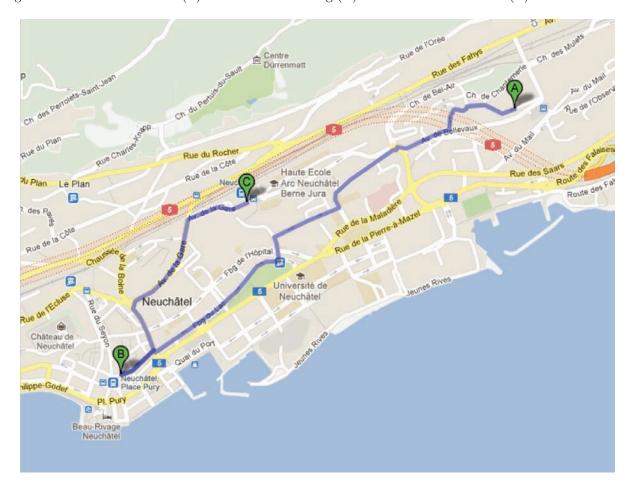


#### 3 Conference Dinner

The conference dinner (Wednesday, 18:30), takes place in the Brasserie du Jura, at Rue de la Treille 7 in the historic part of Neuchâtel.



How to get to the Brasserie Le Jura (B) from the Uni building (A) or from the train station (C):



#### 4 Keynote Talks

We are happy to welcome four keynote speakers at HGS 2013:

A. Dassargues Université Liège, Belgium

Hydrogeosphere and progresses in groundwater modelling: thinking and examples of

 ${\it case studies}$ 

Wednesday,  $9{:}30$  -  $10{:}00$ 

W. Kinzelbach ETH Zürich, Switzerland

To be announced

Wednesday, 13:30 - 14:00

Y.-J. Park Aquanty Inc., Waterloo

Development and Enhancement of the HydroGeoSphere Model: Urban infrastructure,

winter hydrological processes, new surface water flow equations, and more

Thursday, 9:00 - 9:30

E. Sudicky University of Waterloo, Canada

Impact of climate change on surface and groundwater resources over the Canadian

landmass

Friday, 15:15 - 16:00

## 5 Technical Program

| Wednesday | $\mathbf{A.M.}$ | Chair: Philip Brunner | r |
|-----------|-----------------|-----------------------|---|
|-----------|-----------------|-----------------------|---|

| 8:00 - 8:50   | G. Gianni, P. Brunner | Arrival and badge pick-up   |
|---------------|-----------------------|---|
| 8:50 - 9:00   | Philip Brunner        | Welcome of participants   |
| 9:00 - 9:30   | Ed Sudicky            | About Aquanty, HGS and the Future.                                      |
| 9:30 - 10:00  | Alain Dassargues      | Hydrogeosphere and progresses in groundwater modelling: thinking and    |
|               |                       | examples of case studies.*  |
| 10:00 - 10:30 | Coffee break          |   |
| 10:30 - 10:50 | Matthias Munz         | Modelling spatial and temporal variability of surface water-groundwater |
|               |                       | fluxes and heat exchange along a lowland river reach.                   |
| 10:50 - 11:10 | Alicia Sanz-Prat      | Modeling of exchange processes between river and hyporheic zone.        |
| 11:10 - 11:30 | Jie Yang              | Investigating tide and storm surge effects on coastal aquifers using a  |
|               |                       | three-dimensional coupled surface-subsurface approach.                  |
| 11:30 - 11:50 | Samuel Wildemeersch   | Analysis of the influence of grid resolution on discharge and hydraulic |
|               |                       | head simulation using a synthetic catchment.                            |
| 11:50 - 13:30 | Lunch break           |   |

## Wednesday P.M. Chair: Thomas Graf

| 13:30 - 14:00 | Wolfgang Kinzelbach      | To be announced*   |
|---------------|--------------------------|--|
| 14:00 - 14:20 | Jan Fleckenstein         | Simulating GW-SW interactions with HGS - some examples and open      |
|               |                          | questions  |
| 14:20 - 14:40 | Dan Partington           | Quantifying in-stream and overland flow generation mechanisms using  |
|               |                          | HGS.   |
| 14:40 - 15:00 | Pertti Ala-aho           | Modeling groundwater surface water interactions in an esker aquifer. |
| 15:00 - 15:30 | Coffee break             |  |
| 15:30 - 15:50 | Maria Herold             | Groundwater resources under a changing climate - a case study from   |
|               |                          | Lower Saxony, Germany.   |
| 15:50 - 16:10 | Karim Norouzi Moghan-    | Physics-based modelling of erosion at catchment scale.               |
|               | joghi                    |  |
| 16:10 - 16:30 | Guillaume de Schepper    | Numerical modeling of a field scale tile drainage network.           |
| 16:30 - 16:50 | Andrea Brookfield        | Simulating integrated water management in the lower republican river |
|               |                          | basin, Kansas.   |
| 16:50 - 17:00 | Philip Brunner           | Some infos   |
| 18:30         | Workshop dinner, see map | provided above   |

## Thursday A.M. Chair: Jan Fleckenstein

| 9:00 - 9:30   | Yong-Jin Park     | ${\bf Development\ and\ Enhancement\ of\ the\ HydroGeoSphere\ Model:}$    |  |
|---------------|-------------------|---|--|
|               |                   | Urban infrastructure, winter hydrological processes, new sur-             |  |
|               |                   | face water flow equations, and more.*                                     |  |
| 9:30 - 9:50   | Juernjakob Dugge  | ${\it Refreshing Meshing-Generating Triangular Grids for HydroGeoSphere}$ |  |
|               |                   | in an Open-Source GIS Environment.  |  |
| 9:50 - 10:10  | Diane von Gunten  | Model grid simplification to accelerate calibration: A catchment-scale    |  |
|               |                   | case study.   |  |
| 10:10 - 10:30 | Coffee break      |   |  |
| 10:30 - 10:50 | Mehdi Ghasemizade | Catchment scale modeling of surface-subsurface interaction in a pre-      |  |
|               |                   | alpine watershed.   |  |
| 10:50 - 11:10 | Christian Moeck   | Uncertainty of groundwater recharges estimations caused by climate        |  |
|               |                   | model chain variability and model simplification                          |  |
| 11:10 - 11:30 | Thomas Hermans    | Probability perturbation method applied to the inversion of groundwater   |  |
|               |                   | flow models using HydroGeoSphere.   |  |
| 11:30 - 11:50 | Oliver Schilling  | Using tree rings in modeling the water cycle at the lower Tarim River,    |  |
|               |                   | Western China.  |  |
| 11:50 - 13:30 | Lunch break       |   |  |

## Thursday P.M. Chair: René Therrien

| 13:30 - 14:00 | Katharina Vujević   | Density-dependent flow and transport in fracture networks embedded in     |
|---------------|---------------------|---|
|               |                     | low permeability rock.  |
| 14:00 - 14:20 | Eugenia Hirthe      | Optimizing numerical simulation of fracture networks for variable-density |
|               |                     | flow  |
| 14:20 - 14:40 | Marc Walther        | Discretizing a Thermohaline Double-Diffusive Rayleigh Regime.             |
| 14:40 - 15:00 | Sascha Oswald       | Seawater intrusion for a North Sea coastal aquifer in respect to future   |
|               |                     | seawater level rise.  |
| 15:00 - 15:30 | Coffee break        |   |
| 15:30 - 15:50 | Jean Beaujean       | Using HydroGeoSphere with hydrogeological and geophysical data to         |
|               |                     | characterize seawater intrusion.  |
| 15:50 - 16:10 | Walter Illman       | Recent Progress in Hydraulic Tomography and its Potential Applications    |
|               |                     | to Surface Water-Groundwater Interaction Problems.                        |
| 16:10 - 16:30 | Anne Lausten Hansen | What controls the depth to the redox-interface? Preliminary results.      |

16:30 - 16:50 Carlos Guevara

Implementation of the Extended Oberbeck-Boussinesq Approximation for the numerical simulation of variable-density groundwater flow and solute transport in Hydrogeopshere.

#### Friday A.M. Chair: Dan Partington

| 8:30 - 9:00   | Yong-Jin Park        | Numerical secrets of HGS: An overview.*                                 |
|---------------|----------------------|---|
| 9:00 - 9:20   | Stefanie Lutz        | A HGS-based assessment of the potential use of compound specific stable |
|               |                      | isotope analysis in river monitoring of diffuse pesticide pollution.    |
| 9:20 - 9:40   | Stefan Broda         | Conceptual model suitability for reproducing preferential flow in waste |
|               |                      | rock.   |
| 09:40 - 10:10 | Coffee break         |   |
| 10:10 - 12:00 | $\operatorname{ALL}$ | Open discussion on future developments, support and the use of Hydro-   |
|               |                      | GeoSphere   |
| 12:00 - 14:00 | Lunch break          |   |

#### Friday P.M. Co-event at the University of Neuchâtel

| 14:00 - 14:25 | Torsten Braun   | Opening and introduction to the eA4-Mesh project.                     |
|---------------|-----------------|---|
| 14:25 - 14:45 | Daniel Hunkeler | The impact of the eA4-Mesh project on environmental research.         |
| 14:45 - 15:15 | Coffee break    |   |
| 15:15 - 16:00 | Ed Sudicky      | A Physically-Based Modelling Approach to Assess the Impact of Climate |
|               |                 | Change on Canadian Surface and Groundwater Resources.                 |

The talks of Torsten Braun and Daniel Hunkeler are part of the final Dissemination Event on using the wireless mesh networks in the area of Swiss higher education and research. All conference participants are invited to join the talks.

### Saturday A.M.

8:30 - 16:00 René Therrien (approx.)

The numerics of HGS. (If indicated in the registration form)

8:00 - 13:30 Pierre-Yven Jeannin

Excursion to various fascinating local hydrogeological sites, including an underground glacier. The excursion will be led by Pierre-Yven Jeannin, an international authority in Karst Hydrogeology. Helmets will be provided. Good shoes mandatory.



#### 6 Keynote Abstracts

Ed Sudicky A Physically-Based Modelling Approach to Assess the Impact of Climate Change on Canadian Surface and Groundwater Resources. Friday, April-5, 15:15-16:00 It is now generally accepted within the scientific community that the climate is changing, and that future climate change may have significant impact on water resources in both quantity and quality. Alterations of base flow to rivers due to changing subsurface flow patterns, fluctuations in the depth of the groundwater table and the water levels of lakes, and altered groundwater recharge/discharge patterns are examples of possible consequences of future climate change. Quantification of such impacts as driven by plausible climate-change scenarios is essential for policy makers. To date, there are numerous studies concerning this issue in the literature, but many are limited to a relatively small domain, usually up to a watershed or basin scale, and/or they fail to simulate the surface and subsurface flow regimes in a physically-based, fully-integrated manner. In this study, our physically-based model, Hydro-GeoSphere (HGS), is employed to simulate 2D surface water flow on the land surface together with 3D variably-saturated subsurface flow covering the entire Canadian landscape. A globally implicit scheme used to solve the nonlinear surface and subsurface flow and transport equations simultaneously. Various numerical solution and mesh resolution issues are briefly discussed in view of the large computational effort required the handle 3D continental-scale simulations, and to accommodate the highly-complex and wide-ranging terrain over the Canadian land mass. The impact of global warming on Canadian water resources is explored after calibration against historical meteorological, hydrological and hydrogeological data. In this study, we employ future climate predictions from NCAR's Community Climate System Model (CCSM) and the Canadian Regional Climate Model (CRCM) to drive the 3D HGS computations.

Wolfgang Kinzelbach To be announced Wednesday, April-3. 13:30-14:00

Alain Dassargues Hydrogeosphere and progresses in groundwater modelling: thinking and examples of case studies. Present issues about groundwater modelling are not anymore focused to the translation in equations of the different bio-chemico-physical processes to be modelled. Except for very specific cases, one can consider that most of the groundwater related processes have been described and translated in equations. However, huge issues and avenues for progresses are still remaining for an adequate (physically -consistent) modelling: conceptual choices are never perfect, stress factors are less known than often considered, parameters are still badly known, many scale issues affect the parameterisation, calibration/validation and inverse modelling objectives can be discussed, robustness, sensitivity analysis and uncertainty assessment must be improved and CPU time efficiency and parallel processing are still to be increased. One can discuss also different approaches as 'reductionism' versus 'integrationism' (Wood, 2012) when dealing with practical cases and to find an optimal compromise between simplicity and complexity (Doherty, 2011). Two or three illustrative examples will be shortly discussed addressing a) groundwater flow and heat transport in an alluvial aquifer for cooling a future office building; b) simulation of tracer test in a fractured chalk aquifer for protection zones delination; c) integrated modelling at regional scale for assessing impact of climate changes. Wednesday, April-3, 9:30-10:00

Yong-Jin Park Development and Enhancement of the Hydro-GeoSphere Model: Urban infrastructure, winter hydrological processes, new surface water flow equations, and more.

Thursday, April-3, 9:00-9:30

The complexity of the problems associated with water resource analyses has increased unprecedentedly. Despite the growing demand for computer-aided analyses of water-related sive linearization method can suffer from overshooting in issues, numerical models suffer from the overwhelming complexity. For the simulation of integrated surface water and groundwater flow systems, especially in such large-scales, spatial and temporal discretization has already become a limiting factor to achieve an acceptable level of accuracy. Multi-disciplinary analyses in water-related science and engineering have become increasingly popular and further augmented the complexity with more distinct multiple physical, chemical and ecological processes in the hydrological systems. Under the condition that numerical models are deemed to be substantially underdiscretized for the necessary complexity, some of the issues may be circumvented in different ways. Fluid flow and solute transport along linear hydraulic features in surface and subsurface flow systems can be simulated efficiently by adapting one-dimensional approximation. For example in groundwater hydrology, pumping and monitoring wells are treated as highly conductive, vertically-aligned one-dimensional pipes where flow potential can quickly propagate to be equilibrated or groundwater extraction is distributed over the screen interval. For the optimal design of urban infrastructures in water and wastewater engineering, flow through water supply lines and sewer drains are typically modeled in terms of gravity flow in shallow subsurface. In surface hydrology, flow along streams and rivers has been simulated also as one-dimensional open channel flow. Winter hydrological processes such as freezing and thawing of pore water and the accumulation and melting of snow can play an important role to understand general hydrology and water budget, especially in the colder regions. Freezing and thawing of the pore water can be approximated by adapting a one-dimensional analytic solution for vertical heat transport and the snow melting can be effectively simulated using a simple degree-day factor approach. The Manning's surface flow equation states that

surface water flow is proportional to the square root of the head gradient and thus the Newton-Raphson (NR) succesconvergence. In order to resolve this overshooting issue, an approximate equation is introduced that maintains the similar flow characteristics of the original Manning's equation but guarantees the convergence in the NR iterative method. Some additional development and enhancement issues will be discussed in this presentation.

#### 7 Abstracts

# Modeling groundwater - surface water interactions in an esker aquifer

Ala-aho P., Rossi P., Klöve B.

Unconfined esker aquifers are the important source for water supply in Nordic countries affected by the last glaciation. However, the aquifers must simultaneously sustain other important functions, such as provide inflow for groundwater dependent ecosystems and wetlands and provide an environment for recreational use. The interaction between esker aquifers and related lakes and wetlands is not well understood; land use and climate change may impact these complex aquifer systems.

Groundwater surface water interaction at 90 km2 Rokua esker aquifer in northern Finland is studied with numerical modeling using the HydroGeoSphere. Firstly, the modeling exercise aims to understand the effects of peat land drainage to groundwater discharge. The groundwater discharge area is extensively drained to improve forest growth, and the drainage has disturbed the natural groundwater discharge dynamics. Changes in parameterization of overland flow domain in the HGS model will be used to study the effects of hypothetical pre-drainage conditions and conditions after peat land restoration. Hypothesis is that the peat land drainage has the potential to increase groundwater discharge from the aquifer adequately to lower the water table in the Rokua esker aquifer.

Secondly, the model is used to simulate interaction between the aquifer and numerous kettle hole lakes located in the aquifer recharge area. Aim is to explain lake water quality and ecological composition of lakes by their location in the groundwater flow system. The hypothesis is that nutrients are accumulated along groundwater flow paths and nutrient rich lakes are the ones that receive groundwater from long flow paths or a large portion of their water budget constitutes of groundwater inflow. Modeling results will be used alongside with data from groundwater and lake water quality and lake macroinvertebrate species composition to improve the understanding of groundwaters role in lake ecology.

Tentative modeling results show that the fully integrated surface-subsurface flow model can adequately represent the hydrological processes in the complex aquifer system with interconnected lakes and streams. Future work will focus on model calibration and refinement to test the research hypothesis presented above.

#### Using HydroGeoSphere with hydrogeological and geophysical data to characterise seawater intrusion

Beaujean J., Nguyen F., Kenma A., Antonsson A., Engesgaard P.

Water resource management requires characterizing efficiently seawater intrusion at local and regional scale and identifying in real time the seawater/freshwater interface dynamics. Hydrogeological modeling is widely used to predict seawater intrusion if additional natural or manmade factors are modified. These models are currently calibrated using measured heads and salt mass fractions in boreholes, which generally result in sparse data coverage. Within this scope, non to minimally invasive geophysical techniques like electrical resistivity tomography (ERT) or timedomain electromagnetic method are becoming increasingly popular. ERT may be used to constrain seawater intrusion models given its high sensitivity to total dissolved solid contents in groundwater and its relatively high lateral resolution compared to borehole observations. However, the spatial variability of resolution in electrical imaging may prevent the correct recovery of the desired hydrochemical property such as salt mass fraction.

We present here an uncoupled hydrogeophysical inversion to calibrate seawater intrusion models using ERT. It consists in constraining hydrogeological parameters using ERTderived parameters and first requires a geophysical inversion in which geophysical properties are converted to a hydrological property through a petrophysical relationship. The inverse hydrological calibration is then performed on the inferred hydrological properties. In this uncoupled approach we evaluate the feasibility of identifying the hydraulic conductivity and dispersivity in density-dependent flow and transport models from surface ERT-derived mass fraction. Geophysical inversion is performed by using first a smoothness constraint approach and next, a geostatistical constraint in the inversion process. The hydrological inversion is performed using a gradient-based Levenberg-Marquardt algorithm.

Two synthetic benchmarks are tested. They represent a pumping experiment in a homogeneous and heterogeneous coastal aguifer. In the heterogeneous case, a parsimonious hydrological model is built on the basis of the geophysical resistivity model as ERT provides evidence of strong heterogeneities. We show that the mismatch between the targeted and the recovered salt mass fraction occurs from a certain threshold which may be defined as a function of the ERT cumulative sensitivity. We demonstrate the capability of sensitivity-filtered ERT images using surface-only data to recover in both synthetic cases the hydraulic conductivity while underestimating the dispersivity. We attribute the latter mainly to the lack of ERT-derived data at depth, where resolution is poorer, and to a model error introduced by delineation of heterogeneities with geophysical data. In terms of perspectives, we aim at developing a coupled inversion approach based on simultaneous inversion of hydrogeological and geophysical data (resistances) to recover petrophysical and hydrogeological parameters.

#### Conceptual model suitability for reproducing preferential flow in waste rock

Broda S., Blessent D., Aubertin M.

The removal of non-ore rock to access ore depositions comes

along with the production of waste rocks, which may contain reactive sulphidic minerals. Typically, these are placed on the mine site, sloped and contoured into controlled shapes, forming the so called waste rock piles (WRP). The deposition method and the highly heterogeneous hydrogeological and geochemical properties of waste rock have a major impact on water and oxygen movement and pore water pressure distribution in the WRP, controlling hydro-geochemical reactions in the waste rock. The prediction and interpretation of water flow and distribution in WRP is a challenging problem and previous numerical investigations are often found questionable.

This study describes the first-time application of modelling approaches originally designed for groundwater flow in fractured massive rock aguifers to reproduce preferential flow triggered by macropores in waste rock material, using the 3D numerical HydroGeoSphere model. Besides the common equivalent porous media conceptual approach, the dual continuum and the discrete random fracture approach were tested for reproducing distinct, predominantly macroporeand porous media-driven outflows observed at an intermediate laboratory scale column experiment. Outflows obtained with the numerical model applying the basic equivalent porous media approach could not cover the observed macropore-driven drainage period. Increasing model complexity improved model accuracy in terms of reproducing onset of observed drainage periods and total cumulative volumes. However, observed distinct discharge periods and discharge pausing could not be depicted independently of the conceptual model applied.

A sensitivity analysis concludes this study, indicating the necessity of improving knowledge on principal model parameters, such as fracture aperture and location.

#### Simulating integrated water management in the lower Numerical modeling of a field scale tile drainage netrepublican river basin, Kansas, USA

Brookfield A., Ensz A., Stover S., Wilson B.B., Lyon A., Beightel C.

Understanding groundwater-surface water interactions is essential to the effective management of the water resources of the Republican River Basin (RRB), located in Colorado, Nebraska and Kansas. This presentation will describe some of the past and current research activities that quantify and manage water resources of the lower portion of the RRB, emphasizing recent research to link HydroGeoSphere (HGS) to the surface water operations model OASIS for assessing future water management strategies. Surface water and groundwater of the RRB are heavily utilized for agricultural, recreational, industrial and domestic use and has historically experienced severe droughts and floods. In 1942, the three states entered into the Republican River Compact which apportioned the virgin waters of the RRB between the three states. The compact, in turn, paved the way for significant federal investments in the basin for flood control and water supply including a series of dams, reservoirs and irrigation projects along the river valley. Imbalances between water supplies and demands continue in the basin. Continued research is being undertaken by the three states and the Bureau of Reclamation to explore system improvements. As part of this work, the state of Kansas is developing and utilizing a link between HGS and OASIS to evaluate the impacts of current water management strategies and potential infrastructure improvements on the surface and groundwater resources of the Lower RRB. Potential impacts of climate change to the RRB system will also be evaluated. This work emphasizes the need to include groundwater, surface water and their interactions in water management strategies and planning.

# work

De Schepper G., Therrien R., Refsgaard J.C.,

Subsurface drainage is a common agricultural practice in poorly drained production fields to guarantee the productivity of crops and to reduce flooding risks. The impact of shallow tile drainage networks on groundwater flow patterns and associated nitrate transport from the surface needs to be quantified for adequate agricultural management. A challenge is to represent tile drainage networks in numerical models, at the field scale, while accounting for the influence of subsurface heterogeneities on flow and transport.

A numerical model of a tile drainage network has been developed with the fully integrated HydroGeoSphere model for the Lillebk agricultural catchment, which is located in Denmark. The Lillebk catchment includes various tile drainage networks that are monitored regularly, covering 4.7 km<sup>2</sup>. The catchment subsurface is made of Quaternary deposits which consist of a local sandy aquifer with upper and lower clayey till units, confining the aquifer in the upper part. The main modeling objective is to assess the influence of tile drains on the water flow pattern within the confining clayey till unit while accounting for local geological heterogeneities. Using the national-scale geological model for Denmark combined with available local data, a hydrogeological model at field scale has been generated. A proper representation of the tile drains geometry is essential to calibrate and validate the water flow model. HydroGeoSphere allows us to include discrete drains into a model as one-dimensional features, which however requires a very fine mesh discretisation that limits the size of the simulation domain. Because of this limitation, we are testing an alternate approach where the tile drainage network and surrounding porous medium are represented by a dual-continuum formulation, similar to that used to represent fractured porous media, for example. Validating this drain representation method in a model

should allow us to work at larger scale and thus to model

the entire tile drained catchment without having to implement each and every drain, which would induce a very high number of model elements leading to time-consuming simulations.

This contribution will focus on some preliminary simulations designed to validate the dual-continuum approach to represent tile drainage networks. These simulations are also designed to demonstrate the applicability of the approach for 3D variably-saturated flow modelling at the field scale, accounting for local geological heterogeneities.

#### Refreshing Meshing - Generating Triangular Grids for HydroGeoSphere in an Open-Source GIS Environment

Dugge J.

A newly developed plugin for the open source GIS system Quantum GIS is presented that allows to generate unstructured triangular meshes using a graphical user interface. This makes it possible to use spatial data like digital elevation models or bore hole and well locations to guide the mesh development process. The resulting mesh can be exported for use in HydroGeoSphere.

Furthermore, Grok expressions for selecting particular mesh components can be generated, which can then be used to assign boundary conditions or material properties in HGS models.

# Simulating GW-SW interactions with HGS - some examples and open questions

Fleckenstein J., Frei S., Bartsch S., Maier U., Neubauer M., Wiesner V.

Physically based, fully integrated hydrologic models provide a powerful tool to explore the dynamics of GW-SW interactions. Several examples of applications of HGS in coupled GW-SW systems will be presented. Experiences gained in

these applications and open questions will be disscussed.

#### Catchment scale modeling of surface-subsurface interaction in a pre-alpine watershed

Ghasemizade M., Schirmer M., Brunner P.

We intend to simulate the transient behavior of the Rietholzbach catchment, which is a pre-alpine three square kilometer catchment in Switzerland, including temporal and spatial contribution of subsurface flow to stream flow. To achieve this target, we believe that if dominant processes and state variables are identified in a smaller scale, there would be higher chances to simulate the behavior of the catchment fast and generalize the modeling results to the neighboring catchments as well. HydroGeoSphere will be used as a simulation tool in our study. To the knowledge of the authors, the model has rarely been used as a learning tool for testing hypothesis. We intend to apply HydroGeo-Sphere in a heavily instrumented field site in the catchment in order to evaluate the model assumptions in modeling surface water bodies interactions with subsurface media as well as testing some hydrological hypothesis. It is also planned to conduct some new experiments in locations and times that the model fail. We believe the new experiments will provide us with worthwhile data that may reveal some unknown facts.

# Implementation of the Extended Oberbeck - Boussinesq Approximation for the numerical simulation of variable-density groundwater flow and solute transport in Hydrogeopshere

Guevara C., Thomas Graf

Subsurface water systems are endangered due to salt water intrusion in coastal aquifers, leachate infiltration from waste disposal sites and salt transport in agricultural sites.

This leads to the situation where more dense fluid over-

lies a less dense fluid creating a density gradient. Under certain conditions this density gradient produces instabilities in form dense plume fingers that move downwards. This free convection increases solute transport over large distances and shorter times. In cases where a significantly larger density gradient exists, the effect of free convection on transport is non-negligible. The assumption of a constant density distribution in space and time is no longer valid. Therefore variable-density flow must be considered. The flow equation and the transport equation govern the numerical modeling of variable-density flow and solute transport. Computer simulation programs mathematically describe variable-density flow using the Oberbeck-Boussinesq Approximation (OBA). Three levels of simplifications can de considered, which are denoted by OB1, OB2 and OB3. OB1 is the usually applied simplification where variable density is taken into account in the hydraulic potential. In OB2 variable density is considered in the flow equation and in OB3 variable density is additionally considered in the transport equation. The Hydrogeosphere (HGS) groundwater flow and transport numerical model accounted for density driven flow using OB1. OB2 and OB3 were implemented in order to evaluate the differences between the approximation levels in scenarios were large density gradients exist. Results from a laboratory-scale experiment of variable-density flow and solute transport (Simmons et al., Transp. Porous Medium, 2002) are used to investigate which level of mathematical accuracy is required to represent the physical experiment more accurately. Results show that OB1 is required for small density gradients and OB3 is required for large density gradients.

#### What controls the depth to the redox-interface? Preliminary results

Hansen A.L., Ernstsen V., Refsgaard J.C., Therrien R., He X., Jensen K.H.

Nitrate leaching from agricultural areas and the resulting pollution of both groundwater and surface waters constitutes one of the largest challenges in water resources management in Denmark. However, natural transformation of nitrate may occur under anaerobic conditions through denitrification. For denitrification to occur in the saturated zone, nitrate must be transported below the redox interface that delineates the transition from aerobic to anaerobic conditions. Therefore, the amount of saturated zone denitrification in a catchment dependents on the depth of the redox interface and on the water flow patterns. In this study the focus is on the former.

The depth to the redox interface is spatially heterogeneous and can vary several meters within a few hundred meters distance. Furthermore, the location of the interface can only be obtained from information on change in sediment colour or amount of redox active components with depth, but these data are very sparse in most areas. This generates uncertainty on the redox interfaces interpolated from these sparse data and thereby causes uncertainty in nitrate models.

The reason for the variability of depth to the redox interface is at present not fully understood, but is believed to be due to heterogeneity in the amount of reduced compounds in the sediments and local variations in water flow patterns and thereby in the transport of oxidizing components using the inherent reduced compounds (redox capacity). In this study we try to model the development of the redox interface since the beginning of Holocene, where the redox interface is believed to have been at the ground surface.

The study area is the Lillebk catchment on the island of Funen in Denmark. The catchment is situated in a young glacial landscape and the upper unit consists of clayey till of Weichselian age. The redox interface is located within

this till unit. In order to estimate the location of the redox interface in the area 40 boreholes were made along a 1.5 km transect with distances between the boreholes down to 2.5 m. The observed redox depths in the area vary between 1.4 8.6 m. Furthermore, based on a variogram analysis a spatial correlation between the observed redox depths is seen with a correlation length of less than 250 meters, which is smaller than the distances between existing borehole data found in most areas in Denmark.

The objective of this study is to test hypotheses on what controls the location and variation of the redox interface using a new feature in HydroGeoSphere capable of simulating instantaneous reaction between redox capacity in the soil and oxygen in infiltrating water. The test will be done by trying to reproduce the observed geostatistical features on the redox depths in Lilleboek catchment.

#### Probability perturbation method applied to the inversion of groundwater flow models using Hydro-GeoSphere

Hermans T., Scheidt C., Caers J., Nguyen F.

Solving spatial inverse problems in Earth Sciences remains a big challenge given the high number of parameters to invert for and the complexity of non-linear forward models. Techniques were developed to reduce the number of parameters to invert for or to produce geologically consistent simulations from an initial guess. These techniques ask for a prior model to constrain the spatial distribution of the solution. Geostatistical models contain, by nature, information to control the spatial features of the inverse solutions, but the integration of dynamic data into such models remains difficult.

using Matlab® to invert hydrogeological data using multiplepoint geostatistics to build models of pre-defined hydrofa-

pute the forward response of the model and SGems to produce geostatistical realizations. The algorithm only needs the proper definition of all the parameters to be used by HydroGeoSphere (grid matching with SGems, position of the wells, pumping rate, facies properties, boundary conditions, etc.). The PPM algorithm will automatically seek solutions fitting both hydrogeological data and geostatistical constraints. Through the inversion process, the initial geostatistical realization is perturbed. Only geometrical features of the model are affected, i.e. we do not attempt to directly find the optimal value of hydrogeological parameters, but the optimal spatial distribution of facies whose prior distribution is quantified in a training image.

The algorithm can be divided in three steps. In the first step, we use SGems to generate an initial facies model with the multiple-point geostatistical algorithm SNESIM (single normal equation simulation). The facies model is composed of several categories representing hydrological facies (e.g. gravel, sand and clay). It can be conditioned using hard data (borehole data) and/or soft data (e.g. geophysical data). We then run a first flow simulation with HydroGeo-Sphere. This requires defining hydrogeological parameters (porosity, hydraulic conductivity, etc.) for each category of the facies model to create a hydrogeological model. The response of the latter model is compared to the expected one through an objective function. In the second step, a perturbation to the facies model is computed using a single parameter called rD. This perturbation is used to generate a new facies model with SGems and calculate a new objective function value via HGS, as done in the first step. An inner loop optimizes the value of rD. In the third step, we verify if the objective function of the best fitting model is smaller than a predefined value. If it is the case, we stop the We adapted, the "probability perturbation algorithm" (PPM) algorithm, otherwise we go back to step 2 until convergence. We illustrate the methodology with a synthetic example in an alluvial aquifer. The model is based on a training imcies. The algorithm uses HydroGeoSphere (HGS) to com- age depicting gravel channels and clay lenses in a coarse

sand aquifer. We simulate a pumping test and inverse water level data recorded at 9 wells using our implementation of the PPM algorithm. Using this method, it is possible to generate multiple solutions and to derive a posterior probability of the facies distribution.

# ${\bf Groundwater\ resources\ under\ a\ changing\ climate-}$ ${\bf a\ case\ study\ from\ Lower\ Saxony,\ Germany}$

Herold M., Isa M.A., Ryan N.T., Ptak T.

This study will focus on the quantification of the response of a surface water - groundwater system to changing hydraulic and hydrological boundary conditions with expected increased dynamics and a larger spectrum due to a changing climate. The employed surface water - groundwater models are used for process oriented numerical simulations and parameter studies on different scales (i) to characterise the interactions of surface water and groundwater, (ii) to identify the parameters controlling the system dynamics, and (iii) to assess the future impact of climate change on this system. Apart from a large groundwater model (15.000 km<sup>2</sup>), specific parameter studies have been conducted employing two smaller sub-catchment models. Here we present only results from those smaller models. We investigated the effect of land-use change on groundwater recharge, the buffer capacity of the hill slope and the change in inundated areas during a heavy rain event. Additionally, we studied the sensitivity of groundwater recharge towards changes in precipitation and evapotranspiration levels. Finally, the models were run under the conditions of the IPCC scenario A1B and the resulting changes in discharge and groundwater recharge were analysed. Here we could show the possible effects of a changing climate on some components of the water cycle, however, the uncertainty inherent in global climate models is also propagated.

#### Optimizing numerical simulation of fracture networks for variable-density flow

Hirthe E., Graf T., Broda S., Blessent D., Aubertin M. Complex geometries such as fracture networks need irregular meshes with a large number of nodes. Representing fracture networks requires the inclusion of finer elements close to the fractures, increasing the number of nodes. The CPU time increases exponentially with the number of nodes. Optimizing the numerical simulations of complex geometry systems is of high importance. In order to reduce the CPU time while maintaining accuracy, the automatic noniterative second-order time-stepping scheme based on the temporal truncation error proposed by Kavetsky et al. [Water Resour Res, 2002] has been implemented into the code of the HydroGeoSphere model. This time-stepping scheme has been shown to efficiently limit the temporal truncation error to a user-defined tolerance by controlling the time-step size [Hirthe and Graf, Adv Water Resour, 2012]. Moreover, CPU times can be reduced by diminishing the number of nodes present in the mesh. Using a two-dimensional simulation domain of a fractured rock, we are asking the question whether we need to incorporate all fracture network characteristics of a potentially real fracture network, or whether a fracture network can be simplified. Additionally, a case study of unsaturated flow in a waste rock pile is presented, where the presence of macropores -represented by discrete fractures- favor preferential flow, having important effects on geotechnical, geochemical and hydrogeological behaviour. The uncertainty of the main fracture network parameters is studied.

#### Recent Progress in Hydraulic Tomography and its Potential Applications to Surface Water-Groundwater Interaction Problems

Illman W.

The accurate characterization of heterogeneity in hydraulic

parameters such as hydraulic conductivity and specific storage is a topic of great importance in hydrogeology. Recent interest in coupled modeling of surface water and groundwater flow and transport will require better estimates of hydraulic and transport properties within the hyporheic zone and the adjacent subsurface. In this talk, I review the concepts of hydraulic tomography and discuss some applications in porous and fractured geologic media to image heterogeneity in hydraulic parameters. While hydraulic tomography is a robust approach, it is not a panacea technology. Hence, recent research efforts to improve hydraulic tomography are also discussed. After that, I will discuss the potential for utilizing river stage fluctuations and corresponding groundwater level responses to estimate the hydraulic parameters that facilitate the exchange between surface water and groundwater. This new approach has been referred to as river stage tomography. Finally, I discuss the pros and cons of river stage tomography and provide my perspective on research in this area.

A HGS-based assessment of the potential use of compound specific stable isotope analysis in river monitoring of diffuse pesticide pollution

Lutz S., Van Meerveld H.J., Waterloo J., Broers H.P., Van Breukelen B.M.

Compound-specific stable isotope analysis (CSIA) together with its model-assisted interpretation has proven a valuable approach to quantify the extent of organic contaminant degradation in subsurface systems. Whereas CSIA methods for pesticides have increasingly become available, they have not yet been applied to interpret isotope data of pesticides in surface water. Ideally, CSIA data may provide insights into the origin and transformation of pesticides at the catchment scale. We applied the catchment-scale reactive transport model HydroGeoSphere to investigate the usefulness of CSIA data in river monitoring for the assessment of

pesticide degradation. As a first step towards a catchmentwide study, we simulated the transport and transformation of a pesticide in a hypothetical two-dimensional hillslope transect with a river as outlet. The isotope fractionation processes during the transformation of the pesticide were modelled for two elements simultaneously to allow for the quantification of the contribution of two different reaction pathways to the overall degradation. The model results of a steady-state scenario illustrated the strong enrichment in in-stream isotope ratios, which resulted from degradation and long travel times through the hillslope subsurface during average hydrological conditions. In contrast, following a heavy rainfall event that induced overland flow, the simulated isotope signatures dropped to the values of the emission source. Those simulations showed how CSIA can help to distinguish river pollution by pesticides via groundwater exfiltration from direct emission via surface runoff. The simulation was then adjusted to transient conditions with daily data for rainfall and evapotranspiration and one pesticide application per year. As a result, the modelled concentrations and isotope signatures showed small seasonal variations in the river. The variations in in-stream isotope ratios were, however, in the uncertainty range of the CSIA methods, which prohibits the detection of these subtle effects over the seasons. At the same time, this absence of strong isotope variations (except for overland flow events) implies a good reliability of in-stream isotope data since the time of measurement is of minor importance. The simulations also supported the use of the commonly applied Rayleigh equation for the interpretation of CSIA data, since this led to an underestimation of the real extent of degradation of below 20 %, which is a good result in view of the strong mixing of different flow paths in the hillslope discharge. Overall, these first model results support the application of CSIA in the assessment of diffuse pesticide pollution in rivers.

Uncertainty of groundwater recharge estimations cau- to predict the true change in groundwater recharge rates, sed by climate model chain variability and model whereas the simple models over- or underestimate the future simplification groundwater recharge rate. However, differences in model

Moeck C., Brunner P., Hunkeler D.

Estimation of groundwater recharge is essential for sustainable water resource management. However, it is very likely that this key parameter will be affected by predicted changing climatic forcing functions. Therefore, a wide range of different models, differing in their complexity, used to estimate groundwater recharge could be found in the literature to evaluate the effect of climate change. However, model simplification can introduce predictive bias due to simpler model structures, which can give controversy results between different models, especially under climate change. The relative importance of both uncertainties was so far not systematically investigated Therefore, we evaluate how models with various degree of complexity influence the prediction of recharge and secondly how this uncertainty is related to the uncertainty originating from variability among climate model chains.

A highly heterogeneous 2D synthetic model was built to generate recharge data for actual and predicted future weather conditions. Daily values of precipitation and temperature and their changes for future weather conditions of the A1B emission scenario with 10 model chains are applied. Models of simpler models structure were calibrated against groundwater recharge outputs of the complex references model. Different calibration periods were applied to prove the significance of different inputs for the calibration.

Surprisingly good fits for all models can be achieved through
model calibration against the reference recharge period. Howvariations of sediment properties, boundary conditions and
ever, predictive bias occurs by running these models over
several years. Applying climate change with more extreme
weather conditions increases the resulting bias. The potential for model predictive error tends to rise to the extent
to which the climatic forcing function differs from the calibration period. Physically based models are most efficient

This model is a sound basis for investigating quantitatively
variations of sediment properties, boundary conditions and
streambed morphology and also for subsequent generalization of SFW-GW exchange on reach scale river stretches
and beyond.

to predict the true change in groundwater recharge rates, whereas the simple models over- or underestimate the future groundwater recharge rate. However, differences in model results in the trend, (increase or decrease of groundwater recharge) cannot be observed. Comparison of both uncertainties, climate change and model simplification, indicate that the highest uncertainty is related to climate change, but model simplification can also introduce a not negligible predictive error.

#### Modelling spatial and temporal variability of surface water-groundwater fluxes and heat exchange along a lowland river reach

Munz M., Schmidt C., Fleckenstein J., Oswald S.

In this study we used HydroGeoSphere to investigate the spatial and temporal variability of surface water-groundwater (SFW-GW) fluxes and heat exchange along a lowland river reach of the Selke River, Germany. Detailed, high frequent observations of river, groundwater and hyporheic hydraulic heads and temperatures have been conducted along a 100 m long reach since 2011. The complex deterministic, fully-integrated surface-subsurface model incorporates observed hydrological and thermal conditions. Modelling results are used to analyse and quantify water and heat fluxes at the SFW-GW interface and to trace subsurface flow paths within the streambed sediments. The results will improve the understanding of SFW-GW interaction; which control most hydroecological and biogeochemical processes. This model is a sound basis for investigating quantitatively streambed morphology and also for subsequent generalization of SFW-GW exchange on reach scale river stretches and beyond.

#### Physics-based modelling of erosion at catchment scale

Norouzi Moghanjoghi K.

The removal of non-ore rock to access ore depositions comes along with the production of waste rocks, which may contain reactive sulphidic minerals. Typically, these are placed on the mine site, sloped and contoured into controlled shapes, forming the so called waste rock piles (WRP). The deposition method and the highly heterogeneous hydrogeological and geochemical properties of waste rock have a major impact on water and oxygen movement and pore water pressure distribution in the WRP, controlling hydro-geochemical reactions in the waste rock. The prediction and interpretation of water flow and distribution in WRP is a challenging problem and previous numerical investigations are often found questionable.

This study describes the first-time application of modelling approaches originally designed for groundwater flow in fractured massive rock aguifers to reproduce preferential flow triggered by macropores in waste rock material, using the 3D numerical HydroGeoSphere model. Besides the common equivalent porous media conceptual approach, the dual continuum and the discrete random fracture approach were tested for reproducing distinct, predominantly macroporeand porous media-driven outflows observed at an intermediate laboratory scale column experiment. Outflows obtained with the numerical model applying the basic equivalent porous media approach could not cover the observed macropore-driven drainage period. Increasing model complexity improved model accuracy in terms of reproducing onset of observed drainage periods and total cumulative volumes. However, observed distinct discharge periods and discharge pausing could not be depicted independently of the conceptual model applied.

A sensitivity analysis concludes this study, indicating the necessity of improving knowledge on principal model parameters, such as fracture aperture and location.

#### Seawater intrusion for a North Sea coastal aquifer in respect to future seawater level rise

Oswald S., Brunk C., Gräff T.

As part of a project to study the future development of the ecohydrology at the North Sea coast, we simulate seawater intrusion and saltwater upconing for a 15 km long cross-section of the subsurface, aiming for a simulation of the changes to come the next 100 years driven by seawater level rise and land use changes. As first steps hydrogeological data, water level observations and the surface water drainage systems were evaluated and a numerical model was built. Initially two models were tested for the Henry problem, Hydrogeosphere and Feflow, then for the realistic cross-section. Numerical stability and executions times, in case of Hydrogeosphere also on a compute cluster, are major issues for proceeding with this work.

# Quantifying in-stream and overland flow generation mechanisms using HGS

Partington D., Brunner P., Therrien, R., Simmons, C.T.

Understanding the flow generation mechanisms that drive streamflow is critical to managing the resource and the environment is supports. Here we describe the implementation of the Hydraulic Mixing-Cell method to deconvolute the streamflow signal into its constituent flow generation components. Through elucidation of these streamflow generation dynamics, we gain an improved understanding of

# Modeling of exchange processes between river and hyporheic zone

Sanz-Prat A., Cirpka,<br/>O., Selle, B., Blowes, D.  $\,$ 

catchment functioning as simulated by the model.

Based on conceptualized water catchment, coupled flow and transport processes between surface water and the hyporheic zone will be modeled. Because of the usefulness of implementing travel time models for complex dynamic systems, we will be focused on the simulation of hydrological dynamics and different types of reactive systems in three dimensional domains. The objective of this research is to increase the understanding of the conditions in which travel time controls reactive transport processes at catchment scale. For this purpose, we hypothesized that travel time models can provide reliable and representative values of concentration of reactive species if (a) transport mechanisms of dispersion and diffusion should be neglected, such that particles should cross the domain along idealized streamtubes; (b) hydrodynamic processes are slow enough to allow self-organization of reactive zones within the subsurface.

# Using tree rings in modeling the water cycle at the lower Tarim River, Western China

Schilling O., Brunner P., Doherty J., Wang H., Yang P.N., Kinzelbach W.

Increased water use during the last three decades along the upper and middle Tarim River and its tributaries in Western China has caused the lower Tarim River to dry up over a length of about 300 km. In order to forestall the loss of riparian ecosystems along the dried up reach, the Chinese government initiated the Ecological Water Conveyance Project. Periodically, the amount of upstream water drawn from the river for irrigation purposes is reduced; water is thus made available for flow downstream.

Determination of the volumes required for future releases was not possible because of its rather complex geometry requires that the needs of downstream ecosystems be determined. This requires understanding and quantification of water exchange between the river, the vadose zone, groundwater and vegetation. These interactions were simulated for a downstream 2-D cross-section using the HydroGeoSphere tions compare well to the corresponding simulations of the model calibrated against observations of water tables, as well as tree ring data, the latter being a proxy for transpiration. Linear analysis was then employed to quantify the

worth of different components of the observation dataset in reducing the uncertainty of model parameters and of model predictions of interest, and to track the flow of information from elements of the calibration dataset to the different parameters employed by the model. It could be demonstrated, that tree ring records provide a key link in modeling ecosystems dynamics.

# Model grid simplification to accelerate calibration: A catchment-scale case study

Von Gunten D., Woehling T., Haslauer C., Cirpka O. Model calibration is necessary to accurately simulate watershed responses, because the effective parameterization of system properties can not be measured at the appropriate scale. However calibration is sometimes impossible for fully coupled models such as hydrogeosphere, because of their intense computational requirements. To accelerate calibration, we propose here a method which uses a simplified computational grid as a proxy for the more complex simulation model. Our case study is a relatively small catchment (7.5km2) in the North-East of Spain, used principally for agriculture. Based on available data, we constructed a hydrogeosphere model of this catchment using hydraulic parameters derived from general knowledge of the geology and textural data. However the model simulations showed important differences compared to the measured stream hydrograph and water tables readings. Calibration of the model was not possible because of its rather complex geometry and the large model run times. To solve this problem, we created a reduced model with a coarser computational grid. The coarser model has a shorter simulation time (around four times shorter) and hydrograph and water table simulations compare well to the corresponding simulations of the original model. In this presentation, we will compare the two models and explore the effects of model grid reduction. calibration, notably about simulation of evapotranspiration. REFERENCES: Perez A., Abrahao R., Causape J., Cirpka O., Burger C., Simulating the transition of a semi-arid rainfed catchment towards irrigation agriculture, Journal of Hydrology, 2011, 409:663-681

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#### Density-dependent flow and transport in fracture networks embedded in low permeability rock

Vujevic K., Graf T.

Density-driven flow can be a highly efficient mechanism for solute transport in hydrogeological systems, especially if groundwater movement is not determined by head gradients as a driving force. Flow may then be determined by concentration and temperature gradients that generate unstable density layering. Free-convective flow allows solutes to penetrate faster and further into an aquifer than diffusion alone. Number and shape of forming convection cells in homogeneous porous media depend on the prevailing density gradients. The presence of fracture networks may complicate flow patterns because fractures represent high permeability path-ways. Matrix permeability in contrast, is usually orders of magnitude smaller. Nonetheless, molecular diffusion from the fracture into the matrix is possible. Interactions between fractures and the porous matrix and the interdependency of flow and transport in density-dependent problems further increase complexity.

We provide insight into the structural properties of fracture networks that determine flow and transport patterns and the limits of applicability of the equivalent porous medium approach (EPM). We systematically study free-convective flow in continuous, discontinuous, orthogonal and inclined Whether an initially stable, diffusive regime evolves into

discretely fracture networks embedded in a low-permeability rock matrix. Layer stability and convection patterns for different fracture networks are compared to each other and to an unfractured base case representing an EPM. We examine rates of solute transport by monitoring the mass flux at the solute source and relate it to the critical structural properties of the fracture networks.

Results show that for free-convective flow, the EPM approach is not able to reliably represent a fractured porous medium if fracture permeability is more than 5 orders of magnitude larger than matrix permeability. Nonetheless the EPM approach can be a reasonable approximation if the fracture network (i) evenly covers the simulated rock, (ii) shows high fracture density, (iii) is well-connected, (iv) contains fractures whose length is close to the domain size. Fractures tend to destabilise the system and promote convection if fracture spacing is large, fracture aperture is high and fractures form large closed circuits. In that case the fracture network provides continuous high-velocity flow paths throughout much of the domain. Closed circuits are most effective in terms of mass transport if they cover a large area and have a large vertical extension. Simulations of discontinuous fracture networks show that a continuous fracture path between solute source and sink is not necessary for free convection. Therefore, knowledge of the equivalent permeability of a fractured porous medium is not sufficient for the prediction of free convective flow. In addition, the geometry of the fracture network has to be considered.

#### Discretizing a Thermohaline Double-Diffusive Rayleigh Regime

Walther M., Graf T., Kolditz O., Liedl R.

In natural systems, convective flow induced from density differences may occur in near-coastal aguifers, atmospheric boundary layers, oceanic streams or within the earth crust.

a convective (stable or chaotic) regime, or vice versa, depends on the systems framing boundary conditions. A conventional parameter to express the relation between diffusive and convective forces of such a density-driven regime is Rayleigh number (Ra). While most systems are mainly dominated by only a single significant driving force (i.e. only temperature or salinity), some systems need to consider two boundary processes (e.g. deep, thus warm, haline flow in porous media). In that case, a two-dimensional, doublediffusive Rayleigh system can be defined.

Nield (1998) postulated a boundary between diffusive and convective regime at  $RaT + RaC = 4pi^2$  in the first quadrant (Q1), with Rayleigh numbers for temperature and concentration respectively. The boundary in the forth quadrant (Q4) could not exactly be determined, yet the approximate position estimated. Simulations with HydroGeo-Sphere (Therrien, 2010) using a vertical, quadratic, homogeneous, isotropic setup confirmed the existence of the 4pi<sup>2</sup> boundary and revealed additional regimes (diffusive, singleroll, double-roll, chaotic) in Q1. Also, non-chaotic, oscillating patterns could be identified in Q4. More detailed investigations with OpenGeoSys (Kolditz, 2012) confirmed the preceding HGS results, and, using a 1:10-scaled domain (height:length), uncovered even more distinctive regimes (dif- cate that coarsening horizontal spatial discretization mainly fusive, minimum ten roles, supposely up to 20 roles, and chaotic?) in Q1, while again, oscillating patterns were found in the transition zone between diffusive and chaotic regimes in Q4.

Analysis of the influence of grid resolution on discharge and hydraulic head simulation using a synthetic catchment

Wildemeersch S., Goderniaux P., Orban P., Brouyre S., is limited, especially for the coarsest models. Dassargues A.

Large-scale physically based and spatially distributed models are increasingly used in water management. However, Investigating tide and storm surge effects on coastal

at such a scale, flow modeling often requires long execution times. Therefore, a series of choices and simplifications are made for dealing with this issue and obtaining tractable execution times. The most common simplification consists in coarsening the spatial discretization in order to reduce the number of unknowns of the problem, and so the execution times. This coarsening of model grid can limit the accuracy of model results and prevent from simulating properly discharge and hydraulic heads. The objective of the present study is to evaluate the influence of grid resolution on discharge and hydraulic head simulation using a synthetic catchment developed with HydroGeoSphere. Additionally, the capacity of the calibration to compensate for errors induced by a coarse spatial discretization is also investigated. The synthetic catchment is developed for providing reference discharge and hydraulic head observations. These reference observations are then compared with their simulated equivalent obtained with a series of simplified models differing by their horizontal (element size of 250 m, 500 m, 750 m or 1000 m) or vertical spatial discretization (6 layers or 3 layers). The influence of grid resolution on discharge and hydraulic head simulation is investigated using graphics of model fit and performance criteria. The results indideteriorates the simulation of discharge due to a poor representation of groundwater-surface water interactions and runoff. Conversely, coarsening vertical spatial discretization mainly deteriorates the simulation of hydraulic heads due to a poor representation of infiltration and groundwatersurface water interactions. When calibration is performed, an improvement of model performance is observed suggesting that parameter values compensate for errors induced by a coarse spatial discretization. However, this improvement

#### aquifers using a three-dimensional coupled surfacesubsurface approach

Yang J., Graf T., Herold M., Ptak T.

Coastal aquifers are complex hydrologic systems because many physical processes interact: (i) variably saturated flow, (ii) spatial-temporal fluid density variations, (iii) tidal fluctuations, (iv) storm surges overtopping dykes, and (v) surface runoff of storm water. The HydroGeoSphere model is used to numerically simulate coastal flow dynamics, assuming a fully coupled surface-subsurface approach, accounting for all processes listed above. The diffusive wave approximation of the St. Venant equation is used to describe surface flow. Surface flow and salt transport are fully coupled with subsurfacial variably saturated, variable-density flow and salt transport through mathematical terms that represent exchange of fluid mass and solute mass, respectively. Tides and storm surges induce a time-variant head that is applied to nodes of the surface domain. The approach is applied to real cases of tide and storm surge events of the coastal catchment area of Unterweser, Northern Germany (ca. 2500 km<sup>2</sup>). To optimize the simulation and to reduce CPU cost, the actual simulation domain is only a part of the total catchment area: We selected a narrow strip of about 10\*15 km<sup>2</sup>. The 3D model is calibrated using field data previously gathered at the study site. Tides and a storm surge are applied and salinity distribution is observed. Results indicate that the fully coupled approach is effective in the investigation of coastal flow dynamics in 3D aquifers.

## 8 Conference Participants

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