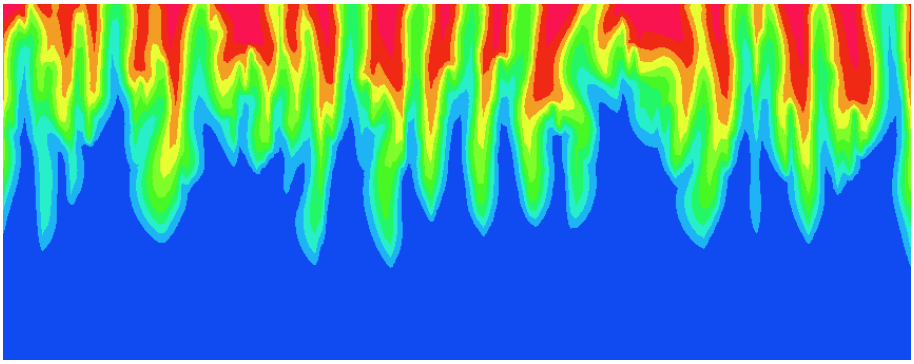
Workshop SITRAM

Advances in the SImulation of reactive flow and TRAnsport in porous Media

University of Pau & Adour Region, France, 2-3 December, 2019

Book of Abstracts



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PREFACE

Welcome to SITRAM 2019!

It is our great pleasure to welcome you to Pau for the Workshop "Advances in the **SI**mulation of reactive flow and **TRA**nsport in porous **M**edia" (**SITRAM**). We hope you will enjoy both the program of the event as well as the beautiful city of Pau.

The SITRAM Workshop is a forum for discussing recent research on the development and applications of both modeling and simulation for coupled transport and geochemistry in subsurface flow. The purpose of this Workshop is to bring together students, researchers and engineers who are active in the broad area of reactive flow and transport in porous media, and to create a fertile forum for presenting research results, exchanging ideas, and initiating collaborations. The Workshop follows other similar events organized in 2015 and 2018 under the umbrella of the MoMaS research group and the National French Research Group MaNu/CNRS GdR 2439. As organizers, we hope there will be more to come in the future

The Workshop will feature presentation on topics including: reactive multiphase flow, the impact of reactions on mechanics (changes on porosity or permeability), discontinuous kinetic reactions, numerical methods for coupling flow, transport and reactions and HPC issues.

A desirable outcome of the Workshop will be the definition of a new benchmark targeted towards two-phase flow with reactive transport in porous media.

This Workshop was jointly organized by the Laboratory of Mathematics and its Applications of PAU - UMR CNRS 5142 of the University of Pau and Adour Region (France) and by the Project-team SERENA of INRIA, the French National Institute for computer science and applied mathematics, in Paris. This event is held in the framework of the National French Research Group MaNu/CNRS GdR 2439 and under the auspices of the French Interpore Chapter (FIC).

This book contains the abstracts of the invited lectures and contributions presented at SITRAM 2019. The scientific program of the Workshop consisted of 20 invited talks and 8 contributed talks. The Workshop was attended by about 50 participants coming from 8 countries: France, Germany, Italy, Morocco, The Netherlands, Norway, Spain and Switzerland. We would like to thank the invited speakers and all of you for your participation at the Workshop.

The Workshop could not have been held without the financial support of the organizing institutions and the following sponsors: the IPRA Research Federation (FR CNRS-UPPA 2952), the French Research Group MaNu/CNRS, Agence pour les mathématiques en interaction avec l'entreprise et la société (AMIES), Investissements d'avenir (CGI) and the Carnot Institute, ISIFoR project (Institute for the sustainable engineering of georesources. We thank them for their financial support. The support of the French Interpore Chapter (FIC) and Société de Mathématiques Appliquées et Industrielles (SMAI) is also greatly acknowledged.
We would like to thank Etienne Ahusborde, Marie Laure Rius and Sophie Hontebeyrie (Uni-

versity of Pau E2S & CNRS, IPRA-LMAP) for their active role in the organization of the logistics of the conference.

On behalf of the organizing committee, we wish you a pleasant and fruitful meeting and hope you enjoy your stay in Pau.

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A NONLINEAR PRECONDITIONER FOR REACTIVE TRANSPORT IN HETEROGENOUS POROUS MEDIA

Laila Amir and Michel Kern

Keywords: Reactive transport, porous media, preconditioning, elimination method, nonlinear systems, Newton-Krylov method.

Reactive transport modeling in porous media involves the simulation of several physico-chemical processes: flow of fluid phases, transport of species, chemical reactions between species. The solution of the system of equations that describes the overall model can be obtained either by a fully coupled approach or by a decoupled approach. In [1] we have introduced a method that tries to combine the advantages of both approaches: it allows a separation of transport and chemistry at the software level, while keeping a tight numerical coupling between both subsystems.

The coupled system, written as a fixed point problem, is solved by a Newton-Krylov method, with a block Jacobian computed from the individual subsystems. However, the size of the nonlinear system obtained is quite large, and the Krylov solvers can stagnate.

In this talk, we present a nonlinear preconditioner [2], based on eliminating some unknowns from the coupled system, and we show its relationship with linear preconditioners methods like block Gauss-Seidel or block Jacobi. We present both heuristic and experimental arguments that show that both linear and nonlinear convergence become independent of the mesh size.

The performance of the method will be illustrated on a well known reactive transport test case: the 1D and 2D MoMaS benchmark.

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LABORATORY AND FIELD SCALE SIMULATIONS OF IN-SITU PYROLYSIS PROCESS

Alfredo Perez-Perez, Marelys Mujica and Igor Bogdanov

Wide CHLOE's experience in numerical simulations of enhanced oil recovery methods (EOR) and most recently the geological carbon storage processes includes various examples of what can generally be called reactive flow models. For instance, the chemical EOR application study which is still in progress and makes part of our current and nearest future research program comprises numerical analysis of lab-scale tests results of secondary and/or tertiary polymer and alkali-polymer flooding. Several series of coreflooding tests have been successfully analyzed using the same *physical* description of heavy oil(s), polymer(s) and O/W emulsion behavior, the *chemical model* being adapted per different alkali types involved (NaOH, NH_4OH ...). Mention that in this study the *chemically* induced significant modifications of fluid properties resulted in the oil production mostly as heavy-oil-in-water emulsion, did not concern at all the physical state of porous matrix.

Much more diverse in *physical and chemical consequences* has finally been the thermal EOR application example, namely, the simulations at lab and field scale of in-situ upgrading (IU) process based on local reservoir oil heating up and exposition to 380ÂřC for reasonably long time. Like in the above case of AP-flooding the first step of numerical analysis was aimed at development of general enough model using the IU lab test results obtained for different experimental setups. In case of typical Athabasca bitumen the initial IU model has incorporated tens of chemical components and reactions which finally generated quasi-solid residue (pyrobitumen) remaining underground, some amount of produced liquid hydrocarbon mixture and considerable volume of gas (C1-C4). The developed model was capable to represent the phase distribution of pseudo-components, the thermal decomposition (pyrolysis) reactions of bitumen fractions and the generation of gases and solid residue under the laboratory conditions. Furthermore, it has been used on one hand for pre-simulations with a purpose to design future IU experiments, and on the other it was validated via application to IU field-scale test published in literature.

In order to better understand the IU field-scale test results, Shell's Viking (Peace River) pilot was analyzed using developed IU model with rigorously adapted kinetic scheme. The appropriate choice of numerical grid was made and the CPU time was reduced using the adaptive mesh refinement technique. The quality of products, the recovery efficiency and the energy expenses obtained with our model were in good agreement with the field test results. Moreover, the bitumen conversion results (upgraded oil, gas and solid residue) from the experiments were compared to those obtained in the field test. Additional analysis was performed to identify energy efficient configurations and to understand the role of key variables, e.g. heating period and rate or the production pressure, in the general IU upgrading performance. Finally, these results illustrated and quantified the global interplay between energy efficiency and productivity indicators.

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Implementation of a chemo-mechanical model to predict the long-term evolution of a bentonite-sand sealing component

Andrés Idiart, Marcelo Laviña, Benoit Cochepin, Antoine Pasteau and Isabelle Munier

The safety of the future deep geological disposal facility for radioactive waste, named Cigéo, is based on the implementation at the closure step of swelling clay seal cores to prevent the water from flowing into the galleries. Their main safety functions rely upon the development and the stability of a swelling pressure that is transferred to the surrounding materials. To predict long-term changes in the swelling pressure, thermo-hydro-mechanical models are typically used. This work is focused on the implementation of physico-chemical processes at the interface between the sealing component and the surrounding materials (concrete support bases, concrete liner, and the surrounding Callovo-Oxfordian claystone). The effects of chemically-induced swelling pressure changes at the full scale are explored here.

A 2D axisymmetric coupled chemo-mechanical model of the sealing system has been developed and implemented in iCP [1], considering water-saturation evolving conditions. The model accounts not only for reactive transport processes of the interaction between the different materials, but also for the mechanical response of the system under such geochemical changes. The mechanical behaviour of bentonite is based on the Barcelona Basic Model [2]. The chemo-mechanical couplings considered in the model include: (1) montmorillonite dissolution, (2) mineral precipitation/dissolution, (3) porewater salinity, and (4) composition of interlayer water (cation exchange reactions). These couplings relate chemical changes with the mechanical behaviour, mainly affecting the void ratio, material stiffness, total suction values and swelling pressure development. The model has been used to assess the chemo-mechanical evolution of the system over 10,000 years as a result of the geochemical alteration of the sealing component.

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Coupling flow, transport and reactions using DuMu^x and Reaktoro

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Keywords: Porous media, reactive transport, code coupling.

DuMu^x [1], a simulator for flow and transport processes in porous media, is coupled to Reaktoro [2], a computational framework for modeling chemically reactive processes. We describe the coupling on a conceptual as well as on a technical level. Several decoupling approaches to solve the resulting coupled problem are investigated by means of representative examples.

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A MULTILAYER MODEL FOR REACTIVE FLOW IN FRACTURED POROUS MEDIA

Alessio Fumagalli and Anna Scotti

Keywords: Porous media, fractures, precipitation, mixed-dimensional.

The presence of fractures has an impact on subsurface flows at all scales: flow tends to focus along highly permeable fractures, which can create "shortcuts" in the domain, or, in the case of cemented fractures, we have low permeability barriers in the domain. In the context of reactive transport fractures can be responsible for fast transport of fluid with different chemical composition with respect to the surrounding matrix: this occurs for instance in geothermal reservoirs where water with different salinity, solutes and temperature is injected in the subsurface. These differences in composition and temperature can trigger transformations such as mineral precipitation, dissolution or replacement, with an impact on porosity and fracture aperture. We propose a model to account explicitly for the presence of fractures and their impact on the flow, transport and reactions. We rely on a geometrically reduced model where fractures can be represented by surfaces or lines coupled with the surrounding porous medium. Moreover, we want to account for the fact that, depending on the speed of the reactions relative to the flow velocity, we can observe a thin layer around fractures where most of the geochemical phenomena are concentrated. This layer is in turn represented as a surface with variable-in-time thickness coupled on one side with the fracture "core", on the other with the bulk porous medium. The equations describing flow and transport are thus a coupled of mixed-dimensional PDEs approximated by means of lowest order mixed finite elements, [1]. We will consider a simple model for mineral precipitation dissolution following [2]. To avoid the occurrence of negative concentrations and oscillations when the amount of precipitate approaches zero we adopt an event location strategy to detect the discontinuity in the ODE describing the reaction part, which is, for this reason, split from advection and diffusion by means of a first-order operator splitting.

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Benchmark of reactive transport tools for unsaturated reactive applications: the case of cement materials carbonation

Bruno Huet

Keywords: Benchmark, Reactivity, Gas diffusion, Drying, Carbonation, concrete.

At every stage of product life cycle, the physics and chemistry of carbonation are ubiquitous to building cementitious materials. Hardening via carbonation, carbonation induced reinforcement corrosion or recycled concrete aggregate carbonation all rely on specific aspects of unsaturated rock/water/gas reactions and transfers.

The monitoring of pH front has long proved as an indicator for service life estimation of concrete structure. Now, the large variety of processes, materials and environmental conditions of interest has called for more robust testing strategies of material properties. Recent studies have focused on gas diffusivity [1], carbonation reaction [2], water sorption and transfer properties for different carbonation degree [3] and coupled mechanisms [4].

Experimental evidence within available datasets on carbonation properties and performance are now available. They cover a range of concrete mix design including cement type, dosage and initial water content. They also a cover a range of environmental conditions, from real atmospheric conditions to industrial gas such exhaust gas from cement plant.

Even if not exhaustive, these datasets could prove to be very useful to validate and benchmark holistic reactive transport model by: 1) selecting the right physics and chemistry at play, 2) highlighting the relevant non-linearity of constitutive laws and 3) quantifying coupled processes.

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ADAPTIVE HIGHER ORDER METHODS FOR POROUS MEDIA AND NON-NEWTONIAN FLUID FLOW PROBLEMS

Birane Kane and Robert Klöfkorn

Keywords: Finite Elements, Discontinuous Galerkin methods, Non-Newtonian Flows, Multiphase flow, Porous Media.

We present adaptive Finite Element and Discontinuous Galerkin discretizations for Porous media flow and non-Newtonian Fluid flow problems. The adaptive approaches implemented allow in most test cases for refinement/coarsening in both the element size, the polynomial degree and the time step size. To our knowledge, this is the first time the concept of local hp-adaptivity is incorporated in the study of such topics. The implementation is based on the new Python frontend Dune-FemPy [2] to the open source framework DUNE [1]. The efficient strategies for parallelization, adaptivity, and load balancing within the framework allow to aim at a range of complex industrial and environmental applications such as Microbially induced calcite precipitation (MICP) as a leakage mitigate solution in CO_2 sequestration [4] and non-Newtonian fluid flow in complex domains.

This work required a combination of a multidisciplinary expertise in state-of-the-art adaptive, higher order discretization schemes for unsteady problems in porous media flow [3] and transport simulation.

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COMPARISON OF SECOND ORDER FINITE VOLUME SCHEMES ON POLYHEDRAL MESHES

Anna Kvashchuk, Robert Klöfkorn, Tor Harald Sandve

Keywords: 2nd Order Finite Volume method, Porous Media, CO2-EOR, Tracer.

Polyhedral grids play an important role in subsurface modeling of flow and transport processes and the application of higher order accurate schemes is important to reduce effects of numerical diffusion, especially for reactive transport. In realistic applications such higher order methods are typically not used because no straight forward extension to polyhedral or corner point grids exists.

In this work we compare different approaches to construct linear reconstructions for second order Finite Volume schemes on polyhedral grids [1]. A variety of second order Finite Volume approaches exist and have been successfully applied to different applications on mostly structured or simplicial grids. For polyhedral grids the absence of a reference element mapping and a possibly high number of neighboring cells make the application of higher order schemes more complicated. We present several different possibilities to construct second order schemes on polyhedral grids. The different schemes are compared in terms of accuracy, runtime, and feasibility of implementation. In addition, we present the performance of the discussed schemes when applied to CO2-EOR cases for real field models, e.g. the NORNE case [2].

The implementation of the presented schemes in based on DUNE (dune-project.org) and OPM (opm-project.org).

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Micro-Macro models: the next generation models for reactive flow and transport problems in porous media?

Peter Knabner

Keywords: Upscaling, multiscale modeling, micro- macro model, evolving porous medium, dissolution/precipitation.

In porous media and other complex media with different length scales, (periodic) homogenization has been successfully applied for several decades to arrive at macroscopic, upscaled models, which only keep the microscopic information by means of a decoupled computation of "effective" parameters on a reference cell. The derivation of Darcy's law for flow in porous media is a prominent example. Numerical methods for this kind of macroscopic models have been intensively discussed and in general are considered to be favourable compared to a direct microscale computation. On the other hand, if the interplay of processes becomes too complex, e.g. the scale separation does not act in a proper way, the porous medium itself is evolving, the upscaled models obtained may be micro-macro models in the sense, that the coupling of the macroscopic equations and the equations at the reference cell is both ways, i.e. at each macroscopic point a reference cell is attached and the solution in the reference cell depends on the macroscopic solution (at that point) and the macroscopic solution depends on the microscopic solutions in the reference cells. At the first glance such models seem to be numerically infeasible due to their enormous complexity (in $d + d$ spatial variables). If on the other hand this barrier can be overcome, micro-macro models are no longer a burden but a chance by allowing more general interaction of processes (evolving porous media, multiphase flow, general chemical reactions, ...), where the microscopic processes "compute" the constitutive laws, which need longer be assumed (similar to the concept of heterogeneous homogenization). We will discuss various examples and in particular numerical approaches to keep the numerical complexity in the range of pure macroscopic models.

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MULTIPHASE CHEMICAL KINETICS MODELING FOR AQUEOUS-MINERALS REACTIVE SYSTEMS

Anthony Michel, Bastien Hamlat, Jocelyne Erhel and Thibault Faney

Keywords: Multiphase reactions, chemical kinetics, discontinuous differential equations.

During the last few years, there has been a growing interest in global formulations of multiphase reactive transport models with a special focus on the complete dissolution of minerals by kinetic reactions involving aqueous species and minerals.

In the specific case of one mineral by reaction and one reaction by mineral, we can introduce a modified model which consists in limiting the dissolution rate when the mineral amount is equal to zero. However, such a discontinuous switching may induce failures in standard implicit solvers and is not compatible with classical mathematical theories. These issues have been solved, by N. Bouillard et al. [1] and J.Hoffman et al. [2], by translating discontinuous switching in complementarity conditions and by using a differential inclusion approach.

In this talk, we will present and justify the "limited kinetics model" introduced by B. Hamlat et al. [3, 4] to extend the range of applications to general systems including any type and number of kinetic reactions. Then we will discuss the mathematical and numerical results obtained and the remaining issues in light of our recent advances.

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On the relevance of discontinuities and geochemical heterogeneity in the reactive transport behavior in fractured rocks

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Keywords: Reactive transport, discrete fracture networks, upscaling, High Performance Computing.

Understanding of groundwater flow and solute transport in discrete fracture networks (DFN) is crucial to assess the safety of deep geological repositories for nuclear waste in crystalline rocks. It is well known that groundwater flow in such environments is controlled by discontinuities, and that traditional continuous porous media theory, based on defining a Representative Elementary Volume does not apply in most cases. However, to simulate the hydrogeological behaviour of such DFN descriptions may lead to unpractical and expensive computational costs. This is the main reason why large research efforts have been devoted to test and developing different methodologies for upscaling from DFN representations to Equivalent Continuous Porous Media approach (ECPM). Successful results in terms of groundwater flow have been achieved in the last decades, but still very limited applicability when solute transport and geochemical processes are considered. In this work, we will show numerical methodologies for solving solute transport and geochemical processes in DFN, and some ideas about future trends for upscaling transport and geochemical properties.

On the other hand, mineral surfaces and pore space in rock are distributed in complex microstructures and their distributions are far from being homogeneous. Such heterogeneities occur at the submillimetre scale and are usually ignored by larger scale traditional reactive transport models based on averaged geochemical parameters. In this work, we use High Performance Computing technology to assess the implications of grain-scale physical and mineralogical heterogeneity on the macroscopic transport and geochemical behaviour of radionuclides. The resulting grain-scale reactive transport models are solved in a supercomputer, and the results are compared with macroscopic upscaled models, where mineral abundance is averaged over the matrix volume.

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Biochemical patterns and waves in underground storage of hydrogen and CO_2

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Keywords: Porous media, bacteria, reactive transport, hydrogen storage, CO2, self-organization, Turing instability, Hopf-Andronov bifurcation, heterogeneous media.

Underground storage of H_2 and CO_2 mixtures in aquifers and their transformation into methane by bacteria can be an efficient technology for the creation of artificial reservoirs of natural gas. The interaction between biochemical reaction and species transport leads to the formation of nonuniform structures in space called autowaves (patterns and waves), which reduces the efficiency of the conversion. The objective is thus to maintain the injection regimes avoiding the formation of autowaves. The theory of autowaves is well developed for two-component systems and much less extended to three- and four-component systems, which is our case. For a given kinetics of the population growth, we have determined, through stability analysis, several types of autowaves that can occur in a storage. Among them we find the Hopf-Andronov fluctuations in time, Turing's oscillations in space, mixed spatial and temporal oscillations, standing waves and traveling waves. We extended our analysis to heterogeneous media (blocks-fractures) and detected new dynamic patterns in the form of flashes randomly traveling over the domain. For all types of the autowaves, we have detected the exact criteria of their existence. We also detected the critical modes of perturbation that provoke fluctuations. The analytical studies have been confirmed by numerical tests. We applied this theory to model the feasibility of storing hydrogen in a depleted gas reservoir. 3D simulations were performed with the open code DuMu^X. Several examples reveal the appearance of spatial autowaves in real conditions.

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Sequential upscaling of multiphase dispersion in porous media

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Keywords: Active dispersion, Darcy-scale heterogeneity, non-equilibrium model.

In this paper we consider the transport of a chemical species in a two phase system with exchange of matter at the interface (so-called active dispersion). The boundary conditions at the interface between the two phases existing within the pore space are either of thermodynamic equilibrium or of reactive type. Saturation changes with the exchange of matter at the interface. The medium itself is characterized by different levels of heterogeneity starting from the pore-scale. In this work, problems related to pore-scale to Darcy-scale upscaling and then to Darcy-scale to Large-scale upscaling are considered.

The first upscaling [1] leads to different problems depending on the boundary conditions and various assumptions, in particular the role of the total mass exchange rate, non-standard terms, etc. The role of geometry, reaction rate on dispersion and tortuosity is investigated for simple 1D/2D/3D unit cells.

The second upscaling is only considered for the case of a local non-equilibrium Darcy-scale model in the case of small variations of density and viscosity with concentration. It leads to a complex coupled problem between Darcy-scale deviations and large-scale averaged values. In particular, the solution exhibits memory and history effects. An algorithm is proposed to solve for the case of small Damköhler numbers (the Diffusive Damköler for low Péclet numbers or the convective Damköhler for high Péclet numbers). The resulting large-scale model is of the non-equilibrium type. The algorithm allows for the calculation of large-scale effective properties such as large-scale relative permeability, large-scale mass exchange coefficients as a function of the large-scale phase saturation.

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NEWTON STRATEGIES FOR IMPLICIT SIMULATIONS OF COUPLED TRANSPORT AND STANDARD CHEMISTRY

Xavier Raynaud

In their simplest formulation, the standard equilibrium equations for chemistry consist of a system of linear equations (mass conservation) and linear equations for the logarithm of the concentrations (equilibrium laws). By nature, a linear and logarithmic scales are mixed and this strong non-linearity creates problem for the convergence of the Newton method. In this talk, we want to introduce two ideas that can be incorporated in a Newton solver to improve its robustness

The first idea originates from [2]. We will discuss the motivation but the outcome consists of using logarithmic variables and a special form of the mass conservation equations. In addition, we use natural physical bounds, as presented in [1]. The result is a solver showing good robustness properties on test cases that we will present.

Transport problems naturally mix components. For an implicit solver, we do not know - a priori - the elements that are present in a computation cell. This information will be given as the result of the computation of the solution of the nonlinear equations. However, to solve the chemical equations, this information is crucial, in particular when using logarithmic variables. Here, we present a strategy that can be used at each Newton step to estimate the appearance or disappearance of species. We will show some numerical experiments with calcite dissolution.

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Evaluation of some models of gas transport at different scales in a deep geological repository

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Keywords: Two-phase flow, gas transport, argilite formation, upscaling, radioactive waste, repository.

The aim of this talk is to present some examples of two-phase flow and two-component (air-water or hydrogen-water) transport problems at different scales based on TOUGH code capabilities, which have been studied in the framework of a safety case of a high level waste (HLW) repository. The first example presented at small scale (meters and days) is that of the simulation of the in-situ PGZ-experiment of nitrogen transport in the Callovo-Oxfordian (COx) argillite. In this example, it is shown the importance of air-entry pressure in hydraulic properties of the COx for enhancement of nitrogen pressure data simulation in the COx. The second example is that of hydrogen transport at cell and module scales (dozen to hundred of meters, thousands of years) of a HLW repository site, where the problem of interfaces is invoked. The last example deals with the problem of the impact of piston flow of hydrogen on radionuclides transport at the scale of the repository site (kilometers, thousands of years), where a simplified repository model is used in order to study this impact. Finally, discussions about some studies on progress are presented, especially modelling of hysteresis, gas-solubility, and geo-mechanics which can have a great impact on gas transport at different scales.

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Multiphase Multicomponent Flow and Reactive Transport (MMF&RT) modeling

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Keywords: Multiphase multicomponent flow, reactive transport, mixtures, density driven flow, chromatographic partitioning, coupled processes.

Development of multiphase multicomponent flow (MMF) simulators can be traced all the way back to the 1970s, and that of reactive transport (RT) codes even earlier. Numerous mathematical and numerical methods have been proposed to couple flow and chemical reactions [3]. Efforts have been made to deal with different specific aspects related to the presence of two or more fluid phases and multiple components, such as dis-/appearance, thermodynamic state of mixtures, coupling, and numerical stability. A significant progress has been done in understanding of the physics of the multiphase flow, i.e. estimation of characteristic properties of homogeneous and heterogeneous porous media. Due to the physical and numerical complexity of the MMF&RT, the problem is often simplified supposing non-reactive components, phases, or loose coupling. Until recently, the gas phase was systematically presented by one gas species only. In models of impure CO_2 injection [1], the gas phase consisted by CO_2(g) . The co-injected impurities were supposed dissolved in brine, hence, the additional amount of brine was injected that changes chemical reactions, fluxes and mass balance. Accurate modeling of phases, of their thermodynamic properties and fluxes is required to describe real aqueous and gas mixtures. Such calculations are numerically demanding because of high degree of freedom. We demonstrate the operator-splitting based approach used in the reactive transport simulator HYTEC for the compressible EOS-based MMF&RT [2]. Modeling of experimental, numerical, and field cases of injection of CO_2 with impurities or tracers show highly coupled physical processes related to complex phase composition, e.g. density driven flow and chromatographic partitioning.

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Thermodynamic modeling of flows through porous media

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Keywords: porous media, thermodynamics, multiphase flow, multicomponent flow, heat transfer.

While chemical reactions are ruled by thermodynamics, flows in porous media are often studied on the basis of hydrodynamics. Nevertheless, several authors [1, 2, 3, 4, 5] have shown over the years that thermodynamics is also a valid foundation for flow modeling.

This talk presents a thermodynamic derivation of heat and mass transfers in porous media. We introduce the classical equilibrium thermodynamics of the different parts of the porous medium (matrix, fluids and interfaces) and apply the local equilibrium assumption on the representative elementary volume (REV) to obtain a consistent thermodynamic description of the porous medium system in the framework of the continuum approach. By working with the balance equations of mass, internal energy and entropy, we derive the local production of entropy. This term includes the dissipation due to interactions and transfers inside the REV (between matrix, fluids and interfaces) and through the REV (fluxes). Assuming the thermal and chemical local equilibria, and a linear regime for flux-gradient relations, we retrieve relations compatible with the well-known laws of Darcy for the fluid velocities and Maxwell-Stefan for the diffusion. The obtained flux-gradient relations for diffusion also include the Soret's and Dufour's effects. The classical capillary pressure curve is obtained as a direct consequence of the equilibrium of the interfaces and is subject to a strong constraint for three or more phases. Finally, we propose a system of partial differential equations for the heat and mass transfers in multiphase and multicomponent flows through porous media. This formulation relies on a unique set of primary variables (no variable switch) and exposes a symmetric structure.

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Geochemical impacts during CO_2 geological storage - feedback from the Lacq demonstration pilot

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Keywords: CO_2 geological storage.

From 2010 to 2013 Total has captured, transported and stored over 50000 tonnes of CO_2 into Rousse depleted gas reservoir, in the vicinity of Pau, in the South West of France. In order to understand the geochemical impacts of the CO_2 injection into a carbonate reservoir, the reservoir rock was characterized in term of mineralogy and chemical composition, and a thermodynamical model was established to equilibrate the minerals, formation water and natural gas priori to production start in 1972. This model enabled to identify reactive pathways due to both gas production and CO_2 injection. This work confirmed that Mano reservoir mineralogy and porosity are largely unaffected by the storage of CO_2. Two interesting findings are that the geochemical impacts are primarily dominated by pressure depletion rather than CO_2 acidity and that the cap rock is kept distant from the CO_2 due to gravity processes within the gas reservoir.

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Comparison of numerical solvers applied to leaching and accelerated carbonation of concrete

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Keywords: Multiphase flow, porous media, carbonation, leaching, porosity change, finite volume.

We study cementitious material subject to carbonation and leaching under accelerated laboratory experiment conditions. Our model consists of two phase flow of water and air in a porous medium, transport of agents: Ca ions in water and CO_2 concentration in air, and above mentioned chemical reactions. Chemical reactions are simplified to nonlinear source terms [1], and are affecting the porosity of the medium. Due to accelerated nature of the setup, carbon dioxide concentration is much higher than usual, which results in a sharp carbonation front.

The position of the carbonation front relative to the mesh has a significant effect on the convergence of scheme. We present a comparison of several solvers highlighting their robustness to this property: global implicit or various iterative operator splitting approaches, solved with standard Newton or RASPEN method [2]. All solvers use vertex centered finite volume method implemented in PDELab module, a part of DUNE project [3].

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Operator-Based Linearization approach for flow and transport with equilibrium and kinetic reactions

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Keywords: Reactive flow and transport, chemical equilibrium, fully-implicit solution, operator-based linearization, element balance formulation.

Increasing demand for energy sources, e.g. complex hydrocarbon reservoirs or geothermal energy, has led to the comprehensive investigation of carbonate reservoirs. These reservoirs are often chemically altered and hence contain a large uncertainty in the spatial distribution of the reservoir parameters. A successful development of these cleaner energy resources and effective management of the associated risks requires an evaluation of the large ensemble of multiphase reactive flow and transport simulations. To solve this problem, we developed an efficient element based reduction technique which can significantly decrease the number of conservation equations and thereby reduce the computational time.

The proposed formulation is based on the consistent element balance reduction of the molar (overall composition) formulation [1]. To predict the complex phase behavior in such systems, we include the chemical equilibrium constraints to the multiphase multi-component negative flash calculations and solve the thermodynamic and chemical phase equilibrium simultaneously [2]. In this solution, the phase equilibrium is represented by the partition coefficients whereas the chemical equilibrium reaction is represented by the activity coefficients model. This provides a generic treatment of chemical and thermodynamic equilibrium within the successive substitution loop of multiphase flash to accommodate precipitation and dissolution. Using the Equilibrium Rate Annihilation matrix allows us to reduce the governing unknowns to the element conservation equations only while the coupling between chemical and thermodynamic equilibrium is captured by a simultaneous solution of modified multiphase flash equations. The element composition of the mixture serves as an input for these computations whereas the output is fractions of components in each phase, including solids.

Next, a finite-volume unstructured discretization in space is applied together with a fully-implicit approximation in time. The resulting complex nonlinear system is parameterized using the Operator-Based Linearization (OBL) approach [3]. The OBL framework transfers the governing nonlinear Partial Differential Equations into a linearized operator-form where the Jacobian is constructed as a product of a matrix of derivatives with respect to state variables and discretization operators. The state-dependent operators are only evaluated adaptively at vertices of the mesh introduced in the parameter-space. The continuous representation of state-dependent operators as well as their derivatives is achieved by using a multi-linear interpolation in parameter-space. This means that the usually time-consuming phase and chemical equilibrium computations, performed on each nonlinear iteration and in every control volume, are only executed when evaluating the operators in the new supporting points, thereby significantly reducing both the linearization time and the number of nonlinear iterations. The simulation of multidimensional problems of practical interest has been performed using the proposed technique. The same approach is later used to simulate the near-wellbore mineral precipitation prevalent in North Sea gas reservoirs.

Equilibrium reactions in typical advection-diffusion problems are usually valid when the rate of the reaction is far greater than characteristic velocity or diffusion. This is typically not true when considering heterogeneous reactions such as complex dissolution/precipitation processes. Therefore, a kinetic reaction module has also been developed within the OBL approach. The newly added module in the OBL framework for multiphase reactive transport and flow is validated for several dissolution regimes at different combination of Damkohler and Péclet numbers. The element based reduction framework, using equilibrium reactions, is compared with the component kinetic reaction framework at different kinetic rates.

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A HYBRIDIZABLE INTERIOR PENALTY DISCONTINUOUS GALERKIN METHOD FOR LOCALLY DEGENERATE ELLIPTIC PROBLEMS

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Keywords: Hybridizable discontinuous Galerkin method, interior penalty stabilization, degenerate elliptic problems.

We design a hybrid variant of the famous Interior Penalty Discontinuous Galerkin (IPDG) method to solve degenerate second-order elliptic problems. This hybrid variant denoted H-IP method is exposed in a unified formalism as it can handle (second-order) diffusion problems, (first-order) advection-reaction problems as well as mixed issues combining both previous mechanisms for a wide range of Péclet numbers, including the delicate situation where the diffusion vanishes on a subdomain. Notably, this unusual circumstance can be easily encountered in the context of mass transport in fractured porous media. It is well-known that the presence of fractures deeply affects the process since they represent preferential fluid flow paths. As a result, the global phenomenon may be governed by a hyperbolic partial differential equation in the fracture, and by an elliptic one in the porous matrix. Let us emphasize that such problems are particularly delicate to solve numerically since the scalar variable can jump at the interface separating hyperbolic and elliptic regions [1]. The class of degenerate elliptic problems has been analyzed by different authors during the last decades, mainly in the context of DG methods (see [2] and the abundant references therein). However, the literature is relatively scarce concerning its resolution by Hybridizable Discontinuous Galerkin (HDG) methods, and this is the purpose of the present work. Several assets render the HDG methods attractive: they are amenable to the static condensation, and coupled degrees of freedom are localized at the mesh skeleton leading to a compact stencil. The robustness and accuracy of the proposed H-IP method are investigated through extensive numerical experiments in two-dimensional space for arbitrary polynomial orders k, including the lowest-order case $k = 0$. Optimal convergence of the scalar variable is generally observed for all investigated regimes.

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Numerical investigation of a fully coupled micro-macro model for mineral dissolution and precipitation

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Keywords: Level set method, multiscale model, porous media, reactive transport, upscaling.

We investigate multiscale models describing mineral dissolution and precipitation processes. Such multiscale models may be derived from detailed pore-scale models applying upscaling techniques. Since mineral reactions alter the porous medium's structure and its bulk properties, the models comprise several levels of couplings. Our model consists of transport equations at the scale of the porous medium (macroscale) while taking the processes of convection, diffusion and reaction into account. They include averaged time- and space-dependent coefficient functions which are in turn explicitly computed by means of auxiliary cell problems (microscale). Structural changes due to dissolution and precipitation reactions result in a time- and space-dependent domain, on which cell problems are defined. The interface between the mineral and the fluid, and consequently the explicit geometric structure, is characterized by means of a level set. Here, information from the transport equations' solutions is taken into account (micro-macroscale). A numerical scheme has been developed which enables evaluating such complex settings. Within this framework the potentially degenerating bulk properties of the medium such as porosity, diffusivity and permeability could be investigated. To reduce computational costs, adaptive methods for controlling the macroscopic steps are investigated. Moreover, we applied our approach to the dissolution of an array of calcite grains in the micro-macro context and validated our numerical scheme.

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3D NUMERICAL SIMULATION OF COUPLED PROCESSES BETWEEN TWO-PHASE FLOWS AND GEOCHEMICAL REACTIONS IN POROUS MEDIA

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Keywords: Two-phase flow, finite volume method, reactive transport, porous media, fully implicit approach, DuMu^X, CO_2 sequestration.

The aim of this work is to develop a parallel code for the coupling between two-phase flows and geochemical reactions in porous media in 3D configurations. The problem is modelled by a highly non-linear system of PDEs (compositional two-phase flow model in porous media) coupled to ordinary or algebraic differential equations (geochemistry)[1].
A fully coupled fully implicit finite volume scheme is developed to avoid splitting errors caused by sequential methods, especially for problems with a strong coupling between flow and reactive transport problems. The latter is implemented in DuMu^X framework, a parallel open-source simulator for flow and transport problems in porous media [2]. Particular attention is paid to the time step strategy to improve the convergence of the Newton method. A heuristic time step strategy is developed to improve the CPU time performance. In this talk, we present 3D test cases for CO_2 injection into a deep saline aquifer, including parallel computing. A numerical convergence study is used to validate our implementation. An analysis of strong and weak parallel scalabilities is also performed. Finally, an advanced comparison with a sequential method developed in [3], is performed in a unified environment. Operator splitting errors are emphasized by an overestimation of the total mass of CO_2 in the sequential method case while the implicit approach is perfectly mass-conservative.

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GLOBAL IMPLICIT SOLVER FOR MULTIPHASE MULTICOMPONENT FLOW IN POROUS MEDIA WITH MULTIPLE GAS PHASES AND GENERAL REACTIONS

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Keywords: PDE reduction method, nested Newton, equilibrium reactions, M++, CO_2.

In order to predict the gas and liquid flow and the efficiency of trapping mechanisms (mineral trapping) for CO_2 storage in deep layers, the system to be solved consists of diffusion-advection-reaction partial differential equations (PDEs), algebraic equations (AEs) and ordinary differential equations (ODEs).

The choice of a suitable formulation of the equations is important for efficient numerical solution. We apply the Kräutle-Knabner PDE reduction method [1] which enables to eliminate the equilibrium reactions based upon specific variable transformations. Separating the resulting remaining PDE/ODE/AE system into a global and a local system, we apply a nested Newton solver method [2] which enables fast and efficient computation of the dynamics of the system by means of the application of parallel solvers to the Finite Element discretized / Finite Volume stabilized PDE system. Our computations of the behavior of the concentrations of the different species of the multiphase multicomponent flow are highly resolved in space and time. We study the mineral trapping scenario [3] using splines derived from experiments for the equations of state (EOS) which describe the interphase mass exchange of CO_2 and the density of CO_2. To this end, we present the work in progress concerning the elaboration and implementation of our methods into the software package M++ for the computation of a recent benchmark which inherits multiple gas phases [4].

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ACCELERATING REACTIVE TRANSPORT SIMULATIONS WITH AN ON-DEMAND LEARNING STRATEGY FOR CHEMICAL EQUILIBRIUM AND KINETICS CALCULATIONS

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Keywords: On-demand learning, chemical equilibrium and kinetics, reactive transport.

Geochemical reaction calculations in reactive transport simulations are extremely costly. These are chemical equilibrium and/or kinetics computations involving many fluid species and rock minerals, which are needed (at least once) in every mesh cell, at every time step of the simulation. As a result, they can account for over 99% of all computing costs in the simulation when realistic chemical descriptions of fluids and rocks are considered in the model. It turns out, however, that many such geochemical calculations, during the course of a reactive transport simulation, have similar (*not identical*) input conditions. As such, by solving key chemical equilibrium and kinetics problems (*determined on-demand during the simulation*), and computing the derivatives of their output with respect to their inputs (*sensitivity derivatives*), we are able to quickly and accurately estimate the majority of subsequent geochemical reaction calculations in the simulation. This is done by applying a first-order Taylor approximation using the currently recorded input/output conditions and their associated sensitivity derivatives. This on-demand learning strategy effectively allows us to **entirely bypass** *(i)* Newton iterations when solving the equations that govern chemical equilibrium (using either Gibbs energy minimization or law of mass action formulations) as well as *(ii)* the integration time steps when solving the ordinary differential equations that govern chemical kinetics. This on-demand learning algorithm can also be used to speed up other costly computations, such as evaluations of fluid properties, equations of state, reaction rates, and so forth. Some reactive transport simulation examples are shown, which demonstrate speedups of several orders of magnitude when solving chemical equilibrium and kinetics calculations with the on-demand learning strategy.

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Evolution of planar fractures: an experimental and reactive transport modelling study

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Keywords: Dissolution, fracture, wormholing, limestone, finite difference method, 2.5 reactive transport model..

The processes that affect the evolution of fracture geometry and reactive transport in limestone fractures were evaluated using an integrated experimental and modeling approach. Flow-through experiments were performed to investigate the alteration of three artificially made planar limestone fractures, which were exposed to HCl-acidified water flow (pH 3.8) at three different rates. Fluid instabilities developed in the fractures because of small fracture aperture variations and naturally occurring heterogeneity in the rock, i.e., the presence of clay spots of higher porosity. The dissolution regime changed from conical to dominant and ramified wormhole with increasing flow rate, i.e., Péclet number. Maps of fracture aperture obtained from X-ray micro-tomography imaging, together with measurements of permeability and analyses of fluid chemistry, provided experimental constraints for modeling. Numerical simulations were performed using a 2.5D continuum reactive transport model to examine the development of flow patterns and the reactivity and permeability evolution over time, and to interrogate the impacts of fluid reactivity, mineral heterogeneity and diffusive boundary layer. The modeling results showed that fracture alteration is very sensitive to initial fluid reactivity and mineralogical heterogeneity, in addition to flow rate. The changes of local transport processes during fracture opening also affected the evolution of fracture reactivity.

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A BENCHMARK FOR THE NUMERICAL SIMULATION OF PORE-SCALE MINERAL DISSOLUTION WITH FLUID-SOLID INTERFACE EVOLUTION

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Keywords: Pore scale, reactive transport, moving boundary, benchmark, review.

This talk presents a benchmark problem for the simulation of single-phase flow, reactive transport and solid geometry evolution at the pore scale [1]. The problem is organized in three parts that focus on specific aspects: flow and reactive transport, dissolution-driven geometry evolution in two dimensions, and a three-dimensional dissolution-driven geometry evolution including an experimental validation.

Five codes are used to obtain the solution to this benchmark problem, including Chombo-Crunch, OpenFOAM-DBS, a lattice Boltzman code, Vortex method, and dissolFoam. These codes cover a good portion of the wide range of approaches typically employed for solving pore-scale problems in the literature, including discretization methods, characterization of the fluid-solid interfaces, and methods to move these interfaces as a result of fluid-solid reactions. Among the discretization methods, one can find finite volumes, Lagrangian methods, grid based methods (stochastic and deterministic).

Results from the simulations performed by the five codes show remarkable agreement both quantitatively based on upscaled parameters such as surface area, solid volume and effective reaction rate and qualitatively based on comparisons of shape evolution. This outcome is especially notable given the disparity of approaches used by the codes.

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Pore-scale modelling of multiphase reactive flow

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Keywords: Pore-scale, dissolution, immiscible flow, microfluidics.

In this talk, we discuss the recent progress in the modelling of multiphase reactive transport at the pore-scale. The dynamics modelling of reactive flow phenomena in reactive environment is complex because it involves the tracking of multiple interfaces that evolve as a function of the details of the reactive transport: on the one hand, the fluid/fluid interface is subject to surface tension forces, on the other hand, the fluid/solid interface moves with chemical reaction at the mineral surface. The approach developed here employs an extended Darcy–Brinkman–Stokes formulation that accounts for the interfacial tension between the two immiscible fluid phases and the moving contact line at the mineral surface [1]. The mass transfer across fluid/fluid interfaces is modeled using an improved Continuous Species Transfer technique that will be described [2, 3]. The simulation framework is validated using an experimental microfluidic device that provides time-lapse images of the dissolution dynamics. The set-up involves a single-calcite crystal and the subsequent generation of CO_2 bubbles in the domain. The experimental dataset can be used to verify other numerical codes along the lines of the recent benchmark on single-phase dissolution at the pore-scale [4].

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