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Book of Abstracts

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Local and global sensitivity analysis of THM consolidation around a point heat source

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Coupled thermo-hydro-mechanical (THM) models are used for assessment of nuclear waste disposal, reservoir engineering and geotechnical engineering. Model-based decision making and optimization require sensitivity analyses (SA) and uncertainty quantification (UQ). Assessment of different UQ and SA methods that work for coupled THM problems on an engineering scale is required. Due to different coupling levels, non-linearities, and large system sizes these analyses can be challenging. For an initial screening, it is advantageous to have an analytical solution that encompasses the most relevant primary couplings, can robustly cover the entire parameter space and remains computationally inexpensive.
Booker and Savvidou (1985) and Chaudhry et al. (2019) provided such an analytical solution for consolidation around a point heat source. We compared different approaches to sensitivity analyses: local (OVAT) and global sensitivity analysis (GSA) based on Sobol indices for different spatio-temporal settings to observe near and far-field effects as well as early- and late-stage system response. We show parameters and interactions that control the results in these different domains and provide physical interpretations. We provide application-oriented conclusions on the conditions which should be met when applying the different methods. The analysis can serve as benchmark for UQ and SA software designed around numerical THM simulators.

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Application of experimental design-based assisted history matching for uncertainty quantification in radioactive waste repositories

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In the performance assessment of nuclear waste disposal concepts, a thorough analysis of uncertainty and sensitivity of the underlying coupled thermo-hydro-mechanical-chemical (THMC) processes over several temporal and spatial scales is necessary. A critical aspect of this analysis is the evaluation of the integrity of the geotechnical and geological barriers for the specific waste repository concept.

For this purpose, we examine the applicability of a design of experiments (DoE)-based assisted history matching workflow using synthetic experimental data —an approach that is commonly used in the oil and gas industry in the context of reservoir modeling.

Based on an analytical solution of a spherically-symmetric thermo-hydro-mechanical problem of a heat source embedded in a fluid-saturated porous medium, we discuss the adaptability of the workflow to the field of radioactive waste disposal research as a potential way to address both, parameter and model uncertainties. We put thereby particular focus on the role of the input parameter distributions on the uncertainty of the model output.

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Derivation of an Effective Dispersion Model for Electroosmotic Flow Involving Free Boundaries in a Thin Strip

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Since dispersion is one of the key parameters in solute transport, its accurate modeling is essential to avoid wrong predictions of flow and transport behavior. In this research, we derive new effective dispersion models.
We consider a simplified geometric setting, i.e. a thin, potentially evolving strip. Within this strip, we investigate reactive ion transport under dominate flow conditions (i.e. for high Peclet number). Electric charges and the induced electric potential (the zeta potential) give rise to electroosmotic flow in addition to pressure-driven flow, while precipitation reactions may lead to a free boundary problem. More precisely, the interface between the precipitate and the fluid is taken into account via the thickness of the layer. To this model, a formal limiting procedure (in a level-set framework) is applied and dispersive terms are stated explicitly for the resulting upscaled models. In doing so, we emphasize the cross-coupling effects of hydrodynamic dispersion (Taylor-Aris dispersion) and dispersion created by electroosmotic flow. Moreover, we study the limit of small and large Debye length.

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Efficient Simulation of Reactive Flow in Reservoirs Rocks at the Pore Scale

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Modelling of reactive flow in digital rocks requires the consideration of geochemistry and Digital Rock Physics (DRP) and relies on the assumption that the examined samples are representative for the properties of interest, which evolve during the simulation of 4D pore alteration. With the prerequisite of high image resolutions and large sample volumes, representative elementary volumes (REV) require numerically challenging domain sizes of 8.5 billion voxels (2048^3) and larger.

Here, we present a highly efficient approach to simulate reactive transport in REV domains based on the Lagrangian transport method. We apply mineral surface-related reaction rates to control the amount of kinetic pore alteration at locations determined by simulating advective and diffusive motion of virtual particles. The dynamic processing of particle-rock interactions allows the high performance required to handle large domains. Simulations at increased time step lengths consider an upscaling of kinetic precipitation and dissolution reactions to account for given mineral-specific reaction rates. We can thus simulate reactive flow at increased time scales.

We present reaction scenarios in typical reservoir rocks, such as the injection of hydrochloric acid into carbonate rock. The goal of this carbonate reservoir stimulation is to increase the permeability by enlarging the pore space. At equal reaction rate, different dissolution patterns develop in the rock, depending on the injection rate and the digital carbonate rock structure. These patterns can be predicted with reactive flow simulations. In them, the injection parameters leading to the most favorable dissolution of the reservoir rock and the correlated permeability increase are determined. In our approach, the reactive flow is modeled as a combined continuum/particle method by a combination of Python coding and the numerical code(s) in the DRP software GeoDict®.
In this ongoing project, numerical experiments qualitatively verify the numerical model. The model reproduces the dissolution patterns from the literature [1,2]. They correspond to the dissolution patterns: face dissolution, wormhole, uniform dissolution, and channeling. The formation of the patterns depends on the fluid velocity, reaction rate, and digital rock structure. We simulate on a carbonate sample from the Grosmont formation (Alberta, Canada) published in a DRP benchmark study [3].

The coupling of our highly efficient flow solver and particle transport simulation with a technically optimized workflow enables reactive transport simulations in sizable geometries at the pore scale. We aim to compare our results with time sequences of μCT-scans of real dissolution processes and offer a suitable tool for predicting the development of digital rock properties during continuous reactions at fluid-rock interfaces.

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A kernel-based approach to NMR Cryoporometry of porous solids

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Porous solids have found wide uses in catalysis, adsorption, molecular separations, gas and energy storage, among others. Indeed, precise structure-function relations of porous structures are rightly obtained when accurate knowledge of the pore structure is available.

At present, most approaches for pore characterisation consider disordered porous materials as individual collection of pores where fluid phase transition occurring in one pore has no effect on adjacent pores. However, pore interconnectivity renders fluid phase behavior in one pore dependent on the phase state in its neighboring pore.

We show systematically how a model of statistical chains of pores can be applied for Nuclear Magnetic Resonance (NMR) cryoporometry of porous solids. By creating a kernel-based approach, considering a varying non-frozen layer thickness between solid core and pore wall and eliminating any a priori assumption of phase transition occurring by metastable or equilibrium transition, we refine the NMR cryoporometry technique.

For verification, we show how this approach works well with ordered materials like MCM-41 porous silica and reveals disorder in SBA-15.

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Efficiency and Accuracy of Micro-Macro Models for Dissolution/Precipitation in Two-Mineral Systems

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We introduce an efficient numerical scheme for flow and reactive transport problems in evolving heterogeneous porous media. Building upon micro-macro models obtained from detailed pore-scale models via periodic homogenization, our approach comprises flow and transport equations on the macroscopic scale including upscaled microscopic information (specific surface area, porosity, effective diffusion and permeability) calculated from representative unit cells. Conversely, the macroscopic solutes'concentrations alter the underlying microstructure by triggering dissolution or precipitation processes. This highly nonlinear bidirectional coupling among both scales poses several numerical challenges. As part of our solution strategy the application of level-set methods provides a convenient and flexible tool to represent even intricate underlying pore-geometries. Using the Voronoi Implicit Interface Method, our framework is also able to accurately describe systems with multiple competing mineral phases. More precisely, complex interactions such as covering processes are accounted for, leading to highly anisotropic structural evolutions. In this way, scenarios beyond the applicability of classical laws for macroscopic parameters such as Kozeny-Carman are accessible with our approach.

We demonstrate the computational efficiency and accuracy of our algorithm by comparing to a purely microscopic simulation approach. For this purpose, the dissolution of an array of dolomite grains within a flow-channel setup is investigated.

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Simulating permeability reduction by clay mineral nanopores in a tight sandstone by combining µXCT and FIB-SEM imaging

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Computer microtomography (µXCT) represents a powerful tool for investigating the physical properties of porous rocks. While calculated porosities determined by this method typically match experimental measurements, computed permeabilities are often overestimated by more than one order of magnitude. This effect increases towards smaller pore sizes, as shown in this study, in which nanostructural features related to clay minerals reduce the permeability of tight reservoir sandstone samples. FIB-SEM tomography was applied to determine the permeability effects of different clay

mineral morphology types at the nanometre scale and Navier-Stokes equations were applied to calculate the permeability of these domains. With this data, Brinkman domains (porous voxels) were defined using microtomography images of a representative sample. The distribution of these domains could be extrapolated by calibration against size distributions measured in FIB-SEM images. For this, we assumed a mean permeability for the dominant clay mineral (illite) in the rock and assigned it to the nanoporous Brinkman domains within the structure. The results prove the applicability of our novel approach by combining FIB-SEM with X-ray tomographic rock core scans to achieve a good correspondence between measured and simulated permeabilities

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Direct Numerical Modelling of Microbially-mediated Degradation in Soil under Unsaturated Conditions

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In soils, microbial communities provide various functions ranging from nutrient cycling to biodegradation of harmful chemical substances. Such functionalities are influenced by the environmental conditions the microorganisms are exposed to. The pore-scale variability of these conditions depends highly on pore size distribution, pore connectivity, water content and mass transfer across the air/water interface, and numerical model approaches would be highly beneficial for a quantitative understanding of such interactions at the pore scale. Previous studies have mainly focused on water-saturated conditions or a simplified representation of porous structure which both may cause a misleading estimate of biodegradation in soil.
The aim of the presented study is to overcome these shortcomings and to disentangle key features contributing to microbially-mediated reactions at the pore scale accounting for unsaturated conditions and maintaining a realistic representation of the soil porous structure. To identify and quantify the key drivers of biodegradation of carbon compounds in soils, we propose a pore-scale Direct Numerical Simulation technique which is able to model the dynamics of air/water/solute transport, explicitly on actual representation of porous structure obtained directly from μ-CT images. We will introduce our novel modeling approach and demonstrate its accuracy and application potential with selected examples.

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Benchmarking Conventional and Machine Learning Segmentation Techniques for Analysis of Digital Rock Physics Properties

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Image segmentation remains the most critical step in Digital Rock Physics (DRP) workflows, affecting modelling results and the digital analysis of rock properties. Conventional segmentation techniques struggle with numerous image artifacts and user biases, which lead to unsatisfying results. Here we introduce the advantages of the machine learning software ilastik to the DRP community.

Images of porous and fractured samples were acquired by X-ray computer tomography and segmented by both conventional methods and machine learning approaches. Porosity, permeability, flow fields, roughness and mechanical aperture were computed. A comparison with conventional segmentation methods highlights the superior capabilities of the machine learning approach, which does not need excessive amounts of training data. Instead, these are provided by the user directly on the dataset, where a constant feedback with ilastik minimizes user bias. Ilastik is easy to use, resource saving and produces high quality segmentations and provides uncertainty calculations as a quantitative measure for evaluating results. For our rock samples, the machine learning segmentation showed the best results and was able to handle every complexity without prior filtering. This comparison highlights the importance of a high-quality segmentation, if considerable variations in physical rock properties is to be considered like of our samples.

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Multi-scale modeling of mineral precipitation and dissolution in porous media

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Mineral precipitation and dissolution processes can alter the pore-scale structure of a porous medium, and hence affect the Darcy-scale flow through the medium. To bridge the gap between the pore-scale changes and their Darcy-scale effect we consider a two-scale model for single-phase flow where the evolution of the pore-scale structures is modeled through a phase-field variable. The phase field approximates the sharp-interface dynamics through an Allen-Cahn equation. The Allen-Cahn equation is in its original form not conservative, but we apply a reformulation which is conservative. The two-scale model is derived through homogenization and conveniently allows for efficient Darcy-scale simulations where the effective parameters, like permeability, are determined through local cell problems. The model is implemented using a multi-scale iterative scheme, applying adaptive strategies on both scales to improve efficiency.

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A new quantitative method to overcome the model-to-experimental data fit problem in multiphase flow in porous media

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Numerical modelling as scientific exercise can increase our process understanding of multiphase flow in porous media. Actual experimental or field data allow calibrating models, as well as testing assumptions and hypotheses within models via model-to-experiment comparisons. Such comparisons are often problematic for highly spatially and temporally resolved data sets like experimental movies: a model will never stand a pixel-by-pixel comparison; instead, weaker methods like perceptual similarity or analysis of spatial moments are traditionally used. Here, we propose a diffused version of the so-called Jaccard index (adapted from image analysis and object recognition) as an objective and quantitative goodness-of-fit metric. In a case study, we compare Invasion Percolation

(IP) models against a laboratory-scale experimental video of gas injection in homogenous, saturated sand. Despite being computationally fast, it is challenging to compare IP models to highly resolved data because of their lack of an explicit notion of time. To overcome this problem and enable an evaluation of the model-to-data fit, we perform a time-matching before applying the proposed Jaccard metric. The combined approach is found to be more objective and reliable than traditional comparison approaches. Further, the diffused nature of the metric allows comparing models to data at different scales of interest.

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Modeling the effect of microscale heterogeneities on soil bacterial dynamics and the impact on soil functions

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Mathematical modeling facilitates the understanding of soil microbial development and their function with respect to habitat and carbon cycling.
Our mechanistic model allows studying the dynamics of bacteria in unsaturated soils. The liquid and gas distributions are calculated according to a morphological model. Various bacteria strains and organic matter are heterogeneously distributed in CT scans of various soil samples.
The bacteria strains grow based on Michaelis-Menten kinetics due to the uptake of oxygen and dissolved organic carbon (DOC). Their development is realized in a cellular automaton framework (CAM). DOC is either present as a carbonaceous solution or hydrolized by a first order kinetics from heterogeneously distributed particulate organic matter (POM) sources. Reactive transport equations for both nutrients oxygen and DOC potentially including a Henry condition are discretized by the local discontinuous Galerkin (LDG) method.
Our simulations show that the impact that heterogeneity in nutrient and bacteria distribution has on overall biodegradation kinetics strongly depends on the scale of interest. We conclude that the heterogeneous spatial structure must be resolved scale-dependently. We include this information into a macro-scale model and estimate the overall CO2 production rate for different soil profiles.

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The impact of wettability, surface roughness & pore space structure on capillary trapping and fluid displacement in 2D and 3D porous media: A µ-CT study and micromodel experiments

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Immiscible fluid displacement in porous media is important in large number of industrial and natural processes. A comprehensive understanding of the combined effects of surface roughness and wettability on the dynamics of the trapping process is lacking in literature. The discrepancy is presumably caused by the surface roughness of the inner pore-solid interface. Herein, we present a comparative µ-CT-study of static fluid-fluid pattern in porous media with smooth (glass beads-GBS) and rough surfaces (natural sands-NS).
For the first time, a global optimization-method was applied to map the characteristic geometrical and morphological properties of NS to 2D-micromodels, exhibiting different degrees of surface

roughness. A realistic wetting model that describes the apparent contact angle (CA) of rough surface as a function surface morphology was proposed. Our results revealed that NS and GBS display opposite trends in terms of the CA-dependence between 5° and 115°. NS depicted a non-monotonous functional CA-dependency, i.e., a transition from maximal-trapping to no-trapping, followed by an increase to medium-trapping. In contrast, GBS showed a sharp transition from no-trapping to maximal-trapping. Since both porous media exhibit similar morphological-properties, we attribute this difference in behavior to surface roughness, that allows complete wetting and hence precursor thick-film flow for NS.

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On the efficiency of the 2D U-net model in the identification of fractures in quenched samples by means of micro-XRCT

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Characterizing the porous materials with high-resolution X-Ray Computed Tomography (micro-XRCT) has emerged as a standard procedure in laboratorial studies in recent years. Despite of technical improvements in the field of XRCT, challenges still remain due to the inherent signal-to-noise ratio and the low contrast of the acquired tomographic data. In order to overcome these challenges, digital image processing methods were conventionally applied, such as non-linear filtering to reduce the noise level, and threshold or morphology-based segmentation techniques. However, these steps often need a skillful operator and a substantial amount of time to identify the most appropriate method and fine-tune its parameters. Recently, by means of Machine Learning (ML) algorithms, the U-net segmentation algorithm showed an impressive performance. In this study, we present and discuss an image segmentation workflow which is applied on fracture networks obtained from quenched crystalline rock samples (Carara marble). The 2D U-net approach is compared to alternative image segmentation tools as hybrid conventional methods (sato and local threshold techniques). The 2D U-net model was successful in capturing the 3D structure of the fracture network efficiently, as well as some local properties like the aperture of a single fracture, while the aforementioned alternative methods have shown various drawbacks.

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Numerical Analysis of Hydro-Mechanically Tested Fractures Under In Situ Conditions

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Analysis of hydro-mechanical measurement data requires a strongly coupled numerical approach to better understand the driving forces throughout hydraulic testing of fractures. Hence, this work proposes a consistent hybrid-dimensional model to study fracture flow under in situ conditions and to discuss the importance of hydro-mechanical effects throughout hydraulic testing of fractures based on a consistent set of flow q, pressure p and fracture opening data δ obtained from measurements conducted at Grimsel Test Site. Analysis of the measurement data is performed by best numerical

fits and a decomposition of the injected fluid volume into volume compensated by the fluid's compressibility and volume created by fracture deformation to increase the understanding of flow in deformable fractures.

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Influence of radiation on evaporation rates: a numerical analysis

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We present a fully coupled soil-atmosphere model that includes radiation in the energy balance of the coupling conditions between the two domains. The model is able to describe evaporation processes under the influence of turbulence, surface roughness, soil heterogeneities. It is shown that evaporation rates are clearly dominated by the diurnal cycle of solar irradiance. During stage-I evaporation maximum temperatures are regulated due to evaporative cooling, but after a transition into stage-II evaporation, temperatures rise tremendously. We compare two different soil types, a coarser, sandy soil and a finer, silty soil and analyse evaporation rates,
surface temperatures and net radiation for three different wind conditions. The influence of surface undulations on radiation and evaporation is analysed and shows that radiation can lead to different local drying patterns in the hills and the valleys of the porous medium, depending on the height of the undulations and on the direction of the sun. At last a comparison of lysimeter measurement data to the numerical examples shows a good match for radiation values but evaporation rates are still overestimated in the model. Possible reasons for the discrepancy between measurement and model data are analysed.

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Simulating pore-scale evaporation with a pore-network model coupled to free flow

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Coupled systems of free flow adjacent to a porous-medium appear almost everywhere in nature and in technical applications. Interface-driven transport and exchange processes govern soil evaporation, fuel cell water management or food drying.

While a discrete, highly resolved (e.g., by means of DNS) description of these systems is computationally very often too expensive, averaged REV-scale approaches may fail to account for important pore-scale effects like local saturation distribution patterns in sufficient detail.

Our novel hybrid model captures pore-scale effects at the interface in ample detail while still maintaining a comparatively low computational effort.

The key feature is a pore-network model which represents the transition region between the porous matrix and the free flow.

Thermodynamic consistency is ensured by appropriate coupling conditions. We follow a monolithic coupling approach such that fluxes of mass, momentum and energy across the domain interfaces are preserved implicitly while no coupling iterations are required.

A fully implicit dynamic pore-network model is used in order to resolve flow and transport processes beyond capillary equilibrium.
The model is implemented in the open-source porous media simulator DuMux
which has recently been extend by the capability to couple an arbitrary number of subdomains.

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Parallel partitioned coupling simulation of fractured porous media

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The numerical coupling of fracture flow and deforming porous media, as it appears in hydraulic stimulation or hydro-fracking, is a challenging problem in reservoir engineering. Due to the often employed mixed dimensional modeling of the problem and the different differential equations used to model the physics in the different subdomains.

We investigate a partitioned black-box coupling approach in order to avoid solving the ill-conditioned system of equations resulting from a monolithic approach. Due to this we can use standard iterative solvers for the linear systems of equations instead of computationally expensive direct solvers. The black-box property of the coupling we follow allows for a simple setup or even reuse of the software needed. We observe that a suitable stabilization technique has to be used to ensure the stability of the coupling.

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Determination of effective transport parameters in porous media –Asymptotic Homogenization from theory to application

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Transport in porous media is central in chemical engineering. An accurate prediction of the effective transport properties is crucial for the assessment and improvement of many processes and applications. Traditionally, effective transport coefficients are determined by experiments or empirical correlations without considering structural properties in a strict way. In contrast, the Asymptotic Homogenization allows a rigorous calculation of effective transport coefficients of anisotropic, porous materials based on structural information [1].
In this work we present an approach to predict effective Knudsen diffusion coefficients of an anisotropic

microporous polymer membrane using the method of Asymptotic Homogenization. The proposed approach lays out the necessary steps to apply Asymptotic Homogenization to an anisotropic porous material. First: visualization and data analysis of the structure, second: the generation of a representative cell geometry and finally the numerical calculation. In addition, an experimental approach was applied to determine the effective Knudsen diffusion coefficients. The results obtained with Asymptotic Homogenization were validated by comparison with the experiments, which showed a remarkable agreement.

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Reactive transport modeling challenges in radioactive waste management in Germany

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Reactive transport and T-H-M processes in porous media often occur in a wide range of subsurface system applications such as nuclear waste disposal and geothermal energy systems. The numerical simulation of the long term behavior of these systems present several challenges to modelers and code developers due to the complexity of the coupled processes and their highly non-linearity. For example, these systems normally present coupled non-isothermal processes, different fluids (i.e. gas, groundwater) and multiple solid phases with different chemical composition. In addition, phase change process, controlled by pressure and temperature may also happen. To further increase the complexity, the long term fluid-rock geochemical interactions could play a role in the system and models should consider chemical reactions and their feedback to the hydraulic and flow field.
In this context our focus is to provide on the holistic scientific view on the safety of nuclear repository systems, quantifying their close –to-reality evolution with regard to physical, chemical and microbiological coupled processes mainly occurring in porous media. Specific objectives comprise the development of modeling capabilities for up-scaling related multi-physical and bio-geochemical processes from lab to field scales and establishing seamless workflows for safety performance assessment.

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Simulation of Thermochemical Heat Storage in the CaO/Ca(OH)2-System on the Micro-Scale

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Thermochemical Energy Storge (TCES) has long been under investigation for prospective applications including the capture of excess heat from industrial processes or storing energy in concentrated solar power plants. Furthermore, TCES in the CaO/Ca(OH)2-System is investigated because of the low price and environmentally friendliness of the reactants. In the project THEMSE, DLR is developing models and simulations for TCES in the CaO/Ca(OH)2-System on the microscopic level.
A geometrical microscale characterization of the material is done using a combination of micro computed tomography (µCT) and scanning electron microscopy (SEM). Where SEM can be used to

resolve fine scale details, up to crystallites, µCT can resolve particles as well as agglomerates of numerous particles. This is complemented by kinetics, measured by thermogravimetric analysis.
The first goal in the project is to explain the measured kinetics using a spatially resolved model, which takes the three-dimensional morphology of the storage material into account. In general, this involves, thermal, hydrodynamic, mechanical, and chemical modeling. However, the first investigations involve a single particle model, where the thermal and hydrodynamic effects can be neglected, and which is solved using finite element simulations.
In this talk, we give an overview over the project and the materials involved and we will show first results from kinetic simulations and experiments.
Simulation

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Feedback between Microbial Accumulation and Hydraulic Properties in Microfluidics and Pore-Scale Simulations

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In the presented work, we investigate accumulation and growth of microbes in microfluidics and its influence on the hydraulic properties of saturated porous media.
The change of porosity over time has been determined by optical microscopy and image segmentation of the water-saturated pore space and the accumulated biomass in the image sequences. Furthermore, the segmented images including the biomass have been used as "digital twin"–a digital representation of the experimental results –for direct numerical flow simulations.
The experimental study indicates the formation of preferred flow pathways with increasing biomass, which is reflected an associated porosity-permeability relationship. Furthermore, an intermittent release of biomass and subsequent filtration have been observed, leading to a stepwise local increase of biomass by filtration.
The numerical simulations were performed by assigning average permeability values to the biomass and solving the Navier-Stokes Brinkman equation in the pore space to get a best match to the experimental data and with this estimating the biomass permeability. In a further attempt, we assigned a permeability distribution on basis of the gray-scale image. The porosity-permeability relationship, effects of the micro porosity on the flow field and the sensitivity of the applied approach will be discussed in the presentation.

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A two-scale phase-field model for dissolution and precipitation of two minerals

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Mineral dissolution and precipitation play an important role in understanding different porous media problems such as geological CO2 sequestration or environmental contaminant transport. Precipitates can significantly alter the pore structure, impacting porosity and tortuosity, and naturally affect reactive transport pathways.

We consider a single phase Navier-Stokes description with solute transport of three dissolved species as well as precipitation and dissolution kinetics of two minerals. The mineral reactions are coupled via a dissolved species bound in both precipitates. The evolving fluid-mineral interfaces are approximated by phase fields using an Allen-Cahn formulation. Using matched asymptotic expansions we show that for shrinking width of the diffusive interface the expected sharp interface model is recovered.

To accurately model the effects of this porescale process on macroscopic behaviour we aim for a two-scale model. We employ periodic homogenization to arrive at a set of macroscopic equations for pressure, velocity and dissolved concentrations coupled to cell problems. These include a phase-field model of mineral distribution yielding effective diffusion and permeability tensors and determining the reactive terms in the macroscopic model.

We present numerical experiments on the pore scale to compare with alternative models of mineral evolution.

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EXPLICIT CONTINUUM SCALE MODELLING OF WATER-BASED IOR/EOR MECHANISMS

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The understanding of the impact of injection water composition on displacement efficiency is a long-standing issue in reservoir engineering; the lowering of injection water salinity may lead to additional oil production, which is considered a low cost and environmentally friendly method for enhanced oil recovery. Several underlying chemical mechanisms have been identified, but the identification of the governing mechanisms is still difficult and very specific to the chemical setting of the reservoir and the injection water composition. In this work, we stepwise implement an explicit chemical description of low-salinity effects in the open-source continuum-scale flow simulator DuMuX, with the goal of designing and interpreting experiments and for upscaling results. We implement two potential mechanisms namely double layer expansion and multicomponent ion exchange. By assuming sets of input parameters, we (a) benchmark simulation results against analytical solutions, (b) we study aspects of dispersive mechanisms on the experimental design of core flood experiments, and (c) we show, how the two mechanisms can experimentally be distinguished.

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Coupled advection-reaction-diffusion processes on an evolving microstructure: analysis and homogenization

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We consider a porous medium composed of solid matrix and pore space, which is completely saturated with a fluid. A dissolved concentration is present in the fluid, which is affected by diffusion and advection as well as reaction at the surface of the solid matrix. This reaction causes the solid matrix to grow or shrink locally. Thus, the microstructure of the porous medium changes, which affects the transport of the concentration. In order to upscale this problem, we consider an advection-reaction-diffusion problem coupled with the Stokes equation in a domain with an evolving microstructure. The mathematically rigorous homogenization of this problem is performed utilizing a transformation to a periodic reference domain and the macroscopic limit problem is determined using two-scale convergence.

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Modelling heterogeneous wetting with Smoothed Particle Hydrodynamics to predict electrolyte distribution in Technical Gas Diffusion Electrodes

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Porous gas diffusion electrodes (GDE) are a crucial part in important electrochemical processes like chlor-alkali electrolysis with oxygen-depolarized cathodes. In this process, the GDE is responsible for ensuring intimate contact between the silver catalyst, the gaseous reactants and the liquid electrolyte. Non-wetting Polytetrafluoroethylene (PTFE) is added in the manufacturing process to prevent the electrode from being flooded. Experimental investigations showed a strong dependence of the PTFE content on the performance of such electrodes [1]. The knowledge of the electrolyte distribution in this structure is essential for further improvement of such electrodes.

Recently, we showed the capability of the Smoothed Particle Hydrodynamics (SPH) method to model these structures based on FIB-SEM images [2]. However, modelling of representative structures is still challenging on larger structures. We present simulation results based on dynamic SPH simulations of the electrolyte imbibition process to estimate the pore entry pressure dependent on wettability effects at the fluid-fluid-solid-interfaces resulting from the PTFE-distribution, external pressure gradients and flow configuration. Incorporating such data in pore networks, can be used to predict electrolyte distribution and transport parameters on a larger scale.

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Arbitrary Multi-Resolution Multi-Wavelet-based Polynomial Chaos Expansion for Data-Driven Uncertainty Quantification

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Several uncertainty quantification techniques were successful used during the past decades. A variety of real-world applications requires to deal with data-driven surrogate models of complex systems. In geophysical applications the amount of available data is often limited, which poses the challenge for the construction of a stochastic discretization. Arbitrary polynomial chaos approximates the dependence of model output on uncertain model parameter by expansion in orthogonal polynomial basis using data-driven principles in a very efficient way. Unluckily the global polynomial representation suffers often from Gibbs'phenomena, especially if non-linear convection dominated problems require to deal with discontinuities.
To face the Gibbs'phenomena and reduce the oscillations of the polynomial representation, we extend the arbitrary polynomial chaos framework by the multi-resolution Ansatz using piecewise polynomials based on the underlying raw data. We enhance our approach by a multi-wavelet based stochastic adaptivity that assures a significant reduction of the computational costs.
Numerical experiments show the performance and confirm the accuracy of non-intrusive implementation of the introduced methods in a non-linear hyperbolic scenario driven by several uncertain parameters. The use of the carbon dioxide storage benchmark scenario allows to compare the presented methodology with other stochastic discretization techniques applied to this benchmark.

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Physics Informed Neural Network for porous media modelling

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Artificial Neural Networks (ANNs) have gained immense popularity for data-driven modelling and surrogate modelling. Increasing research has been conducted to implement ANNs to solve porous media flow problems, such as predicting the dynamics of multiphase flow and for contaminant transport in groundwater. However, because ANNs are black-box models that lack interpretability and neglect physical laws, the predictions are often not physically plausible –unless the available training data are so exhaustive and abundant that they can teach fundamental principles. Recently, a Physics Informed Neural Network (PINN) approach was proposed to tackle these issues. PINNs improve the prediction accuracy of ANNs by introducing additional regularization term in the form of physical laws, thus training the network to obey the prescribed laws. In our work, we study how the physical knowledge can be implemented to model porous media flow problems. We implement the physics-based regularization as proposed in the PINN framework, as well as design the architecture of our PINN based on known mathematical forms of the physical laws and based on similarity with existing numerical simulation schemes. The suggested approach improves not only the accuracy, but also the physical plausibility of the model predictions, even at smaller amount of training data.

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Modelling fluid-driven fractures in partially saturated porous materials

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Fluid-driven fractures are frequently used in the energy sector, even though the control of these processes is still widely based on empirical methods. To enlarge the knowledge of the ongoing processes and prevent severe geological consequences, a systematic theoretical understanding of fluid-driven fractures in porous media is crucial. Since soils are generally partially saturated, this contribution focuses on a triphasic approach.

In this regard, a continuum-mechanical model for hydraulically induced fractures is presented on the basis of the Theory of Porous Media and the phase-field approach to fracture. The material is described on the macroscopic scale as an immiscible mixture of a solid phase, representing the solid skeleton, and two fluid constituents, namely a liquid and a gaseous pore fluid. By use of this model, capillary effects are taken into account. Moreover, the fracturing process is modeled with a phase-field approach, characterising a diffuse crack pattern. Hereby, the crack propagation in the solid skeleton is driven by the pressure field of the injected fluid.

The resulting set of coupled partial differential equations is implemented in the finite-element solver PANDAS. Numerical examples showing the coupled processes of crack propagation in partially saturated porous materials are discussed.

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Image-based characterization of multi-phase flow in porous media

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Understanding the physics of immiscible two-phase flow in porous media is not a straightforward process due to a number of factors, i.e. the fluid or the solid matrix properties, and the solid-fluid interaction.
Given the pronounced effects of pore-scale geometry and pore-fluid configuration on two-phase flow, various attempts have been made to embed these parameters in a macroscopic continuum, i.e. mean-field, models. However, these models fail to incorporate the effect of small-scale topological features, e.g. phenomena related to trapping mechanisms in the evolution of the flow.
The ultimate objective of our work is to develop an enhanced (image-based) data-integrated continuum model for two- and multi-phase flow for applications on larger scales. To achieve this goal, we study the effects of the pore structure (topology and geometry) on the flow in combination with the phase diagram proposed by Lenormand et al. 1988. Artificial porous media, micro-models, with distinct properties regarding their geometry were designed and manufactured. We then performed experiments for a series of combinations between the capillary number and the viscosity ratio in order to put Lenormand's phase diagram to test, and identify the effect induced by the topological characteristics, in combination with the fluid properties and the boundary conditions.

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Uncertainty quantification and global sensitivity analysis for coupled porous-medium and free-flow problems

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Coupled porous-medium and free-flow problems appear in various industrial and environmental applications, e.g. surface-groundwater interaction, industrial filtration, and evaporation processes. Mathematical models for such coupled problems contain several effective parameters that have uncertain nature. Quantification of these uncertainties is crucial for accurate modelling and simulation of coupled flow problems.

In the current work, we consider the Stokes equations describing fluid flow in the free-flow domain, single-phase Darcy's law in the porous medium and the classical set of interface conditions (conservation of mass, balance of normal forces and the Beavers-Joseph condition for the tangential velocity). The crucial question is how sensitive is the coupled model to such uncertain parameters as the Beavers-Joseph coefficient, the permeability of the interfacial zone and the location of the sharp fluid-porous interface.

Polynomial chaos based techniques are widely used for uncertainty quantification as computationally very efficient approaches. The arbitrary polynomial chaos is often applied due to the flexibility of its data-driven design. Sobol-index based sensitivity analysis allows to quantify the influence of the single uncertain parameters or parameter combinations on the variance of the model. Transferring this concept to coupled flow problems, we can localize the relevant uncertain model parameters and focus computational resources on them.

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An SPH approach for pore-scale resolved simulations of fluid flow through porous media

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We employ fully-Lagrangian Smoothed Particle Hydrodynamics (SPH) as a simulation method to model pore-scale resolved flow by means of weakly-compressible Navier-Stokes equations. The solver allows massively parallel CPU and GPU computations and showed a sufficient scaling behaviour as well as numerical accuracy \cite{osorno2019}. The implementation includes constitutive models for both Newtonian and Non-Newtonian fluids as well as for flow with immersed solid particles. Applications are the evaluation of effective (coarse-grained) model parameters like intrinsic permeability and the analysis of near field forces of suspended solid particles. We focus on 3-D pore-scale resolved computations of single-phase fluid flow through reservoir rocks for high Reynolds numbers aiming to show a smooth transition of effective intrinsic permeability and tortuosity from creeping flow to a weak inertia regime. An additionally field of interest are solid particles immersed in a fluid as it can be found in suspensions or sedimentation processes. We therefore present a modeling approach for fluid flow containing solid aggregates. Notable model specifications are the surface-coupled fluid–solid interaction forces and the contact forces between solid aggregates. We investigate the motion of suspended solids (in Newtonian and Non-Newtonian carrier fluids) and moreover discuss their interaction with fluid and the surrounding porous material \cite{kijanski2020}.

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Validation and calibration of coupling concepts for Stokes-Darcy problems

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Coupled free-flow and porous-medium flow systems appear in many environmental and technical applications (surface-groundwater flows, industrial filtration, water-gas management in fuel cells). Interaction between these flow regions is dominated by interface driven processes and the coupled problem is sensitive to the choice of interface conditions.

We study coupled Stokes-Darcy problems and consider two sets of interface conditions: the classical conditions (conservation of mass, balance of normal forces, Beavers-Joseph condition) and newly developed coupling conditions for arbitrary flows. Effective parameters appearing in the classical conditions and the location of the sharp fluid-porous interface are uncertain. We find the optimal interface position by comparing macroscale simulation results to pore-scale resolved models. To compare velocity and pressure, the pore-scale results are averaged using several strategies (volume averaging, Voronoi partition). The interface position providing the minimal difference between the averaged pore-scale values and the macroscale ones is optimal. For the new interface conditions for arbitrary flows all effective parameters are computed based on the pore geometry and chosen interface location. For model validation, we compare these interface conditions to the classical ones with the optimal interface position.

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An Uncertainty-Aware Bayesian Framework for Validation of Flow Models in Porous Media

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In the field of modeling, *validation* refers to simple comparisons that constitute plotting the model results against experimental data to provide a visual assessment of agreement or lack thereof. Firstly, these comparisons tend to provide qualitative rather than quantitative assessments and are clearly insufficient as a basis for making decisions regarding model validity. Second, naive comparisons often disregard or only partly account for existing uncertainties in the experimental observations or the model input parameters.

These pitfalls give rise to the need for an uncertainty-aware framework that includes a validation metric. To address this need, we have developed a statistical framework that incorporates a fully Bayesian probabilistic modeling technique. A Bayesian perspective on a validation task yields an optimal bias-variance trade-off against the experimental data and provide an integrative metric for model validation that incorporates parameter and conceptual uncertainties. Additionally, to accelerate the validation process for computationally demanding flow and transport models in porous media, the framework is equipped with a model reduction technique, namely Bayesian Sparse Polynomial Chaos Expansion. We demonstrate the capabilities of the aforementioned Bayesian validation framework by applying it to several applications for validation as well as uncertainty quantification of flow and transport models in porous media.

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Dynamic Mechanical Analysis (DMA) for High Performance Concrete: A Means for Damage Analysis

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High Performance Concrete (HPC) is in the focus of current research and construction projects, due to its outstanding stiffness and durability.

HPC is a low porous medium, which means that when dealing with HPC, hydro-mechanical interaction phenomena between its solid matrix and its pores and potential fractures have to be accounted for, especially if the pore space is fully saturated with a pore liquid. In addition, under harmonic excitations (micro-) fractures evolve and the inherent pore space of the sample is significantly changed. Nevertheless, because of their relatively small apertures,
these fractures may be difficult to resolve in a considered Representative Volume Element with established non-destructive imaging techniques like X-Ray Computed Tomography.

In contrast to this, frequency-dependent effective material properties obtained in amplitude-sensitive forced harmonic oscillation experiments can provide an insight into the damage process of a liquid saturated porous medium. With regard to the heterogeneous pore space and the stiffness contrast between pores and fractures, resulting pressure differences lead to Squirt-flow-type phenomena on the micro-scale of HPC. The inherent effective response of the material, measured in frequency-dependent material properties, is a 'fingerprint' of the damage process of the material.

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Modeling of solute transport in drying porous media: transition from micro to macro scale

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The understanding of the transport mechanisms involved in drying of capillary porous media initially saturated with saline water is key to many processes. In order to predict the evolution of salt concentration in a porous medium, the macroscopic continuum models (CMs) are commonly employed. However, the predictive aptitudes of the CMs are still questionable at this stage. In this work, we solve the classical CM, i.e. the one-dimensional advection-diffusion equation, for salt transport in an isothermally drying capillary porous medium for the limiting condition of capillary-dominated regime. The solution of the continuum model is compared with three-dimensional microscopic pore network simulations. The results of both models are analyzed in terms of local salt concentration profiles and the ability of the continuum model to reciprocate the pore network simulation results is assessed. Moreover, we characterize the process of fragmentation in the liquid phase through pore network Monte-Carlo simulations, whereby the results are statistically analyzed and the probability is computed for first solid crystals to appear in the fragmented liquid phase elements. We observe that salt enrichment is more pronounced in the fragmented liquid elements due lack or significant hindrance to back-diffusion as a result of discontinuity in the liquid phase.

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An open, modular and flexible micro X-Ray Computed Tomography system for porous media research

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The capability which micro X-Ray Computed Tomography (μXRCT) as a non-destructive imaging technique offers is meanwhile well known and often used for the microstructural characterization of porous media. In this contribution, we present a modular μXRCT system, where the focus from the beginning was on a high flexibility and a large available space for in-situ experimental setups. To accomplish this, a modular and open concept was applied, which allows changes on every hard- and software level. To maximize the chamber for quasi-static in-situ setups, the system was installed on an optical table which is inside an accessible lead shielded cabin, comparable to the environmental conditions in tomography beamlines located at synchrotron radiation facilities. Latter allows a realistic preparation of experimental setups for further transient investigations in such high X-Ray flux facilities. The presented work motivates and demonstrates an alternative solution for researchers that do not want to have the limitations related to commercial available XRCT benchtop devices. A performance study of the system is given and some typical application examples, all open access published, demonstrate what can be done and how good the data set quality is.

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A Numerical Model for Enzymatically Induced Calcite Precipitation

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One of the key issues of underground gas storage is the long-term security of the storage site. Amongst the different storage mechanisms, cap-rock integrity is crucial for preventing leakage of the stored gas due to buoyancy into shallower aquifers or, ultimately, the atmosphere. This leakage would reduce the efficiency of underground gas storage and pose a threat to the environment.

An emerging biomineralization method is enzymatically induced calcium carbonate precipitation (EICP). A new conceptual and numerical model for EICP is presented. The model has been calibrated and validated using quasi-1D column experiments designed to provide the necessary data for model calibration. The challenge is constructing a predictive model for the permeability reduction by EICP is to quantify the complex interaction between flow, transport, adsorbed enzyme, and reaction kinetics.

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A mixed-dimensional discontinuous Galerkin scheme for fluid flow through fractured porous media with fractures of non-constant aperture

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We study a fractured porous medium at a macroscopic scale such that fractures can be modeled individually. Based on a mixed-dimensional model for Darcy's flow, where fractures are represented by (n − 1)-dimensional interfaces between n-dimensional subdomains, we consider a mixed-dimensional discontinuous Galerkin scheme to numerically solve the coupled flow problem. The convergence of the scheme is validated through two- and three-dimensional numerical experiments. We especially consider the case of fractures with non-constant aperture, for which we propose a new modification of the scheme and confirm its convergence through numerical experiments. Moreover, especially for fractures of non-constant aperture, we numerically examine the model error due to approximations in the derivation of the mixed-dimensional model.

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Asymptotic analysis of immiscible two-phase flow with moving contact line in a thin strip

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We consider a model for the flow of two immiscible fluids in a two-dimensional thin strip of varying width. This represents an idealization of a pore in a porous medium. The interface separating the fluids forms a freely moving interface in contact with the wall and is driven by the fluid flow and surface tension. The contact line model incorporates Navier slip boundary conditions and a dynamic and possibly hysteretic contact angle law.
We assume a scale separation $\varepsilon \ll 1$ between the typical width and the length of the thin strip. Based on asymptotic expansions and letting ε approach zero, we derive effective models for the two-phase flow. These models form a system of differential algebraic equations for the interface position and the total flux. The result is a Darcy-type equation for the flow, combined with a capillary pressure - saturation relationship involving dynamic effects.
Finally, we provide some numerical examples to show the effect of a varying wall width, of the viscosity ratio, of the slip boundary condition as well as of having a dynamic contact angle law.

Keywords:
Asymptotic expansions;
Two-phase flow;
Freely moving interface;
Dynamic contact angle;
Thin strip;
Upscaled models

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Towards data-integrated simulation of growth and regression of tumours in brain tissue

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In this project we study data-integrated modelling of tumour growth and regression in brain tissue. We expect that the combination of data-integrated approaches with continuum-mechanical models results in faster and more reliable simulations, allowing for potential clinical applications.
Following the framework of the macroscopic Theory of Porous Media (TPM), the relevant microscopic components of the overall aggregate are volumetrically averaged and considered as superimposed constituents with internal interactions. Basically, a solid and a fluid phase are distinguished. These phases are build up by accumulating components. In particular, the solid phase consists of healthy φ^{Sh} and tumorous tissue cells φ^{St}. The interstitial fluid φ^{I} contains a base liquid φ^{Is} with the dissolved components; nutrients φ^{In}, mobile cancerous cells φ^{It} and vascular endothelial growth factors (VEGF) φ^{Iv}.
The mathematical formulation of the model consists of governing coupled partial differential equations, that are solved using the finite-element method. Thereby the spatial domain is discretised by numerically stable Taylor-Hood elements and the temporal domain by an implicit Euler scheme. Presented numerical examples show the processes of proliferation, apoptosis, necrosis, angio- and lymphangiogenesis. Proceeding from these reference solutions, the model enrichment with data-based techniques, such as surrogates, model-order reduction or machine-learning tools is discussed.

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A subcell-enriched Galerkin method

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In this presentation, we will discuss a generalization of the enriched Galerkin (EG) method. The key feature of our scheme is an adaptive two-mesh approach that, in addition to the standard enrichment of a conforming finite element discretization via discontinuous degrees of freedom, allows to subdivide selected (e.g. troubled) mesh cells in a non-conforming fashion and to use further discontinuous enrichment on this finer submesh. We prove stability and sharp a priori error estimates for a linear advection equation by using a specially tailored projection and conducting some parts of a standard convergence analysis for both meshes. By allowing an arbitrary degree of enrichment on both, the coarse and the fine mesh (also including the case of no enrichment), our technique is very general in the sense that our results cover the range from the standard continuous finite element method to the standard discontinuous Galerkin (DG) method with (or without) local subcell enrichment.

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Experimental Investigation of Chemical Assisted CH4/CO2 Exchange in Porous Medium

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We investigate CH4/CO2 hydrate exchange in unconsolidated porous media with and without hydrate former. CO2 rich gas injection into a natural gas hydrate reservoir is proposed as a novel technique to produce natural gas and simultaneously store CO2 without disturbing the geological settings. This method is limited by mass transport due to hydrate film acting as a barrier at the liquid/gas interface. The very low CO2 diffusivity through these films causes delay in CH4/CO2 exchange. A few simulation studies suggest that adding a small concentration of surface active chemicals can improve the diffusivity through hydrate film. To confirm, we formed CH4 hydrate from gaseous CH4 and a solution containing a small concentration of different chemicals (surfactant, amino acid, and methanol). Pure CO2 is injected into this reservoir to initiate CH4/CO2 exchange. P-T and GC analsyis is carried out using high pressure cell and unconsolidated sand (particle size 0.9-1.6 mm). CH4/CO2 mixed hydrate are formed at reservoir conditions (P = 50-65 bar and T = 1.0-3.0℃). Changes in CO2 and CH4 concetration in vapor are measured. The results showed that 5% methanol was able to enhance methane production and CO2 storage efficiency as well as reduced the risk of reformation.

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Numerical modeling of hydro-thermo-mechanical processes in fluid-saturated fractured rocks

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Consideration of thermo-hydro-mechanical processes is essential for the understanding of fluid transport in rocks, e.g. associated with geothermal heat provision, as well as for many engineering applications dealing with physico-chemical interactions between fluids and solids at elevated temperatures. The fluid transport in hydraulically open fractures in porous rock is particularly important for the characterization of fracture interaction e.g. in geothermal reservoirs.
We investigate networks of thin fractures that are embedded in a matrix containing several fault zones, which are modelled as large-scale homogeneous features with enhanced permeability and porosity. Therefore, the fractures are modeled with a sharp interface formulation in a three-dimensional poroelastic matrix with varying properties. Here, classical balance equations are combined with a Couette-Poiseuille-type flow in the dimensionally reduced fractures. This enables us to investigate more complex networks of fractures with low aperture.
Different geometries of fracture networks are investigated and benchmarked against classical thermo-poromechanical formulations. We analyse inhomogeneous boundary conditions to mimic pumping tests from a borehole in a fluid-saturated reservoir.
Our goal is to model the thermo-hydro-mechanically coupled processes and fracture interactions within natural fractures around a borehole, aiming to predict the reservoir behavior.

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Experimental Methods and Imaging for Enzymatically Induced Calcite Precipitation in micro-fluidic devices

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Enzymatically Induced Calcite Precipitation (EICP) in porous media can be used as an engineering option to achieve targeted precipitation in the pore space. It is associated with an alteration of porosity and, consequently, permeability. A major source of uncertainty in modelling EICP is in the quantitative description of permeability alteration due to precipitation based on conventional porosity-permeability relations [1]. To improve REV-scale models, we investigate the effect of EICP on hydraulic properties in micro-fluidic experiments, measuring the pressure drop to calculate the permeability while quantifying the change in porosity by optical microscopy as well as X-Ray Computed Tomography (XRCT). The results of the study show the enormous benefits and insights of combining both microscopy and XRCT with hydraulic measurements in micro-fluidic devices. This allows for a quantitative analysis of the evolution of precipitates while monitoring the influence on the permeability, and thus improves the interpretation of monitored flow data dependent on changes in pore morphology.

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The Influence of Motility on Bacterial Accumulation in a Microporous Channel

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Swimming microorganisms are often encountered in confined, porous geometries where also an external flow is present, e.g. in filters or inside the human body. To investigate the interplay between microswimmer motility, confinement and external flows, we developed a model for swimming bacteria based on point coupling to an underlying lattice Boltzmann fluid. With this implementation, straight swimming motion interrupted by random reorientation events reproduces the motility pattern of the run-and-tumble bacterium E. coli. We present the application of the model to the study of bacterial dynamics in a simplified porous geometry: A rectangular channel with a single cylindrical obstacle. In accordance with experimental measurements, the results show asymmetric accumulation behind the obstacle only when the bacteria are active and an external flow is present[1]. We quantitatively compare bacterial densities from simulations to the experiments and investigate the physical mechanisms that lead to accumulation.

[1] M. Lee et al.: *The Influence of Motility on Bacterial Accumulation in a Microporous Channel*, Soft Matter, 2020, DOI: 10.1039/D0SM01595D

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Hydro-mechanical continuum modelling of fluid percolation through salt rock

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Underground salt caverns for storing hydrogen offer a promising option to reduce CO₂ emissions by improving the utilization of volatile renewable energy sources.

Simulations play an important role in predicting the long-term stability of caverns. Salt rock limits the infiltration of hydrogen into the contour due to its favourable low permeability, however pressure driven percolation may create non-linear pathways for the fluid and damage the cavern. Depicting this effect accurately in simulations may pose crucial for assessing the long-term stability correctly.

By introducing an extension to a permeability model by Olivella and Alonso we can capture the non-linear fluid behaviour using continuum models. Based on the quasi-isotropic arrangement of potential flow paths the model is able to reproduce percolation experiments on salt rock specimens in terms of breakthrough pressure as well as preferential path orientation and locality. The model is implemented in the scientific open-source framework OpenGeoSys6.

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Data-driven homogenization based on neural networks for permeability estimation

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The intrinsic permeability is a crucial parameter which characterizes and quantifies fluid flow through porous media. Correct estimation of permeability is important for physically consistent modeling and accurate numerical simulation of flow and transport processes in porous media. While the computation of permeability via mathematical homogenization is possible for simple periodic porous media, albeit computationally expensive, more complex structures represent a problem where neural networks can contribute.

We test the applicability of neural networks for an accurate estimation of permeability. Our research results verify the convolutional neural networks to be optimal for this task, as the permeability is primarily characterized by the underlying geometrical configuration of porous media. The predicted permeability is accurate for both two-dimensional and three-dimensional geometries, which we model by employing a voxel representation. The created datasets contain a variety of different geometries in order to properly test the networks ability to generalize. A fully trained convolutional

neural network requires a fraction of the computation time required by mathematical homogenization in order to accurately predict the permeability.

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Wetting transition and freezing of ionic liquids in nano-confining conducting porous media: an effective Thomas-Fermi screening approach

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Hierarchical porous electrode materials are promising candidates for next generation energy storage due to their combination of a large surface to volume area with controlled meso-/macroporosity to overcome slow diffusion in nanopores. However, at the nanometer scale the standard image charge approach for electrostatics close to metallic interfaces breaks down due to the finite screening in any real metal. Recent experiments revealed a freezing transition of ionic liquids between surfaces of varying metallicity.

We here develop an effective approach to deal with any real metal using the Thomas–Fermi formalism in which electrostatic screening is described through the behavior of a charged fluid whose Debye length sets the screening length λ. This easy-to-implement molecular method captures the electrostatic interactions upon varying λ from insulator to perfect metal conditions.

Applying this strategy to a nanoconfined ionic liquid, an unprecedented wetting transition is found upon switching the confining medium from insulating to metallic. The wetting behavior at imperfect metals is identified to induce freezing of strongly charged liquids in confinement, which raises new challenging questions on the complex behavior of charged systems in the vicinity or confined within surfaces with important applications such as electrowetting/switching for energy storage, lubrication, catalysis, etc.

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Pore-specific Wetting in PEFC Catalyst Layers Elucidated by Small Angle X-ray Scattering

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In polymer electrolyte fuel cells (PEFC), the water management is crucial for achieving high performance. Although the knowledge about water management in the catalyst layer is continuously improving, it has not been fully understood so far. In the past decade, an extensive range of methods for *ex-situ* and *operando* imaging of water in the porous structures of the PEFC has been explored, mainly x-ray and neutron imaging methods [1,2]. However, they are insufficient to explain the mechanism of catalyst layer saturation. Here, we introduce small angle x-ray scattering (SAXS) as

a characterizing tool, able to fit to the length scale of pores in the catalyst layer (29-183 nm) [3]. We confirmed the feasibility of the SAXS-based catalyst layer wetting study with *ex-situ* and *in-situ* wetting of Pt/C catalyst layers. Random morphological model was developed and applied to aid data interpretation. This insight of wetting phenomena in PEFC catalyst layer is valuable for advancing materials development.

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Unravelling pore-scale processes in geomaterials

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To fully understand the macroscopical behavior of geomaterials, their pore scale properties and processes have to be understood. The stone's mineralogy and pore structure strongly affect key internal pore scale processes. To explore these dynamic pore-scale processes, several non-destructive 3D and 4D methods are currently available. Unravelling pore-scale processes in combination with pore scale modelling is an essential step towards understanding and predicting a geomaterial's macroscopic behavior correctly.

The presentation discusses the current possibilities and challenges in non-destructive pore-scale imaging of geomaterials and how this data can be used as input for fluid flow models and their validation. Additional new developments at the synchrotron and on lab-based X-ray systems related to material characterization as well as to the understanding of pore-scale processes are discussed. Examples will be given of different experiments related to the characterization and the imaging of dynamic pore scale processes in geomaterials.

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The role of porous media for water transport in plants

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A longstanding question in biology is how plants are able to operate a transport system under negative pressure without continuously developing large gas bubbles, which would reduce sap transport from roots to leaves. This is a highly puzzling process because the water transported is saturated with gas and includes insoluble, amphiphilic lipids, which can act as strong surfactants. We speculate that transport under negative pressure is possible thanks to porous cell walls between neighbouring conduits. The 200 to 1,000 nm thick porous cell walls are estimated to have a porosity of 80%, and 20 nm wide pore constrictions. They play a crucial role as safety valves, and together with the local surface tension of lipids at gas-liquid interfaces may produce surfactant coated nanobubbles. Experimental evidence showed that partial removal of the porous cell walls in stem segments does not allow water transport under negative pressure, while electron microscopy confirmed the presence of surfactant-coated nanobubbles in plant sap. Further work on multiphase interactions between gas, surfactants, water, and solid substances are needed to provide a more complete mechanistic understanding of plant water transport, which would also be useful to develop evaporation-driven transport devices that do not rely on fossil fuels.

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The Theory of Porous Media with Applications in Environmental Engineering, Biomechanics and Materials Science

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Many materials show a multiphase composition and have a distinct microscopic structure. Examples of multiphase materials are saturated or partly saturated porous material like soil, concrete but also steel and biological tissue like cartilage or bone. Their substructures are e.g. pores, fibres with different orientations or cells which can be influenced by bio-chemical reactions. The high complexity of those kind of material makes it reasonable to consider homogenization approaches and multiscale techniques in order to find an effective modeling access for the numerical simulation. This is even more the case since modern experimental methods as CT-scanning or MRI imaging give us the opportunity to get a deep insight into the microscale structure. Thus, we will present a combined multiphase-multiscale approach for the description of those kinds of materials. The method is based on the well-known Theory of porous media (TPM), a continuum mechanical homogenization approach founded on the mixture theory in combination with the concept of volume fraction. Depending on the material, we will combine the TPM with reasonable multiscale techniques such as FE2, POD-ODE, or the Phase Field method.

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Beyond Kozeny-Carman: Predicting the Permeability in Porous Media

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An accurate modeling of the permeability and diffusion coefficient is essential for predictive flow and transport models. Well-established relations are proposed by Kozeny-Carman for the permeability, which relates the scalar permeability coefficient to the porous medium's porosity. In order to capture the porous medium's structure in more detail, further models include fitting parameters, geometric, or shape factors. Some models additionally account for the tortuosity, e.g. via Archie's law. Contrarily to these approaches, upscaling methods directly enable to calculate the full, potentially anisotropic, effective permeability tensor without any fitting parameters. As input only the geometric information in terms of a representative elementary volume is needed. To compute the permeability-porosity relations, supplementary cell problems must be solved numerically on this volume and their solutions must be integrated. We apply this approach to provide easy to use quantitative permeability-porosity relations that are based on representative single grain, platy, or blocky soil structures. Similarly, we determine the effective diffusion coefficient and make the derived relations explicit by interpolation of the obtained data.

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The Role of Local Instabilities in Fluid Invasion into Permeable Media Studied by in situ X-Ray Microtomography

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Considering the paradigmatic case of random piles of spheres, fluid front morphologies emerging during slow immiscible displacement with a global front velocity of 3 μm/s are investigated in real time by X-ray micro–tomography and quantitatively compared with model predictions. Controlled by the wettability of the bead matrix two distinct displacement patterns are found with a transition region of about $\Delta\theta \approx 30^\circ$ separating both regimes. Within each regime the displacement behavior is fairly insensitive to the exact contact angle [1].

A compact front morphology emerges if the invading fluid wets the beads while a fingered morphology is found for non–wetting invading fluids, causing the residual amount of defending fluid to differ by one order of magnitude. The corresponding crossover between these two regimes in terms of the advancing contact angle is governed by an interplay of wettability and pore geometry and can be predicted on the basis of a purely quasi–static consideration of local instabilities that control the local progression of the invading interface as similarly introduced by Cieplack and Robbins for 2D systems [2], [3]. In particular the absence or the appearance of 'Burst-Instabilities'where the local instability occurs when the pressure in a throat exceeds the required filling pressure can be used to distinguish the transition between both wetting regimes. For the non-wetting system where the local front progression occurs mainly by 'Burst-Instabilities'an interconnected and very extended network of invading and defending phase develops at later times. The interconnected network of the defending phase is slowly drained by gutter flow leading to an increased residual saturation which is reached only after a substantial flush of the invading phase. If time allows, also the situation of bead and grain packs consisting of heterogeneous bead sizes, grain shapes or heterogeneous wettability will be discussed in brief.

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