International Conference on Numerical and Mathematical Modeling of Flow and Transport in Porous Media

Dubrovnik, Croatia, 29 September – 3 October 2014

Book of Abstracts

Organized by:

Faculty of Science, University of Zagreb, Zagreb, Croatia

Laboratoire de Mathématiques et de leurs Applications, University of Pau & CNRS, France

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Contents

PREFACE

Welcome to the International Conference on Numerical and Mathematical Modelling of Flow and Transport in Porous Media (NM2PorousMedia), held at Dubrovnik, Croatia, September 29 – October 3, 2014. This Conference was jointly organized by the Faculty of Science of the University of Zagreb (Croatia), and the Applied Mathematics Laboratory of the University of Pau & CNRS UMR 5142 (France).

The aim of the conference is to bring together researchers, scientists, engineers, and students to exchange and share their experiences, new ideas, and research results about modelling, analysis and simulation of flow and transport in porous media and application to problems including subsurface hydrology, petroleum exploration, contaminant remediation, carbon sequestration and nuclear waste storage.

Topics of the conference:

- Numerical modelling and simulation of flow and transport in porous media.
- Modelling, analysis, and simulation of multiphase multicomponent compositional flow in porous media.
- Modelling, analysis, and simulation of flow and reactive transport in porous media.
- Discretization based on advanced finite element, finite volume, or discontinuous Galerkin methods of flow and transport in porous media.
- High performance computing for multiphase flows.
- Numerical analysis of methods for flow and transport in porous media.
- Mathematical modelling and analysis of flow and transport in porous media.
- Multi-scale and/or adaptive algorithms for flow and transport in porous media.
- Upscaling and/or homogenization.
- Advances in pore-scale modelling and upscaling.
- Theory and computation of porous media flows.
- Coupled models and domain decomposition in geosciences.
- Non-equilibrium models for flows in porous media.
- Computational methods in geophysical inverse problems.
- Mathematics and computation in geosciences.
- Flow and transport simulation of oil reservoir engineering, groundwater hydrology, geological storage of carbon dioxide, deep geological repository for radioactive waste, bioremediation, solid-fluid problems, diffusion in materials, electromagnetic field applications, complex flow phenomena, and others.
- Environmental, technical and biomedical applications involving porous media.

This conference contains 7 invited talks and 36 contributed talks and 7 posters. It is attended by 63 participants from 30 different countries: Albania, Algeria, Austria, Belgium, Canada, Croatia, Czech Republic, Denmark, France, French Guiana, Germany, India, Israel, Italy, Mexico, Morocco, The Netherlands, Norway, Russia, Kingdom of Saudi Arabia, Slovakia, South Korea, Spain, Sweden, Switzerland, Tunisia, Turkey, United Kingdom, USA and Venezuela.

The conference could not have been held without the financial support of the organizing institutions and the following sponsors: Faculty of Science of the University of Zagreb; Ministry of Science, Education and Sport of Republic of Croatia; Laboratoire de Mathématiques et de leurs Applications, Institut Pluridisciplinaire de Recherche Appliquée dans le domaine du Génie Pétrolier, Université de Pau & des Pays de l'Adour; Centre National de la Recherche Scientifique, France; and FEI Visualization Sciences Group. We thank them for their financial support. The support of SMAI: Société de Mathématiques Appliquées et Industrielles and INTERPORE, International Society for Porous Media is also greatly acknowledged.

Last, but not least, we want to acknowledge all participants for their contribution and efforts in making the conference an interesting, pleasant and successful event.

Wishing you a pleasant and fruitful meeting and hope you enjoy your stay in Dubrovnik.

Organizing committee:

- Mladen Jurak, University of Zagreb, Croatia (Co-Chair).
- Brahim Amaziane, University of Pau & CNRS, France (Co-Chair).
- Etienne Ahusborde, University of Pau & CNRS, France.
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- Faculty of Science, University of Zagreb.
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List of Invited plenary speakers:

- Grégoire Allaire, Ecole Polytechnique, France.
- Peter Bastian, IWR, University of Heidelberg, Germany.
- Gregory A. Chechkin, Moscow Lomonosov State University, Russia & Narvik University College, Norway.
- Zhangxing Chen, University of Calgary, Canada.
- Yalchin Efendiev, Department of Mathematics & ISC Texas A&M University, USA.
- Alexandre Ern, University Paris-Est, CERMICS , ENPC, France.

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- Centre National de la Recherche Scientifique.
- INTERPORE, International Society for Porous Media.
- SMAI: Société de Mathématiques Appliquées et Industrielles.
- FEI Visualization Sciences Group.

HOMOGENIZATION OF ELECTROKINETIC FLOWS IN POROUS MEDIA: THE ROLE OF NON-IDEALITY

G. Allaire

We study the homogenization (or upscaling) of a system of partial differential equations describing the non-ideal transport of a N-component electrolyte in a dilute Newtonian solvent through a rigid porous medium. Realistic non-ideal effects are taken into account by an approach based on the mean spherical approximation (MSA) model which takes into account finite size ions and screening effects. We first consider equilibrium solutions in the absence of external forces. In such a case, the velocity and diffusive fluxes vanish and the equilibrium electrostatic potential is the solution of a variant of Poisson-Boltzmann equation coupled with algebraic equations. Contrary to the ideal case, this nonlinear equation has no monotone structure. However, based on invariant region estimates for Poisson-Boltzmann equation and for small characteristic value of the solute packing fraction, we prove existence of at least one solution. When the motion is governed by a small static electric field and a small hydrodynamic force, we generalize O'Brien's argument to deduce a linearized model. Our second main result is the rigorous homogenization of these linearized equations and the proof that the effective tensor satisfies Onsager properties, namely is symmetric positive definite. We eventually make numerical comparisons with the ideal case. Our numerical results show that the MSA model confirms qualitatively the conclusions obtained using the ideal model but there are quantitative differences arising that can be important at high charge or high concentrations. This is a joint work with Robert Brizzi, Jean-François Dufrêche, Andro Mikelić and Andrey Piatnitski.

G. Allaire
Ecole Polytechnique, France
gregoire.allaire@polytechnique.fr

HIGH-PERFORMANCE COMPUTING FOR FLOWS IN POROUS MEDIA

P. Bastian

Simulation of flow and transport processes in porous media provides a formidable challenge and application field for high-performance computing. Relevant continuum-scale models include partial differential equations of elliptic, parabolic and hyperbolic type which are coupled through highly nonlinear coefficient functions. The multi-scale character and uncertainties in the parameters constitute an additional level of complexity but provide also opportunities for high-performance computing.

This talk will focus on the efficient solution of single and two-phase flow with discontinuous Galerkin methods. These schemes are comparable in efficiency (measured in accuracy per computation time) to simple cell-centered schemes but offer the opportunity to increase arithmetic intensity substantially in the assemble as well as the solve phase. For high-order schemes we exploit the tensor product structure using sum factorization which renders the work per degree of freedom almost independent of the polynomial degree. For the fast solution of the arising linear systems in the elliptic case a hybrid preconditioner based on subspace correction in the conforming finite element subspace is employed. Scalability and robustness of this preconditioner for the elliptic model problem and the full two-phase problem is investigated on a moderate number of processors including the Intel Phi architecture.

P. Bastian
IWR, University of Heidelberg, Germany
peter.bastian@iwr.uni-heidelberg.de

On homogenization of liquid crystals

G. Chechkin and T. P. Chechkina

We study a homogenization problem for the system of equations of liquid crystals dynamics (dynamics of nematics or nematodynamics). We consider a simplified Ericksen-Leslie system for incompressible medium with inhomogeneous density. Assuming the initial distribution of the density to converge to the limit distribution, we construct the limit (homogenized) problem and prove the strong convergence of solutions of the initial problem to a solution of the homogenized problem.

Also we prove the existence and the uniqueness theorems for the full Ericksen-Leslie system of equations.

G. Chechkin
Moscow Lomonosov State University, Russia & Narvik University College, Norway
chechkin@mech.math.msu.su

How can parallelization recover more oil?

Z.J. Chen

For large oil and gas heterogeneous fields, vast amounts of seismic, geologic and dynamic reservoir data yield high-resolution geological models. These models involve mega (million) to giga (billion) grid block cells. Recent advances in the development of a general parallel reservoir simulator platform are capable of the solution of field simulations of these sizes within minutes. These parallel simulations provide increased recovery of oil and gas resources, due to a full utilization of available data and a better understanding of the chemical and physical mechanisms involved, process design and uncertainty analysis. This talk will present these advances in the development of a general parallel reservoir simulator platform on CPUs and GPUs. Applications to the black oil, compositional and thermal simulators will be addressed.

Z. J. Chen
University of Calgary, Canada
zhachen@ucalgary.ca

MULTISCALE MODEL REDUCTION TECHNIQUES FOR FLOWS IN HETEROGENEOUS POROUS MEDIA

Y. Efendiev

Many porous media problems have multiscale nature. Due to disparity of scales, the simulations of these problems are prohibitively expensive. Some types of upscaling or model reduction techniques are needed to solve many multiscale problems. In this talk, we discuss a few known techniques that are used for problems with scale separation and focus on Generalized Multiscale Finite Element Method (GMsFEM) that has been recently proposed for solving problems with non-separable scales and high contrast. The main objective of the method is to provide local reduced-order approximations for linear and nonlinear PDEs via multiscale spaces on a coarse computational grid. In the talk, we briefly discuss some main concepts of constructing multiscale spaces and applications of GMsFEMs.

Y. Efendiev
Department of Mathematics & ISC Texas A&M University, USA
efendiev@math.tamu.edu

COMPATIBLE DISCRETE OPERATOR SCHEMES FOR ELLIPTIC PROBLEMS ON POLYHEDRAL MESHES

A. Ern

Compatible discrete operator schemes aim at preserving structure properties of the continuous problem at the discrete level. We analyze a class of such schemes for a model elliptic problem. The cornerstone in the design of the scheme is the discrete Hodge operator linking discrete gradient and fluxes. We present the two abstract properties to be satisfied by this operator to achieve convergence. Then, we focus on the design of this operator using the concept of local gradient reconstruction. We discuss links with other classical and more recent schemes from the literature. Finally, we present numerical examples and outline extensions to other model problems.

A. Ern
University Paris-Est, CERMICS , ENPC, France
ern@cermics.enpc.fr

A MIXED FINITE VOLUME METHOD FOR NONLINEAR SECOND-ORDER ELLIPTIC PROBLEMS

F. Benkhaldoun, A. Mahamane and M. Seaid

We present a mixed finite volume method for the discretization of the second-order nonlinear elliptic boundary value problems. The discretization results with a system of nonlinear algebraic equations for which a Newton-Krylov algorithm is applied. We also describe an adaptive procedure in the finite volume method by monitoring a posteriori error estimator in the computational domain. This residual type estimator is established for linearized problems and it is used for adaptive refinement using unstructured grids. The performance and the effectivity of the mixed finite volume method are examined on a variety of practical numerical examples. It has been found that the proposed adaptive mixed finite volume method offers a robust and accurate approach for solving second-order nonlinear elliptic boundary value problems, even when highly nonhomogeneous diffusion coefficients are used in the simulations.

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F. Benkhaldoun
LAGA, Université Paris 13, Villetaneuse, France
fayssal@math.univ-paris13.fr

A. Mahamane
LAGA, Université Paris 13, Villetaneuse, France
mahamane@math.univ-paris13.fr

M. Seaid
School of Engineering and Computing Sciences, University of Durham, United Kingdom
m.seaid@durham.ac.uk

AVIZO, 3D IMAGE ANALYSIS AND QUANTIFICATION

F. Arnaud and A. Sanchez-Erostegui

Avizo is an advanced 3D analysis software application for exploring and understanding materials structures and properties, in a wide range of materials science research areas and for many types of materials (porous media, metals and alloys, fibrous materials, composites...). It helps engineers, scientists and researchers gain greater and faster insight into 2D/3D images and numerical simulation data, with applications in Materials Sciences, Oil & Gas, Geosciences, Mining, Engineering and Simulation.

The presentation will highlight the possibilities offered by Avizo Fire in terms of:

- Visualization and exploration of data from CT, microscopy, etc
- Processing and improvement of images
- Automatic and assisted segmentation
- Advanced measurement and quantification
- Pore/grain distribution
- Porosity, tortuosity, pore connectivity
- Correlative CT / SEM imaging
- Results presentation

F. Arnaud, A. Sanchez-Erostegui
FEI Visualization Sciences Group, Bordeaux, France
fabien.arnaud@fei.com, alejandra.sanchez-erostegui@fei.fr

AVIZO, FROM IMAGE TO SIMULATION

F. Arnaud and A. Sanchez-Erostegui

Avizo is an advanced 3D visualization and analysis software application used for exploring and characterizing core samples and digital rock data sets. It offers a comprehensive software platform to run advanced digital routine or special core or core analysis for:

- Advanced segmentation
- Physical property calculation (absolute permeability, âĂę)
- 3D model reconstruction and meshing
- Simulation pre- and post-processing tools
- Finite element analysis results visualization
- Custom algorithm integration
- Advanced result presentation

F. Arnaud, A. Sanchez-Erostegui
FEI Visualization Sciences Group, Bordeaux, France
fabien.arnaud@fei.com, alejandra.sanchez-erostegui@fei.fr

A DISCRETE FRACTURE MODEL FOR TWO-PHASE FLOW WITH MATRIX-FRACTURE INTERACTION

E. Ahmed, J. Jaffré and J. E. Roberts

We consider a discrete fracture models for two-phase flow with matrix-fracture interaction. The fractures are considered as (n-1)-dimensional interfaces in an n-dimensional domain. The model was presented in [1]. It results in a system of equations in both the n-dimensional matrix domain and in the (n-1)-dimensional fracture domain. The matrix domain is effected by the fracture flow through a Robin type boundary condition along both sides of the fracture, while the fracture takes into account the flow in the matrix by means of a source term representing the discontinuity across the fracture of the flux, both wetting phase and total. We also take into account the fact that the rock-type in the matrix is different from that in the fracture so that the capillary pressure and relative permeability curves for these two domains are different. We will present numerical experiments. To construct our program we coupled 3-D and 2-D two-phase flow simulators from the MATLAB Reservoir Simulation Toolbox (MRST) from SINTEF. Meshes were obtained by P. Laug using the 3-D tetrahedral mesh generator GHS3D and the surface mesh generator BLSURF from the Inria team Gamma3.

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E. Ahmed
Inria, Rocquencourt, France & ENIT-Lamsin, Tunis, Tunisia
elyes.ahmed@inria.fr

J. Jaffré
Inria, Rocquencourt, France
jerome.jaffre@inria.fr

J. E. Roberts
Inria, Rocquencourt, France
jean.roberts@inria.fr

NONLINEAR TRANSPORT FLOW THROUGH ELASTOVISCOPLASTIC POROUS MEDIA

G. Alduncin

Nonlinear transport-flow through elastoviscoplastic porous media is variationally analyzed. Mixed variational formulations of the poro-mechanical system are given via composition duality methods, establishing solvability results on the basis of duality principles. Composition duality compatibilities are classical interior domain conditions as well as surjective coupling operator properties. The conformation of the model-system corresponds to constrained transport phenomena driven by a compressible Darcian flow, in a quasistatic elastoviscoplastic deformable subsurface media, modelled variationally by a primal evolution mixed transport, a dual evolution mixed flow and a dual evolution mixed quasistatic deformation. For computational purposes, proximation realizations of primal and dual marching time schemes, implicit and semi-implicit, are derived, determining corresponding conditions for convergence to stationary states of the system.

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G. Alduncin
Instituto de Geofísica, Universidad Nacional Autónoma de México, México
alduncin@geofisica.unam.mx

Investigating the role of tortuosity in the Kozeny-Carman equation

R. Allen and Shuyu Sun

The Kozeny-Carman (KC) equation proposes a relationship between permeability and porosity, as well as tortuosity, and has been the subject of many published works in the porous media community. Authors propose modifications to the KC equation or propose a new KC constant after fitting their pore-scale simulation results to the original KC equation.

Since the KC constant is empirically derived, it will depend on the definition used for tortuosity [1]. Tortuosity is often expressed as a function of porosity, however it has been suggested that tortuosity is dependent only on the pore geometry [2].

In this work, we generate random porous media samples and use a Stokes solver to obtain the permeability tensor [3]. We obtain the tortuosity tensor using different approaches that have been previously reported in literature. We investigate the impact that these tortuosity definitions have on fitting pore-scale simulation results to the KC equation.

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R. Allen
Computational Transport Phenomena Laboratory, KAUST, Kingdom of Saudi Arabia
rebecca.allen@kaust.edu.sa

S. Sun
Computational Transport Phenomena Laboratory, KAUST, Kingdom of Saudi Arabia
shuyu.sun@kaust.edu.sa

A non-linear Beavers–Joseph interface condition derived from a kinetic energy balance

P. Angot, M. Belliar and C. Zaza

The numerical simulation of a fluid flow over a porous bed involves very different length scales. Macroscopic models using Ochoa-Tapia–Whitaker (OTW) and Beavers–Joseph (BJ) laws represent the small scale phenomena coupling the flow in the free-fluid and in porous media as an interface of discontinuity associated with specific boundary conditions. While the BJ condition is well acknowledged for a Stokes flow, the presence of non-linear convective terms seems to introduce a nearly linear dependence of the slip coefficient with the fluid Reynolds number at the interface Re_i [3] for Re_i below 20. A vector jump embedded boundary condition (JEBC) for interface coupling was used to study the well-posedness of both BJ and OTW models [1]. Following [2], we introduce in the JEBC condition a jump of the kinetic energy. This allows us to propose a Beavers–Joseph law with a non-linear slip coefficient which depends linearly on the ratio of the Darcy velocity to the slip velocity. Our direct numerical simulations results support this modified condition for Re_i below 20.

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P. Angot
Aix-Marseille Université & I2M UMR 7373 CNRS, France
philippe.angot@univ-amu.fr

M. Belliard
CEA DEN/DANS/DM2S/STMF/LMEC, France
michel.belliard@cea.fr

C. Zaza
CEA DEN/DANS/DM2S/STMF/LMEC & I2M UMR 7373 CNRS, France
chady.zaza@latp.univ-mrs.fr

COMPARING DIFFERENT NUMERICAL METHODS FOR TWO-DIMENSIONAL COUPLED WATER AND SOLUTE TRANSPORT IN POROUS MEDIA

S. M. Baviskar and T. J. Heimovaara

We compare different numerical methods for two dimensional (2D) coupled water and solute transport model in porous media by Richards equation (RE) and non-sorbing, single component, solute transport by advection dispersion equation (ADE). In this research numerical approximations like finite element method (FEM) and finite difference method (FDM) are used for spatial discretization. In spite of similar initial and boundary conditions, verification of different numerical approximations showed differing results due to emerging numerical diffusions. FEM discretization was carried out in COMSOL [1] and in FAESOR [2]. In FAESOR mixed-based RE discretized on qudratic finite elements showed better performance than head-based RE with default linear finite elements inbuilt in COMSOL. In FDM solutions mixed-based RE had improved results because of inter nodal hydraulic conductivity averaging method. Conventional solutions for ADE on Euler nodes produces numerical diffusions caused by erroneous evaluation of the advection term. Using numerical technique called marker-in-cell (MIC) by Gerya [3] which uses Lagrangian principles, we remove these strong oscillations. Different iteration process for convergence are investigated concluding mixed-based RE formulated in FDM and ADE formulated in MIC has least numerical diffusions.

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S. M. Baviskar
Geo-Engineering Section, Technical University of Delft, Netherlands
s.m.baviskar@tudelft.nl

T.J. Heimovaara
Geo-Engineering Section, Technical University of Delft, Netherlands
t.j.heimovaara@tudelft.nl

Two-phase flow relative permeability determination using lattice Boltzmann method at the pore scale

S. Ben Hadj Hassine, M. Dymitrowska, V. Pot and A. Genty

Experimental determination of macroscopic two-phase flow properties of porous media such like relative permeability remains challenging in the case of very low permeable media like argillites. As an alternative method, simulations were made on a pore scale with a lattice Boltzmann approach in 3D reconstructed images of real samples obtained by X-ray tomography at fine resolution (0.7 μm).

We implemented the Rothman and Keller [1] two-phase flow lattice Boltzmann model using a Two Relaxation Time collision operator [2]. In order to cope with the samples size (10^7 fluid sites), the model was implemented on a GPU device and parallelized using CUDA. It was tested against classical static and dynamic flow analytic problems. In real 3D connected porosity, we performed two-phase flow computations and deduced relative permeability curves.

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S. Ben Hadj Hassine
IRSN, Fontenay aux Roses, France
seifallah.benhadjhassine@irsn.fr

M. Dymitrowska
IRSN, Fontenay aux Roses, France
magdalena.dymitrowska@irsn.fr

V. Pot
INRA, Thiverval-Grignon, France
vpot@grignon.inra.fr

A. Genty
CEA, Saclay, France.
alain.genty@cea.fr

AN ADAPTIVE FINITE VOLUME METHOD FOR OIL RECOVERY PROBLEMS IN POROUS MEDIA

F. Benkhaldoun, A. Mahamane and M. Seaid

In this contribution we investigate the numerical performance of an adaptive cell-centered finite volume method for solving oil recovery problems in porous media. The proposed finite volume method uses the cell-centered techniques to discretize the diffusion operators on unstructured grids. The method is second-order accurate, it can be applied on general unstructured adaptive grids, it does not require serious restrictions on the angles of triangles, and it can be easily incorporated in an existing finite volume code for hyperbolic systems of conservation laws. The adaptation criteria is based on monitoring the saturation in the computational domain during its transport process. Numerical results are presented for several test problems two-phase flows in porous media with both isotropic and anisotropic coefficients.

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F. Benkhaldoun
LAGA, Université Paris 13, Villetaneuse, France
fayssal@math.univ-paris13.fr

A. Mahamane
LAGA, Université Paris 13, Villetaneuse, France
mahamane@math.univ-paris13.fr

M. Seaid
School of Engineering and Computing Sciences, University of Durham, UK
m.seaid@durham.ac.uk

POROUS MEDIA FLOW CALCULATIONS WITH HEXAHEDRAL MIXED FINITE ELEMENTS

N. Birgle, J. Jaffré and J. E. Roberts

In reservoir simulation as well as in many other domains of application, hexahedral grids in combination with locally conservative cell-centered discretization techniques are preferred for modelling flow and transport in porous media. In particular it is easier to follow geological layers with hexahedra than with rectangular solids. In addition, hexahedral grids generally require fewer cells than tetrahedral grids. Numerical models based on mixed finite elements have many properties that make them especially appropriate for flow models: they produce an approximation to the Darcy flux as well as to the pressure and they are locally conservative. However, the classical mixed finite elements of Raviart-Thomas-Nedelec do not give satisfactory results for hexahedral grids.

For this reason an appropriate composite mixed finite elements have been developed using a subdivision of the hexahedron into 5 tetrahedra. However this method could not be extended to the case of deformed cubes with nonplanar faces. Therefore a new composite mixed finite element with a subdivision of the hexahedron into 24 tetrahedra has been developed. At the same time a posteriori error estimators have been constructed. Numerical results will be shown for experiments relevant to flow in the subsurface around a waste storage site.

N. Birgle
Inria, Rocquencourt, France
nabil.birgle@inria.fr

J. Jaffré
Inria, Rocquencourt, France
jerome.jaffre@inria.fr

J. E. Roberts
Inria, Rocquencourt, France
jean.roberts@inria.fr

Upscaling of Lattice Boltzmann simulations in heterogeneous media and related reduced order modelling techniques.

D. L. Brown, J. Li, M. Ghommem and V. M. Calo

In this talk, we will discuss the application of the Lattice Boltzmann Method (LBM) to fluid flow in porous media. LBMs have been used extensively fluid mechanics simulations, and by adding forcing terms it is able to describe flow in porous media [1]. These inputed permeability fields may be very complex and contain many scales and have high-contrast. Such media can be computationally expensive, and to expedite the calculation we present an upscaling algorithm where many local problems are computed to calculate coarse scale properties. Then, the computation can be carried out on the coarse grid [2]. In addition, a technique of using model reduction techniques to quickly and efficiently calculate upscaled quantities will be presented. By reformulating the LBM into a matrix vector product, reduced order modelling techniques can be utilized. Taking fine resolution snapshots a well suited basis can be constructed and computation is done on a significantly smaller dimensional subspace [3]. This algorithmic methodology of the reduced order modelling will be presented along with computational results.

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D. L. Brown, J. Li, M. Ghommem, V. M. Calo
Center for Numerical Porous Media, KAUST, Kingdom of Saudi Arabia
donaldbrowdr@gmail.com

AN UPWIND FINITE VOLUME METHOD ON NON-ORTHOGONAL QUADRILATERAL MESHES FOR THE CONVECTION DIFFUSION EQUATION IN A POROUS MEDIUM

S. Buitrago, G. Sosa and O. Jiménez

Traditionally, the finite difference method has been applied to solve numerically the PDE governing fluid flow on a rectangular mesh in porous media for its easy implementation and computational efficiency. The aim of this work is to solve the two-dimensional convection diffusion equation on a non-rectangular grids formed only by quadrilaterals honoring the internal structures of a reservoir (preferential flow channels, faults, areas of high permeability contrast, changes in sediment type, etc.), taking into account different physical configurations of the porous medium. To take advantage of the good representation of the domain through these meshes, the finite volume method was used, which is conservative and facilitates the treatment of the boundary conditions. In this method the convection diffusion equation is integrated on each quadrilateral (control volume) of the mesh, thus obtaining the integral form of the equation. The velocity value in the face of each quadrilateral is determined according to the direction of the flow (upwind scheme). After approximating the integrals involved and taking into account the boundary conditions, a discrete equation in each control volume showed up. Finally, a large sparse linear system is obtained, generally non-symmetric and ill-conditioned, which can be solved by iterative methods such as GMRES with incomplete LU preconditioning. Different scenarios were considered varying boundary conditions (Dirichlet and Neumann type), source term, and diffusion constant fluid velocity. The results are consistent with the physical interpretation of each configuration.

S. Buitrago
Universidad Simón Bolívar, Venezuela
sssbuitrago@yahoo.es

G. Sosa
Universidad Simón Bolívar, Venezuela
giselle1701@gmail.com

O. Jiménez
Universidad Simón Bolívar, Venezuela
oswjimenez@usb.ve

NXFEM FOR SOLVING NON-STANDARD TRANSMISSION PROBLEMS

D. Capatina, R. Luce, N. Barrau et H. El-Otmany

We are interested in the numerical approximation of Darcy and/or Stokes equations in a domain containing a thin layer, with highly discontinuous permeability matrix or viscosity. This academic problem is a first approach in modelling, for instance, flows in fractured porous media or flows of biological fluids (where the thin layer is a membrane).

Due to the small thickness ε of the layer, and hence to the difficulty to mesh it, we work with the limit problem obtained as ε goes to 0 in the weak formulation. Thus, the equations in the layer are replaced by adequate transmission conditions between the neighbouring domains.

We justify the passage to the limit for both Darcy and Stokes equations and then we propose a well-posed finite element approximation of the limit problems, based on NXFEM [1]. On the one hand, this method has the advantage to treat discontinuities which are not aligned with the mesh. This is done by imposing the couplings across the discontinuities weakly, by means of Nitsche's method, and by doubling the degrees of freedom on the cells cut by the interface. A judicious choice of the stabilization parameters yields robustness with respect to both the geometry and the physical coefficients, see [2]. On the other hand, NXFEM allows us to take into account in a natural way the non-standard transmission conditions previously derived. Numerical tests showing the relevance of the method will be presented.

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D. Capatina
LMAP & CNRS, University of Pau, France
daniela.capatina@univ-pau.fr

R. Luce
LMAP & CNRS, University of Pau, France
robert.luce@univ-pau.fr

N. Barrau
LMAP & CNRS, University of Pau, France
nelly.barrau@univ-pau.fr

H. El-Otmany
LMAP & CNRS, University of Pau, France
hammou.elotmany@univ-pau.fr

FEM MODELLING OF MEMBRANE CAPACITIVE DEIONIZATION (MCDI) FOR COMPLEX STREAMS

D. Cardoen, B. B. Sales, J. Helsen and A. Verliefde

MCDI is a desalination technology which utilizes ion exchange membranes (IEM) and porous carbon electrodes to remove ions through storage in the electrical double layer (EDL). It efficiently desalinates water with moderate salt content (e.g. in domestic water softening, [1]). To broaden its application range, MCDI of 'mixed' streams (e.g. biomass hydrolysates, [2]) is investigated.

A COMSOL Multiphysics FEM model for MCDI is constructed, applied to salt streams and then expanded to mixed streams. A macroscale model is coupled to a 1D micropore model for ion storage in the EDL. The former models laminar mixing by spacer elements in the feed channel, Donnan potential-driven ion transport across the IEMs, and mass transport through the electrode macropores by an effective medium approximation. In the latter, modified Poisson-Nernst-Planck equations correct for steric interactions and solvent effects, and a Robin type boundary condition couples with electrolyte concentrations and potential in the macropores.

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D. Cardoen
VITO, Separation and Conversion Technology, Belgium
Ghent University, Particle and Interface Technology, Belgium
dennis.cardoen@vito.be

B. B. Sales, J. Helsen
VITO, Separation and Conversion Technology, Belgium

A. Verliefde
Ghent University, Particle and Interface Technology, Belgium

MODELLING THE FATE AND TRANSPORT OF ENGINEERED NANOPARTICLES IN POROUS MEDIA

N. K. Copty

In recent years engineered nanoparticles have been proposed for numerous applications including in-situ groundwater remediation. A critical step for the development of such technology is the effective deliverability of the nanoparticles suspension to the zone of contamination. Because of their relatively high surface energy, bare nanoparticles may undergo significant aggregation and deposition within the porous media, thereby limiting its transport. To enhance the mobility of engineered nanoparticle, surface coating with various materials have been considered. This paper reviews the factors influencing the fate and transport of engineered nanoparticles in porous media. In particle the effect of nanoparticle concentration on its mobility is examined. The nanoparticle considered in this study is poly(acrylic acid) (PAA) supported magnetite (Fe2O3). The transport experiments were conducted in a water-saturated sand-packed column for nanoparticle suspensions. Particle size analysis of the synthesized nanoparticle solutions showed that PAA provides good size stability. Time-moment analysis of the engineered nanoparticle breakthrough curves, on the other hand, revealed that nanoparticles mass recovery from the column decreased consistently with dilution, with greater attenuation, sharper fronts and longer tails compared to that of the tracer. To further interpret the experimental results, a nanoparticle transport model that accounts for deposition/detachment kinetics was developed. The best agreement between the observed breakthrough curves and model simulations was obtained using a kinetic time-dependent deposition term with finite deposition capacity and a kinetic detachment term. Different numerical techniques are considered for the solution of the governing differential equations. The model results suggest that the decrease in mass recovery with decrease in input particle concentration may be due to time-dependent blocking that hinders further deposition. The implications of these results on the use of engineered nanoparticles for groundwater remediation applications are discussed.

N. K. Copty
Institute of Environmental Sciences, Bogazici University, Istanbul, Turkey
ncopty@boun.edu.tr

Monte Carlo analysis of macrodispersion in 3D heterogeneous porous media

A. Dartois, A. Beaudoin, J-R. De Dreuzy and S. Huberson

The influence of molecular diffusion, isotropic and anisotropic dispersions on the macrodispersion in 3D heterogeneous porous media was investigated by means of large scale numerical simulations. The permeability is a Gaussian correlated field with a lognormal distribution. A stochastic approach was used for the computation of the macrodispersion coefficients through a monte-carlo analysis. Comparisons between 2D and 3D simulation show very similar behavior. However, the impact of molecular diffusion and dispersion is much stronger in 3D. The results were obtained using the PARAallel DISpersion module from the H2OLAB platform. For several simulations, the particles trajectories have been drawn on a 3D permeability field to serve as a visual support for our analysis. The required post-treatments and visualization were achieved with Matlab and Gocad.

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A. Dartois
Institut P' (UPR CNRS 3346), University of Poitiers, France
arthur.dartois@univ-poitiers.fr

J-R. De Dreuzy
Geosciences (UMR CNRS 6118), University of Rennes 1, France

COUPLING FLUID AND POROUS-MEDIA FLOWS: MODELLING AND NUMERICAL METHODS

M. Discacciati, P. Gervasio and A. Quarteroni

Two possible concepts are presented for coupling the Stokes and the Darcy equations to model the filtration of incompressible fluids through porous media. First, we consider a macroscopic approach that relies on suitable conditions at the interface between the fluid and the porous medium to impose the conservation of mass and of stresses. Mathematically, this method allows to reformulate the Stokes/Darcy problem as an equivalent equation defined only on the interface, and we present possible numerical methods to solve effectively such reduced problem [1]. On the other hand, we propose a coupling strategy that does not consider any specific interface condition, but introduces a thin transition region between the fluid and the porous medium. From the mathematical point of view, this method leads to an optimal control problem defined on the boundary of the transition domain [2]. We compare these approaches theoretically and we present simulations of some test cases of physical relevance.

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M. Discacciati
UPC BarcelonaTech, Spain
marco.discacciati@upc.edu

P. Gervasio
Università di Brescia, Italy
gervasio@ing.unibs.it

A. Quarteroni
École Polytechnique Fédérale de Lausanne, Switzerland
alfio.quarteroni@epfl.ch

A SIMULATION STUDY OF REACTIVE FLOW IN 2-D INVOLVING DISSOLUTION AND PRECIPITATION IN SEDIMENTARY ROCKS

T. Dutta and S. Sadhukhan

A porous rock structure is simulated in 2-D by using the relaxed bidisperse ballistic deposition model.We solve the Navier-Stokes equation using finite difference method to study the velocity distribution of fluid flowing through it under a constant pressure gradient. Reactive flow of a fluid is simulated using a random walk algorithm.The reactive solute carried through the fluid, mimicked by a random walker, is allowed to interact with the minerals in the rock. A walker is capable of either advection or diffusion, which it decides stochastically as a function of Peclet number. Dissolution and precipitation probabilities are calculated depending on the Damkholer number, interface area and concentration. Precipitation occurs only through the cations that are released in the solution due to dissolution. These combined dissolution-precipitation reactions change the porosity, permeability and pore geometry of the sedimentary rock. We follow the temporal changes of these properties as functions of the Peclet number, concentration of the reactive solute and ratio of Damkholer numbers of dissolution to precipitation. The final flow property is decided by a combination of these parameters.

T. Dutta
Physics Department, St. Xavier's College, Kolkata, India
tapati_mithu@yahoo.com

S. Sadhukhan
Physics Department, Jogesh Chandra Choudhury College, India
Suptisadhukhan@gmail.com

Explicit and implicit numerical methods for some advection dominated problems of transport and flow in porous media

P. Frolkovič

In this talk we deal with finite volume methods for some advection dominated problems with applications in contaminant transport [1] and flow with moving groundwater table [2]. We focus on recent semi-implicit in time numerical methods for advection equation [3, 4]. The methods have no restriction on the time step due to the stability, they are second order accurate for smooth solutions and they can be used in conservative form. In each time step linear algebraic system of equations must be solved and that can be realized efficiently by Gauss-Seidel type of iterations due to special structure of resulting matrices. In general the semi-implicit methods may require a nonlinear stabilization procedure to insure the discrete min-max property for numerical solution.

We discuss the advantages and disadvantages of the new semi-implicit methods [3, 4] with respect to some explicit in time numerical methods [1, 2, 5] for several relevant examples.

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P. Frolkovič
Faculty of Engineering, Slovak University of Technology in Bratislava, Slovakia
peter.frolkovic@stuba.sk

Homogenization of reaction-diffusion processes in a two-component porous medium with a non-linear flux-condition on the interface

M. Gahn, P. Knabner and M. Neuss-Radu

The periodic homogenization of a system of microscopic non-linear reaction diffusion equations in a porous medium consisting of two components separated by an interface is performed. One of the components is connected, the other one is disconnected and consists of periodically distributed inclusions. The model is motivated by the transport of different species through the membrane of organelles into the cytoplasm of a plant cell. The differential equations in the different domains are coupled by a non-linear flux-transmission condition on the boundary of the organelles, which describes the exchange of substances through the interface and involves multi-species reactions. For this system existence and uniqueness is proved by a fixed-point argument and to derive the macroscopic problem the methods of two-scale convergence in periodic domains and on periodic surfaces are used. For the convergence results of the nonlinear reaction-rates the strong two-scale convergence is applied. Especially to pass to the limit in the non-linear transmission condition on the boundary of the organelles, we employ the strong two-scale convergence on the surface. This is given by an unfolding argument and a compactness criterion for spaces of the form $L^2(\Omega, B)$ with a Banach-space B.

M. Gahn
Friedrich-Alexander-University Erlangen-Nuremberg, Germany
markus.gahn@fau.de

P. Knabner
Friedrich-Alexander-University Erlangen-Nuremberg, Germany
knabner@math.fau.de

M. Neuss-Radu
Friedrich-Alexander-University Erlangen-Nuremberg, Germany
maria.neuss-radu@math.fau.de

Modelling of flow transport in porous media, from pore scale to non-Darcy flow

R. Gooya, H. O. Sorensen and S. L. S. Stipp

When the fluid velocity in a porous media increases because of an increasingly high pressure gradient, the flow no longer follows Darcy's law. The Forchheimer (Fo) model is the most common way to describe this non-Darcy behavior. When the Fo number, which is $\beta\rho v/\mu$, reaches a certain value, and this depends on the rock type, the flow behaviour deviates from the expected one. Non-Darcy flow parameters, such as β, have historically been extracted from macroscopic experiments but with the improvements of X-ray microtomography, complex microstructure can be characterized in natural porous media, and the non-Darcy flow parameters can be determined. The current work presents data from a carbonate reservoir rock, has been imaged using X-ray microtomography, where voxel (volume pixel) size is 650 nm. A volume of 100^3 voxels from the image was selected for pore scale modelling of fluid transport. By applying a finite volume code and solving Stoke's equations for porous media over a range of pressure gradients, the non-Darcy flow parameters have been extracted for this complex carbonate rock. Results show that non-Darcy flow for this carbonate rock start around Fo = 0.005. This number shows that carbonate rocks have a complex structure which non-Darcy behaviour starts in lower velocities.

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R. Gooya, H. O. Sorensen, S. L. S. Stipp
Nano-Science Center, Department of Chemistry, University of Copenhagen, Denmark
gooya@nano.ku.dk, osholm@nano.ku.dk, stipp@nano.ku.dk

Numerical Upscaling by a Localized Orthogonal Decomposition

P. Henning, A. Målqvist and D. Peterseim

In this talk, we given an introduction and overview on recent developments for the Localized Orthogonal Decomposition (LOD) multiscale method. The central idea of the LOD is to construct an optimal low dimensional generalized finite element space, that incorporates any desired variations of data functions, independent of their structure. The multiscale space is constructed by finding the orthogonal complement of the kernel of an interpolation operator with respect to a problem specific scalar product. The operator maps into a classical 'coarse' finite element space. We show general rigorous convergence results for various types of equations, such as linear and nonlinear elliptic problems with heterogenous, rapidly varying coefficients. Furthermore, we present numerical examples on problems with high contrast and conductivity channels and we present an application of the framework to the Buckley-Leverett equation.

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P.Henning
ANMC, École polytechnique fédérale de Lausanne, Switzerland
patrick.henning@epfl.ch

A. Målqvist
Department of Mathematical Sciences, Chalmers University of Technology and University of Gothenburg, Sweden
axel@chalmers.se

D. Peterseim
Institut für Numerische Simulation, University of Bonn, Germany
peterseim@ins.uni-bonn.de

A REGULARIZED ELLIPTIC-PARABOLIC MODEL FOR THE TRANSPORT IN POROUS MEDIA

O. Lafitte

We show that the coupling of the Richards' equation for a saturated-unsaturated porous medium and of its mechanical behavior (which is degenerate (non parabolic) when the medium is saturated, see, for example, [1]), leads to a more regular problem, hence leading to existence and uniqueness with suitable data.
This comes from the observation that the complete system writes

$$\begin{cases} \mathrm{div}(\sigma(u,v) - hId) = f \\ \omega = \frac{1}{2}(\partial_x u + \partial_y v), \theta = \omega S(h) \\ \partial_t \theta = \mathrm{div}(K(h)\nabla h) \end{cases}$$

where ω is the trace of the deformation tensor and θ is the moisture given, for example, by the van Genutchen law. This system implies

$$\partial_t(\theta(h)) = \omega S'(h)\partial_t h - \frac{C_0}{2} S(h)\mathrm{div}(K_T^{-1}(L\partial_t h)) = F$$

where $L\phi = \left(\partial_x(V_s\phi), \partial_y(V_s\phi)\right)^T$, K_T is the deformation tensor.
This system writes $\mathcal{M}(\partial_t h) = \mathrm{div}(K(h)\nabla h)$.
Introduce N such that $-\mathrm{div}(K_T^{-1}(L\partial_t h)) = N(\partial_t h)$. Using

$$(N\phi, V_s\phi) \geq \frac{\alpha}{C_p}\|S(h)^{\frac{1}{2}}\phi\|^2,$$

the coupled problem leads to a parabolic-elliptic equation on the water pressure h, $\mathcal{M}$ being elliptic.

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O. Lafitte
LAGA, Université Paris 13, Sorbonne Paris Cité, France
lafitte@math.univ-paris13.fr

Development of an adaptive mesh refinement strategy for the Melodie software simulating flow and radionuclide transport in porous media

M.-H. Le, H. Amor, M. Bourgeois and F. Benkhaldoun

This talk presents the recent developments of the MELODIE software which aims to simulate the physico-chemical phenomena involved in the release and in the migration of the radionuclides in the domain under investigation from the repository to the geosphere outlets. The interesting phenomena is modelled by a system combining the Darcy flow equation and the diffusion-convection concentration equation. The present work consists in developing and evaluating an adaptive mesh strategy for industrial application purpose. A guaranteed *a posteriori* error estimator, derived thanks to an $\mathbf{H}$(div)-conforming flux reconstruction, is computed and followed by an appropriate method of local refinement and coarsening of the mesh elements in two- and three- dimensional cases. Several features related to the complexity of the algorithm and to the numerical implementation will be discussed.

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M.-H. Le, H. Amor, M. Bourgeois
IRSN/PRD-DGE/SEDRAN/BERIS, BP 17 - 92262 Fontenay-aux-Roses Cedex, France
minh-hoang.le@irsn.fr, hanen.amor@irsn.fr, marc.bourgeois@irsn.fr

F. Benkhaldoun
LAGA, Université Paris 13, 99 Av. J.B. Clément 93100 Villetaneuse, France
fayssal@math.univ-paris13.fr

EFFECT OF PERIODIC FORCING ON STABILITY OF INCLUSION IN POROUS MEDIA

T. Lyubimova, D. Lyubimov and A. Ivantsov

It is known that a planar displacement front in a porous medium is unstable if the displacing fluid has lower viscosity than the displaced one. The instability is associated with development of penetrating fingers of the less viscous fluid. They grow due to lower friction with porous matrix. The process is virtually unimpeded by viscous momentum transfer, which is negligible in porous media. This mechanism explains the short-wave nature of the instability. Thus, any method of suppressing short-wave perturbations can significantly affect the stability of the entire front. One such method is based on periodic forcing in the front-normal direction.

In practice the displaced fluid often forms compact inclusions surrounded by the displacing fluid. In this case we should consider displacement fronts on both sides of the inclusion. To study the effect of vibrations on such systems, we consider the problem of gravity-controlled vertical motion of an initially spherical inclusion of a heavier fluid within a lighter fluid in a porous medium. Calculations performed using the level set method showed that, if the periodic forcing is weak, the droplet evolution is similar to the evolution in the absence of vibrations, i.e. it is dominated by instability developing in the vicinity of one of the droplet poles and disintegration of the droplet. Sufficiently strong periodic forcing, however, can completely suppress the instability. Further increase of the intensity of vibrations leads to another instability, localized near the equator of the droplet, i.e. in the area where vibrations are tangential to the interface.

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T. Lyubimova
Institute of continuous media mechanics UB RAS, Russia
lyubimovat@mail.ru

D. Lyubimov
Perm State University, Russia
lubimov@psu.ru

A. Ivantsov
Institute of continuous media mechanics UB RAS, Russia
aivantsov@gmail.com

COMPARATIVE ANALYSIS OF COMPOSITIONAL TWO-PHASE FLOW MODELLING IN HETEROGENEOUS MEDIA BETWEEN THE DISCRETE EVENT SIMULATION METHOD COUPLED TO A SPLIT NODE FORMULATION AND CLASSICAL TIMESTEP-DRIVEN APPROACHES

R. M. Manasipov and J. E. Mindel

Numerical simulation of multiphase flow processes brings about issues related to stiff problems in non-linear parabolic equations as well as restrictions to the characteristic time steps in different regions of the domain due to heterogeneity and/or cell size variations. Discrete Event Simulation (DES) has been already implemented and applied to modelling of stochastic and deterministic processes [2].

A DES approach is proposed in this work and is meant to, among other features, mitigate the mentioned issues by maintaining the explicit nature of the underlying numerical scheme. The background spatial discretization method is the combined Finite Element–Finite Volume [1] coupled to a split node approach for material interfaces. The methodology as a whole is applied to compositional two phase flow of CO_2 in saline aquifers. Classic time-step-driven approaches to these problems have been already well studied, hence several benchmark cases are presented to perform a comparative analysis including the difference in approaches to the treatment of material interfaces.

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R. M. Manasipov
Montanuniversitaet Leoben, Austria
roman.manasipov@unileoben.ac.at

J. E. Mindel
Montanuniversitaet Leoben
julian.mindel@unileoben.ac.at

The effect of sorption on linear stability for the solutal Horton-Rogers-Lapwood problem

B. Maryshev

This abstract presents the results of linear stability analysis within the solutal analogue of HRL problem [1] with sorption of solid particles. The solid particles are treated as solute within the continuous approach. Therefore, we consider the infinite horizontal porous layer saturated with mixture (carrier fluid and solvent) with concentration difference between the layer boundaries. The solute sorption is modelled in accordance with the standard linear MIM model [2].

First, the instability of steady horizontal seepage through this layer is studied analytically. The critical values of parameters have been found. It is known that for the HRL problem the seepage makes the critical mode oscillatory, but the stability threshold remains unchanged. In contrast, if the sorption is taken into account, the stability threshold varies. In last case the critical value of solutal Rayleigh-Darcy number is increased versus that for the standard HRL problem.

The second part is devoted to investigation of instability for time-modulated horizontal mixture seepage. In this case the parametric excitation of convection is observed. The ordinary differential equation have been obtained for description of convection onset. The last equation is analyzed numerically by the Floquet method. Domains in the problem parameter space, where the uniform state is stable, are found.

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B. Maryshev
Institute of continous media mechanics UB RAS, Perm, Russia
bmaryshev@icmm.ru

EVENT-BASED NUMERICAL SIMULATION OF SLIGHTLY COMPRESSIBLE TWO-PHASE FLOW IN HETEROGENEOUS POROUS MEDIA APPLIED TO CO_2 INJECTION IN SALINE AQUIFERS

J. E. Mindel and R. M. Manasipov

Classic simulation of transport processes has long suffered from CFL restrictions that are eventually difficult to address when dealing with complex systems and non-linear phenomena, and may thus have severe impact on results and/or runtime. We present the implementation of an asynchronous event-based methodology for simulation of isothermal slightly compressible flow in heterogeneous porous media with the intent of increasing simulation efficiency.

In the test cases presented, supercritical CO_2 is injected as a tracer field in a water saturated medium. A finite volume discretization in unstructured meshes is used and results are benchmarked with similar classical timestep-based implicit and explicit schemes, showing particular increase in efficiency when the active phenomena is confined to a limited number of cells, large variations exist in the cell sizes, and considerable variation is present in the rock permeability.

An in-house C++ fluid flow in porous media code library was used for this proof-of-concept implementation of this methodology.

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J. E. Mindel
Montanuniversitaet Leoben, Austria
julian.mindel@unileoben.ac.at

R. M. Manasipov
Montanuniversitaet Leoben, Austria
roman.manasipov@unileoben.ac.at

Flow in fractal fractured-porous media: macroscopic model with super-memory, appearance on non-linearity and instability

M. Panfilov

We consider the single-phase flow described by the linear diffusion equation in multiscale self-similar fractured-porous medium, which represents an infinite set of self-similar double porosity media. At each scale the medium consists of a highly permeable network of connected channels and low permeable blocks. The characteristic scale of heterogeneity is small (ε), the ratio between the channel and block permeability at each scale is ε^2.

It is known that in a two-scale ε^2-medium the diffusion equation changes its type after averaging and transforms to an integro-differential equation, which means the appearance of the long-term memory. For the multiscale case, the averaging can be represented as an iterative set of two-scale homogenization procedures. Each step of averaging leads to the appearance of memory and progressive memory accumulation. Then at each step of averaging, the macroscale model changes its type and even the result of the second step can not be predicted. The objective was to determine the limit macroscopic model for the infinite number of scales.

By the method of induction, described in [1], we have obtained the macroscale model for an arbitrary number of scales, and its limit for the infinite hierarchy. The limit model represents the system of two equations with "super-memory", which is an integro-differential operator whose kernel is the solution of another (local) integro-differential equation. The local integro-differential equation is nonlinear. The appearance of the nonlinearity is caused by the infinite process of memory accumulation.

The numerical solution of the local nonlinear problem and the form of the kernels was obtained through the Laplace transform.

We have revealed next that the obtained macroscopic model with super-memory proves a new type of the instability with respect to a complex parameter responsible for the medium heterogeneity. Due to the stability analysis we obtained the stability threshold for this parameter.

The first results have been published in [1].

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Mikhail Panfilov
LEMTA, University of Lorraine and & CNRS, France
michel.panfilov@univ-lorraine.fr

MULTISCALE ALGORITHMS FOR OPTIMAL DESIGN OF MICROFLUIDIC DEVICES

S. I. Petrova

The problem of optimizing the shape design of advanced technological devices and systems arises in many practical applications. In the last years, the microfluidics has attracted a lot of attention in physics, chemistry, engineering, biotechnology, and medicine. This new scientific field concerns the behavior and precise control of small volumes of fluids (typically in amounts of microliters or nanoliters) which are geometrically restricted at a microscale. Recently used technologies have allowed the rise of chip–based miniaturized laboratories to control the fluid flow electronically.

We focus on the design of acoustically driven microfluidic biochips placed on a piezoelectric substrate. These devices are equipped with a lithographically produced network of channels and reservoirs to transport droplets for a chemical analysis. Successful applications of the biochips are in pharmaceutics and clinical diagnostics. Multiscale algorithms based on the homogenization approach are used to split the mathematical model, governed by the compressible Navier–Stokes equations, into two subproblems at different time scales. Our aim is to design the geometry of the channel network in order to achieve a maximal pumping rate for the microfluidic transport. The optimal design problem is subjected to partial differential equations as equality constraints and to the inequality constraints on the design variables which restrict the fluid filled channels. Primal–dual interior–point algorithms based on path–following barrier methods are used for the solution of the nonlinear optimization problem.

S. I. Petrova
University of Applied Sciences, Bielefeld, Germany
svetozara.petrova@fh-bielefeld.de

Particle methods for transport in porous media at the pore scale

P. Poncet and R. Chatelin

In this talk, we present the coupling between a viscous fluid in a porous medium at the pore scale and a transport of species whose concentration has an impact on the fluid viscosity. This describes the context of several engineering configurations such as micro-emulsion, shear-thinning or Herschel-Bulkley fluid with variable threshold.

We consider the Stokes flow $-\mathrm{div}(2\mu \mathrm{D}) + \nabla p = f$ in a domain Ω denoting the fluid domain, where $\mathrm{D} = (\nabla u + \nabla u^T)/2$ is the strain rate, μ is the kinematic viscosity, p is the pressure and u is the fluid velocity.

The species concentrations α follow a diffusion-transport equation $\partial_t \alpha + u \cdot \nabla \alpha - \eta \Delta \alpha$, where μ and α are linked by means of a relation $\mu = \phi(\alpha)$ or $\mu = \phi(\alpha, \mathrm{D})$.

We will discuss numerical strategies for Lagrangian methods in order to perform large scale simulations (up to 1024^3), comparing immersed boundaries [4] and panel methods [5] to penalization [2, 3] with recent improvements on memory saving [1].

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P. Poncet
LMAP & CNRS, University of Pau, France
philippe.poncet@univ-pau.fr

R. Chatelin
Toulouse Institute of Mathematics, UMR CNRS 5219, Team MIP, Toulouse, France

MIGRATION OF CONTAMINANTS IN FRACTURED-POROUS MEDIA IN THE PRESENCE OF COLLOIDS: EFFECTS OF KINETIC INTERACTIONS

T. Reiche, U. Noseck and I. Blechschmidt

In the context of the assessment of the long-term safety of a repository for radioactive waste in a deep crystalline rock the role of colloidal particles with respect to the transport of radionuclides in the geological formation is investigated. Colloids are typically characterized by high sorption ability and therefore can considerably enhance the transport of radionuclides. Among others, field experiments performed in a shear zone at the Grimsel Test Site (GTS) in Switzerland indicate that the sorption processes for contaminants on mobile and immobile colloids are kinetically controlled and that the colloid filtration proceeds according to a linear kinetic approach. To enable the modelling of those experiments an appropriate model of colloid-facilitated contaminant transport in fractured-porous media is developed. The physical system is modeled as a single planar fracture with adjacent full saturated porous rock matrix. Contaminants can diffuse into the rock matrix but colloids cannot because of their large size. In the mathematical model the one dimensional advective contaminant transport along the fracture is coupled with contaminant diffusion into the rock matrix perpendicular to the fracture. Radioactive decay and sorption processes for contaminants in the rock matrix (linear equilibrium sorption), on the fracture surface (linear equilibrium as well as linear kinetic reactions) and on the mobile and filtered colloids (linear kinetic approach) are taken into account. The model for colloid transport includes filtration of colloids in the fracture as well as their remobilization. A useful approach is developed that can be applied to adequately describe a natural system (crystalline rock) with our double-porosity model (single fracture integrated into porous rock). Numerical solution are obtained using an implicit finite difference scheme (Crank-Nicolson) and realized in the transport code entitled COFRAME. The transport code is verified using some existing analytical solutions and further successfully qualified by comparison of calculated results with the data from field experiments (dipol tests for investigation of colloid-facilitated transport). Some sets of simulations are performed to study the effect of kinetics for sorption of contaminants on colloids and on the fracture surface and for interaction of colloids with the fracture surface.

T. Reiche
Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Theodor-Heuss-Str. 4, 38122 Braunschweig, Germany
Tatiana.Reiche@grs.de

U. Noseck
Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Theodor-Heuss-Str. 4, 38122 Braunschweig, Germany
Ulrich.Noseck@grs.de

I. Blechschmidt
NAGRA Hardstrasse 73, 5430 Wettingen, Switzerland
Ingo.Blechschmidt@nagra.ch

FINITE VOLUME-EDGE FINITE ELEMENT SCHEME FOR A TWO-COMPONENT TWO-COMPRESSIBLE FLOW IN NONHOMOGENEOUS POROUS MEDIA

B. Saad and M. Saad

In this work, we present the convergence of a combined finite volume nonconforming finite element scheme on general meshes for a partially miscible two-phase flow model in anisotropic porous media. This model includes capillary effects and exchange between the phase. The diffusion term, which can be anisotropic and heterogeneous, is discretized by piecewise linear nonconforming triangular finite elements. The other terms are discretized by means of a cell-centered finite volume scheme on a dual mesh. The relative permeability of each phase is decentred according the sign of the velocity at the dual interface. The convergence of the scheme is proved thanks to an estimate on the two velocities which allows to show estimates on the discrete gradient of global pressure and the translates on time and on space of the mass of each phase and consequently compactness results are established in the case of degenerate relative permeabilities. A key point of the scheme is to use particular averaging formula for the dissolution function arising in the diffusion term. We show also a simulation of CO_2 injection in a water saturated reservoir and nuclear waste management. Numerical results are obtained by in-house numerical code.

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B. Saad
King Abdullah University of Science and Technology, CEMSE
4700 KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia
bilal.saad@kaust.edu.sa

M. Saad
Ecole Centrale de Nantes, 1, rue de la Noé, BP 92101, 44321 Nantes, France
Mazen.Saad@ec-nantes.fr

Numerical tools to investigate the AMCs cross-contamination between wafers and FOUPs: transient analysis of mass transfer

N. Santatriniaina, J. Deseure, T. Q. Nguyen, H. Fontaine, C. Beitia and L. Rakotomanana

This work investigates the mass transfer of the Airborne Molecular cross Contamination (AMCs) between the Front Opening Unified Pod (FOUP) and wafer (silicon substrates) during the microelectronics devices manufacturing. Such cross-contamination phenomena lead to detrimental impact on production yield in microelectronic industry and a predictive approach using modelling and computational methods is a very strong way to understand and qualify the AMCs cross contamination processes. The FOUP is made of polymeric materials and it is considered as a heterogeneous porous medium, thus the modelled processes are the contamination of two-component in transient flow under isothermal conditions. The present methodology is, first using the optimization methods with the analytical solution in order to define the physical constants of various materials which have been studied experimentally and separately, and the second using the finite element method including these physical constants and relevant interface condition. The behavior of the AMCs in analysis was determined thanks to the switch of Dirichlet to Neumann condition. The model framework preserves the classical forms of the diffusion and convection diffusion equations and yields to consistent form of the Fick's law. Most results are correlated with the experimental measurements. This methodology is relevant for the applications we focused on the dynamics of cross-contamination mainly on the evolution of the concentration level and the profile through the polymeric material, and finally on the effect of the material.

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N. Santatriniaina, L. Rakotomanana
Mathematical Research Institute & CNRS, University of Rennes 1, France.
nirina.santatriniaina@univ-rennes1.fr

J. Deseure,
LEPMI & CNRS, University of Joseph Fourier, Grenoble, France.

T. Q. Nguyen, H. Fontaine, C. Beitia
CEA, LETI, MINATEC Campus, 17 rue de martyrs, 38054 Grenoble, France.

Study of the role of spatial heterogeneities in the vicinity of a CO_2 injection well.

I. Sin, J. Corvisier and V. Lagneau

The composite near-well injection zones demonstrate a strong spatial heterogeneity and highly reactive coupled physicochemical processes. This heterogeneity has an impact on the injectivity and integrity of the storage. The interpretation of both pilot and experiment can be usefully supplemented by numerical modelling of reactive transport to quantify some phenomena that are difficult to measure at the storage scale. The present study shows the development of a two-phase flow module in the reactive transport software HYTEC [1]. The resolution is built on a water pressure/gas saturation formalism, a fully implicit method and on a Voronoi-based finite volume discretization. The method was tested and compared against a self-similar solution [2]. The effects of gravity and heterogeneity (spatial variations of the absolute/relative permeability) are observed on reference test cases.

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I. Sin, J. Corvisier, V. Lagneau
Ecole des Mines ParisTech, Centre de Géosciences, Fontainebleau, France
irina.sin@mines-paristech.fr

GEOMETRY MODELING OF OPEN-CELL FOAMS FOR EFFICIENT FLUID FLOW AND HEAT TRANSFER COMPUTATIONS USING MODIFIED KELVIN CELLS

E. Werzner, M. Mendes, J. Storm, M. Laurinat, S. Ray and T. Trimis

Open-cell foams find application in various fields of technology such as heterogeneous catalysis and separation systems. Due to the irregular structure of such porous media, the accurate representation of their geometry requires to consider a representative number of pores, which can cause high computational cost for numerical simulations. One approach to address this problem is the idealization by periodic foam geometries, whose geometric properties, e.g. porosity or strut width, are similar to the real foam. This allows to perform simulations of a single representative geometry element using periodic boundary conditions and implies a remarkable reduction of computational effort.

For the present study, three different modifications of the Kelvin cell have been generated and tested regarding their ability to accurately capture the fluid-dynamic and thermal behavior inside a highly porous open-cell foam, whose detailed geometry parameters are known from a computed tomography (CT) scan. The evaluation is based on a comparison of hydrodynamic permeability, which has been obtained from solving the conservation equations for mass and momentum using the lattice-Boltzmann method (LBM), along with effective thermal conductivity of the solid material, determined by the average steady-state heat flux computed using the finite volume method (FVM).

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E. Werzner, M. Mendes, M. Laurinat, S. Ray
Chair of Gas and Heat Technology, Institute of Thermal Engineering,
TU Bergakadamie Freiberg, Germany
marcel.laurinat@student.tu-freiberg.de, ray@iwtt.tu-freiberg.de
J. Storm
Chair of Solid State Mechanics, Institute of Thermal Engineering, TU Bergakademie, Freiburg
dimosthenis.trimis@kit.edu
D. Trimis
Chair of Combustion Technology, Engler-Bunte-Institute, Karlsruhe Institute of Technology, Germany
dimosthenis.trimis@kit.edu

Buoyancy driven dispersion in a layered porous rock

A. W. Woods and A. Farcas

We investigate the longitudinal dispersion of a passive tracer by a gravity driven flow in a porous medium consisting of a series of independent horizontal layers connected to a constant pressure source. We show that in a formation of given vertical extent, the flux is almost independent of n, the number of layers, and that as $n \to \infty$, the flux asymptotes to the multiple 1.06 of that in a single layer of the same total depth. The flow speed in each layer is approximately uniform, but gradually increases with layer depth. As a result, if a pulse of tracer is released in the flow it will migrate more rapidly through the lower layers, leading to longitudinal dispersion of the tracer. Eventually, the location of the tracer in the different layers may become separated in space so that a sufficiently distant observation well would detect a series of discrete pulses of tracer rather than the original coherent input, as would occur in a single permeable layer. At long times, the standard deviation of the longitudinal tracer distribution asymptotes to a fraction of order 0.1 of the position of the centre of mass, depending on the number of layers and the overpressure of the source.

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A. W. Woods
BP Institute, University of Cambridge, United Kingdom
andy@bpi.cam.ac.uk

A. Farcas
BP Institute, University of Cambridge, United Kingdom
adrian@bpi.cam.ac.uk

On the rate of dissolution of a trapped plume of gas in an anticline

A. W. Woods and S. Norris

Gas generated from waste emplaced in a geological disposal facility (GDF) may, depending on site-specific geology, accumulate under buoyancy in a structural trap to form a gas plume. The bulk of the gas is expected to be hydrogen, but minor species, including radionuclide-bearing gases, may be generated. Over time, this plume may gradually dissolve into ground-water, producing a cloud of hydrogen gas-saturated water which is transported downstream along with any radionuclides associated with the gas. This changes the transport mechanisms and hence risks associated with the gas reaching the surface. Once dissolved, the mobility of the gas is substantially reduced, and the transport of any radionuclides associated with GDF-derived gas residual is subsequently associated with the dispersion processes in the groundwater flows. Here, we develop a simplified model of the diffusion controlled dissolution of hydrogen from such a trapped plume and hence estimate the longevity of such a gas plume. We also use the model to estimate the spatial distribution of the cloud of hydrogen-saturated water once the gas plume is fully dissolved. We find that with typical solubilities of hydrogen in water and on the basis of assumptions regarding the rate of groundwater flow, the dissolution of a gas volume of order 100 m^3 may require tens of thousands of years as the groundwater flows past the gas. Also, depending on stratigraphy the aquifer geometry and the background groundwater flow rate, this may produce a cloud of gas-saturated water which extends several kilometres downstream of the repository GDF.

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A. W. Woods
BP Institute, University of Cambridge, United Kingdom
andy@bpi.cam.ac.uk

S. Norris
NDA, Harwell, Oxfordshire, United Kingdom
simon.norris@nda.gov.uk

Reactive transport modelling of carbonate diagenesis on unstructured grids

A. Yapparova

Reactive transport modelling code was implemented as part of CSMP++ software library, which employs finite element finite volume method for solution of PDEs on unstructured grids. Sequential non-iterative approach was used for coupling the chemistry module with transport [1]. System of nonlinear algebraic equations, that describes a geochemical system under thermodynamical equilibrium, is solved using KINSOL, from SUNDIALS [3].

A benchmark against the well-known calcite dissolution dolomite precipitation test case from [2] was performed and results are in a good agreement.

Calcite dolomitization was simulated on a 2d cross-section model with realistic geology including alternating carbonate and sandstone layers and the following results are presented: evolution of calcite and dolomite dissolution-precipitation fronts and consequent porosity/permeability change. While trying to capture the chemistry and geology accurately, we were aiming to speed up the running time by code optimization and parallelization.

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A. Yapparova
Department Mineral Resources and Petroleum Engineering, MontanÐşniversität Leoben, Austria
alina.yapparova@unileoben.ac.at

Complete dynamic modelling for a membrane distillation process

F. Eleiwi and T. M. Laleg-Kirati

This work presents a complete dynamic modelling of a membrane distillation process. The complete model contains two consistent models; the first is for the process of the membrane distillation and is based on 2D advection-diffusion equation [1], and the second is a modified 1D heat equation of a porous media for the membrane itself [2]. A full description of the temperature diffusion phenomenon across the feed container, membrane, permeate container and boundary layers of the membrane is tackled. An analysis of mass transfer through each phase of the process is provided. Heat conduction and convection mechanisms that take place inside the process are explained in terms of mathematical parameters, in addition to justification for process behavior during transient and steady state phases. Production rates can be maintained and fabrication recommendations for membrane can be granted by applying control theory techniques and optimization methods on the complete dynamic model. Simulations were performed over the complete model with real membrane specifications. Plots of vapor mass transfer along the process, evolution of membrane boundary temperature with time, and temperature difference between membrane boundary layers are included.

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F. Eleiwi
CEMSE, KAUST, Saudi Arabia
fadi.eleiwi@kaust.edu.sa

T. M. Laleg-Kirati
CEMSE, KAUST, Saudi Arabia
meriem.kiratii@kaust.edu.sa

Spatio-temporal distribution of water table depth, depending on hydrological and meteorological conditions

J. Grižić

Slavoian oak (Quercus robur L.), one of the national symbols of Croatia, is dominant and economically most valuable species in Slavonia proved to be sensitive to changes of groundwater levels (dominant for average annual groundwater levels ranging from 1.6 to 4.3 m). The goal of this project is to find spatio-temporal distribution of groundwater levels depending on hydrological (water levels of rivers in the area and piezometric levels) and meteorological conditions (mean monthly air temperature, monthly precipitation and monthly evapotranspiration) using Richards model simulations in Dumux - a free and open-source simulator for flow and transport processes in porous media. Porous media is considered to be homogeneous using mean soil as well as model parameters for loam.

J. Grižić
GEKOM-Geophysical and ecological modeling Ltd. Zagreb, Croatia
jelena.grizic@gmail.com

LOCALIZED ORTHOGONAL DECOMPOSITION TECHINQUES FOR THE MIXED FINITE ELEMENT METHOD

F. Hellman, P. Henning and A. Målqvist

For flow in porous media, rapidly varying heterogeneities in permeability fields are a significant issue in the construction of reliable numerical approximations under economical computational costs. In this work, we therefore apply the recent theory for the localized orthogonal decomposition (LOD) finite element multiscale method to the mixed finite element method for Poisson's equation. The LOD concept allows to formulate effective multiscale methods that do not rely on any regularity or scale separation in the data functions. Recent works show that high contrast and even conductivity channels can be efficiently treated with the LOD. In this talk we present a new Mixed-FEM LOD with corresponding rigorously derived convergence rates. Furthermore, mass conservation properties of the multi-scale solution are studied.

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F. Hellman
Department of Information Technology, Uppsala University, Sweden
fredrik.hellman@it.uu.se

P. Henning
ANMC, Ecole polytechnique fdérale de Lausanne, Switzerland
patrick.henning@epfl.ch

A. Målqvist
Department of Mathematical Sciences, Chalmers University of Technology and University of Gothenburg, Sweden
axel@chalmers.se

Determination of soil parameters using experimental data from centrifugation experiments

J. Minár

We have a centrifuge with the radius approximately 70 cm. At one arm we have an injection chamber, from which the water infiltrates into the sample. Next to it is the sample and subsequently an extraction chamber, where the water is collected. On the opposite arm of the centrifuge, we have two moving counterbalancing weights, which are used to equalize centrifuge force during the execution of the experiment. Under the chambers and the sample we have a scanner, which is used to measure the amount of water in injection chamber and extration chamber. Our additional measurement is a position of weights in the opposite arm, which are used to calculate centrifuge force.

In our numerical simulation, we have used the modified Richards equation for centrifugal scenario to model water movement. Several parametric fundamental relations describing saturation-pressure and saturation-permeability can be applied in the model. We have chosen few parametric classes of these relations (e.g. van Genuchten – Mualem, Brook-Corey – Burdine, e.t.c.). Then we have optimized free parameters to minimize discrepancy between experimental measurements and simulated measurements.

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J. Minár
Faculty of Civil Engineering, Slovak University of Technology in Bratislava, Slovakia
minar8@gmail.com

IMPACT OF MODEL APPROXIMATIONS ON SOIL WATER DYNAMICS IN DRIP IRRIGATION

P. Stange and N. Schütze

For modelling drip irrigated crop production, an adequate description of the soil water dynamics is crucial. Although these processes are three-dimensional under single drippers and drip lines, a simple bucket model approach (root zone as a reservoir) is implemented in most current crop growth models (e.g. AquaCrop). Only few crop growth models are able to use a 1D (e.g. APSIM) or 2D description of the soil water dynamics (e.g. Daisy). This study aims to quantify the information losses that occur by simplifying the water flow processes by several examples. The soil water dynamics were simulated for different soils on the basis of the Richards' equation for variably-saturated water flow. The model was used to generate a 1D, a 2D and a 3D setup of different layouts of drip irrigation system. The simulation results show that for specific cases the simplification of the soil water dynamics may fail due to remarkable information losses. Therefore it is important to test each different type of simplified model against more realistic 3D models before using them in drip irrigation modelling.

P. Stange
Institute of Hydrology and Meteorology, TU Dresden, Germany
peter.stange@tu-dresden.de

N. Schütze
Institute of Hydrology and Meteorology, TU Dresden, Germany
ns1@rcs.urz.tu-dresden.de

Natural methane hydrate instability with respect to its inhomogeneities

K. Tsiberkin and T. Lyubimova

We present the studies of multiphase flows with phase transitions in porous medium which contain water, methane and methane hydrate. The main goal of the work is analysis of methane hydrate stability in natural systems. We consider several kinds of hydrate layer perturbations. First, a localized spherical inclusion (a bubble) of fluids within hydrate is studied. It does not lead to instability with small initial radius and matrix permeability. An analytical self-similar solution of sphere solidification problem and bubble lifetime estimates are obtained. The simulations of large-scale bubbles shows the strong fluid flows exist and make hydrate unstable in that case. Second, the dynamics of vertical channel penetrating the methane hydrate is simulated. Large channel in high-permeable medium causes an upward flow of warm gas from underlying layers, and hydrate dissociation begins at the layer top. Finally, the criteria of gas flow instability within liquid-saturated medium are determined. It corresponds with bubble instability simulation results. The numerical modelling is performed with our own FORTRAN-90 code uses explicit finite-difference schemes and OpenMP parallel technique.

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K. Tsiberkin
Perm State University, Russia
kbtsiberkin@psu.ru

T. Lyubimova
Institute of Continuous Media Mechanics UB RAS, Russia
lyubimovat@mail.ru

SIMULATION OF SELF-DIFFUSIVITY OF WATER IN STOCHASTICALLY RECONSTRUCTED POROUS BODIES

M. Vesely, P. Capek, V. Hejtmanek, J. Lang, M. Peksa and M. Kocirik

Porous solids exhibit complex microstructures and their three-dimensional (3D) models have to catch irregular pore structure. The 3D microstructure models are usable for understanding and predicting of effective (macroscopic) transport properties. We obtained 3D stochastic replicas of three α-alumina samples using a simulated annealing method. The reconstruction method was based on a set of two-dimensional (2D) random cuts through the samples with subsequent computation of microstructural descriptors. The common way of verifying this computational methodology has been based on the comparison of macroscopic transport properties such as permeability, effective Knudsen diffusivity and effective ordinary diffusivity. We propose self-diffusion of a liquid filling pore space as another experimental method to do it. Effective self-diffusivities of water in the porous samples are determined using PFG (pulsed field gradient) NMR. We also compare results of the PFG NMR experiments and theoretical calculation of the self-diffusivity.

M. Vesely, P. Capek
Institute of Chemical Technology, Prague, Czech Republic
veselyr@vscht.cz, pavel.capek@vscht.cz

V. Hejtmanek
Institute of Chemical Process Fundamentals of ASCR, Prague, Czech Republic
hejtmanek@icpf.cas.cz

M. Peksa
Charles University, Prague, Czech Republic & University Leipzig, Germany
mikulas.peksa@uni-leipzig.de

M. Kocirik
J. Heyrovsky Institute of Physical Chemistry of ASCR, Prague, Czech Republic
milan.kocirik@jh-inst.cas.cz

Contributors

List of participants

AHMED, Elyes
Inria, Rocquencourt, France.
ahmed_elyes@yahoo.com

ALDUNCIN, Gonzalo
Instituto de Geofísica, Universidad Nacional Autónoma de México, México.
alduncin@geofisica.unam.mx

ALLAIRE, Grégoire
Ecole Polytechnique, France.
gregoire.allaire@polytechnique.fr

ALLEN, Rebecca
Computational Transport Phenomena Laboratory, KAUST, Kingdom of Saudi Arabia.
rebecca.allen@kaust.edu.sa

AMAZIANE, Brahim
LMAP & CNRS, University of Pau, France.
brahim.amazianeu@univ-pau.fr

ARNAUD, Fabien
FEI Visualization Sciences Group, Bordeaux, France.
fabien.arnaud@fei.com

BASTIAN, Peter
IWR, University of Heidelberg, Germany.
peter.bastian@iwr.uni-heidelberg.de

BAVISKAR, Shirishkumar M.
Geo-Engineering Section, Technical University of Delft, Netherlands.
s.m.baviskar@tudelft.nl

BIRGLE, Nabil
Inria, Rocquencourt, France.
nabil.birgle@inria.fr

BOURGEAT, Alain
Université Lyon1, Lyon, France.
alain.bourgeat@univ-lyon1.fr

BROWN, Donald
Center for Numerical Porous Media, KAUST, Kingdom of Saudi Arabia.
donaldbrowdr@gmail.com

BUITRAGO, Saul
Universidad Simón Bolívar, Venezuela.
sssbuitrago@yahoo.es

CAPATINA, Daniela
LMAP & CNRS, University of Pau, France.
daniela.capatina@univ-pau.fr

CARDOEN, Denis
VITO, Separation and Conversion Technology, Ghent University, Particle and Interface Technology, Belgium
dennis.cardoen@vito.be

CHECHKIN, Gregory
Moscow Lomonosov State University, Russia & Narvik University College, Norway.
chechkin@mech.math.msu.su

CHECHKINA, Tatiana
Department of Higher Mathematics, Moscow Engineering Physics Institute, Russia.

CHEN, Zhangxing John
University of Calgary, Canada.
zhachen@ucalgary.ca

COPTY, Nadim K.
Institute of Environmental Sciences, Bogazici University, Istanbul, Turkey.
copty@boun.edu.tr

DARTOIS, Arthur
Institut P' (UPR CNRS 3346), University of Poitiers, France.
arthur.dartois@univ-poitiers.fr

DISCACCIATI, Marco
UPC BarcelonaTech, Spain.
marco.discacciati@upc.edu

DORVILLE, René
Laboratoire CEREGMIA EA 2440, IUFM de Guyane, Cayenne, Guyane Française.
rene.dorville@orange.fr

DUTTA, Tapati
Physics Department, St. Xavier's College, Kolkata, India.
tapati_mithu@yahoo.com

EFENDIEV, Yalchin
Department of Mathematics & ISC Texas A&M University, USA.
efendiev@math.tamu.edu

ELEIWI, Fadi
CEMSE, KAUST, Kingdom of Saudi Arabia.
fadi.eleiwi@kaust.edu.sa

ERN, Alexandre
Université Paris-Est, CERMICS, ENPC, France.
ern@cermics.enpc.fr

FROLKOVIČ, Peter
Faculty of Engineering, Slovak University of Technology in Bratislava, Slovakia.
peter.frolkovic@stuba.sk

GAHN, Markus
Friedrich-Alexander-University Erlangen-Nuremberg, Germany.
markus.gahn@fau.de

GENTY, Alain
CEA, Saclay, France.
alain.genty@cea.fr

GOOYA, Reza
Nano-Science Center, Department of Chemistry, University of Copenhagen, Denmark.
gooya@nano.ku.dk

GRIŽIĆ, Jelena
Geophysical and ecological modeling Ltd. Zagreb, Croatia.
jelena.grizic@gmail.com

HELLMAN, Fredrik
Department of Information Technology, Uppsala University, Sweden.
fredrik.hellman@it.uu.se

HENNING, Patrick
ANMC, Ecole Polytechnique Fdérale de Lausanne, Switzerland.
patrick.henning@epfl.ch

ISLAHUDDIN, Muhammad
Building Physics Section, Department of Civil Engineering, KU Leuven, Belgium.
islah.islahuddin@bwk.kuleuven.be

IVANTSOV, Andrei
Institute of Continuous Media Mechanics UB RAS, Perm, Russia.
aivantsov@gmail.com

JAFFRÉ, Jérôme
Inria, Rocquencourt, France.
jerome.jaffre@inria.fr

JURAK, Mladen
University of Zagreb, Croatia.
jurak@math.hr

LAFITTE, Olivier
LAGA, Université Paris 13, Sorbonne Paris Cité, France.
lafitte@math.univ-paris13.fr

LE, Minh-Hoang
IRSN/PRD-DGE/SEDRAN/BERIS, Fontenay-aux-Roses Cedex, France.
minh-hoang@irsn.fr

MANASIPOV, Roman M.
Montanuniversität Leoben, Austria.
roman.manasipov@unileoben.ac.at

MARYSHEV, Boris
Institute of Continous Media Mechanics UB RAS, Perm, Russia.
bmaryshev@icmm.ru

MILIŠIĆ, Josipa Pina
University of Zagreb, Croatia.
Pina.Milisic@fer.hr

MINÁR, Jozef
Faculty of Civil Engineering, Slovak University of Technology in Bratislava, Slovakia
minar8@gmail.com

MINDEL, Julian E.
Montanuniversität Leoben, Austria.
julian.mindel@unileoben.ac.at

PANFILOV, Mikhail
LEMTA, University of Lorraine and & CNRS, France.
michel.panfilov@univ-lorraine.fr

PETROVA, Svetozara
University of Applied Sciences, Bielefeld, Germany.
svetozara.petrova@fh-bielefeld.de

PONCET, Philippe
LMAP & CNRS, University of Pau, France.
philippe.poncet@univ-pau.fr

REICHE, Tatiana
Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Braunschweig, Germany.
Tatiana.Reiche@grs.de

ROBERTS, Jean
Inria, Rocquencourt, France.
jean.roberts@inria.fr

SAAD, Bilal
Center for Numerical Porous Media, KAUST, Kingdom of Saudi Arabia.
Bilal.Saad@kaust.edu.sa

SAAD, Mazen
Ecole Centrale de Nantes, Nantes, France.
Mazen.Saad@ec-nantes.fr

SANCHEZ-EROSTEGUI, Alejandra
FEI Visualization Sciences Group, Bordeaux, France.
alejandra.sanchez-erostegui@fei.com

SANTATRINIAINA, Nirina
Mathematical Research Institute & CNRS, University of Rennes 1, France.
nirina.santatriniaina@univ-rennes1.fr

SEAID, Mohammed
School of Engineering and Computing Sciences, University of Durham, United Kingdom.
m.seaid@durham.ac.uk

SIN, Irina
Ecole des Mines ParisTech, Centre de Géosciences, Fontainebleau, France.
irina.sin@mines-paristech.fr

STANGE, Peter
Institute of Hydrology and Meteorology, TU Dresden, Germany
peter.stange@tu-dresden.de

TSIBERKIN, Kirill
Perm State University, Russia.
kbtsiberkin@psu.ru

VESELY, Martin
Institute of Chemical Technology, Prague, Czech Republic.
veselyr@vscht.cz

VRBAŠKI, Anja
University of Zagreb, Croatia.
avrbaski@math.hr

WERZNER, Eric
Institute of Thermal Engineering, TU Bergakadamie Freiberg, Germany.
Eric.Werzner@iwtt.tu-freiberg.de

WOODS, Andrew W.
BP Institute, University of Cambridge, United Kingdom.
andy@bpi.cam.ac.uk

YAPPAROVA, Alina
Department Mineral Resources and Petroleum Engineering, Montanuniversität Leoben, Austria.
alina.yapparova@unileoben.ac.at

ZAZA, Chady
CEA DEN/DANS/DM2S/STMF/LMEC & I2M UMR 7373 CNRS, France.
chady.zaza@latp.univ-mrs.fr

ŽGALJIĆ KEKO, Ana
University of Zagreb, Croatia.
ana.zgaljic@fer.hr