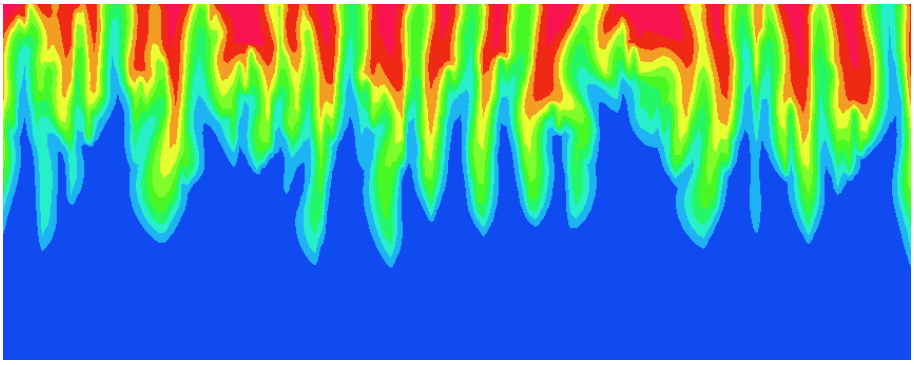
Workshop SITRAM21

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

December 8-10 2021, Inria, Paris



Program Committee:
Etienne Ahusborde and Brahim Amaziane (UPPA E2S & CNRS, IPRA-LMAP)
Michel Kern (INRIA Paris, SERENA)
Stefan de Hoop and Denis Voskov (TU Delft)

Contents

PREFACE

Welcome to SITRAM 2021!

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

The SITRAM Workshop is a forum for discussing recent research on the development and applications of both modeling and simulation for coupled transport and geochemistry in subsurface flow. The purpose of this Workshop is to bring together students, researchers and engineers who are active in the broad area of reactive flow and transport in porous media, and to create a fertile forum for presenting research results, exchanging ideas, and initiating collaborations. SITRAM21 is a follow-up to the first edition SITRAM19 that took place in Pau in December 2019, and gathered more than 40 researchers from eight different countries. SITRAM19 followed other similar events organized in 2015 and 2018 under the umbrella of the MoMaS research group and the National French Research Group MaNu/CNRS GdR 2439. As organizers, we hope there will be more to come in the future.

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

A session of the Workshop will be dedicated to a new benchmark targeted towards two-phase flow with reactive transport in porous media.

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

This book contains the abstracts of the invited lectures and contributions presented at SITRAM 2021. The scientific program of the Workshop consisted of 22 talks. The Workshop was attended by about 80 participants coming from 8 countries: France, The Netherlands, Germany, Italy, Morocco, Norway, Great Britain and Canada. We would like to thank the speakers and all of you for your participation at the Workshop.

The Workshop could not have been held without the financial support of the organizing institutions and the following sponsors: the IPRA Research Federation (FR CNRS-UPPA 2952), the French Research Group MaNu/CNRS and the Carnot Institute, ISIFoR project (Institute for the sustainable engineering of georesources. We thank them for their financial support. The support of the French Interpore Chapter (FIC), InterPore and Société de

Mathématiques Appliquées et Industrielles (SMAI) is also greatly acknowledged.

We would like to thank Derya Gök (INRIA Paris) for her active role in the organization of the logistics of the conference.

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

Etienne Ahusborde and Brahim Amaziane (UPPA E2S & CNRS, IPRA-LMAP)
Michel Kern (INRIA Paris, SERENA)
Stefan de Hoop and Denis Voskov (TU Delft)

Contributors

List of participants

ABUAISHA, Murad
murad.abuaisha@mines-paristech.fr

AHUSBORDE, Etienne
LMAP & CNRS, University of Pau, France.
etienne.ahusborde@univ-pau.fr

AIT-MOUHEB, Naila
Forschungszentrum Juelich.
n.ait.mouheb@fz-juelich.de

AJEDDIG, Younes
younes.ajeddig@univ-pau.fr

AL NAZER, Safaa
Université du Littoral Côte d'Opale, LMPA & CNRS - Université Libanaise, LaMA-Liban.
safaa_nazer@hotmail.com

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

AMIR, Laila
FSTG, Univ. Cadi Ayyad, Marrakech, Morocco.
l.amir@uca.ma

ANDRIANOV, Nikolai
nia@geus.dk

ARISKINA, Kristina
kristina.ariskina@univ-pau.fr

BANSHOVA, Shin
University of Bergen.
shin.banshoya@uib.no

BASTIDAS, Manuela
INRIA.
manuela.bastidas-olivares@inria.fr

BERRE, Inga
University of Bergen.
inga.berre@uib.no

BEGUINET, Adrien
adrien.beguinet@universite-paris-saclay.fr

BOUREL, Christophe
bourel@univ-littoral.fr

CHABAB, Salaheddine
salaheddine.chabab@univ-pau.fr

CHEVALIER, Jérémy
jeremy.chevalier2603@gmail.com

COCHEPIN, Benoit
ANDRA - Châtenay-Malabry, France.
benoit.cochepin@andra.fr

DE HOOP, Stephan
TU Delft, Delft, The Netherlands.
S.deHoop-1@tudelft.nl

DEISSMANN, Guido
Forschungszentrum Juelich.
g.deissmann@fz-juelich.de

DELAGE SANTACREU, Stéphanie
stephanie.delage@univ-pau.fr

DONG, Zhaonan
INRIA Paris.
zhaonan.dong@inria.fr

DURAN, Omar
University of Bergen.
omar.duran@uib.no

EL OSSMANI, Mustapha
University Moulay Ismaïl, Meknes, Morocco.
m.elossmani@ensam.umi.ac.ma

ETANGSALE, Grégory
gregory.etangsale@univ-reunion.fr

FAILLE, Isabelle
IFP Energies nouvelles, Rueil-Malmaison, France. isabelle.faille@ifpen.fr

FLAURAUD, Eric
IFP Energies nouvelles, Rueil-Malmaison, France. eric.flauraud@ifpen.fr

FUMAGALLI, Alessio
MOX Laboratory, Politecnico di Milano.
alessio.fumagalli@polimi.it

GAYELLE, Fahed
gayelle.fahed@etu.univ-nantes.fr

GOUASNOUANE, Omar
gouasnouane@gmail.com

HAJIZADEH JAVARAN, Mohammad Reza
mrhj75@gmail.com

HERNANDEZ ANGULO, Luis Roberto
luis.hernandez@univ-grenoble-alpes.fr

HILHORST, Danielle
Danielle.Hilhorst@math.u-psud.fr

HORNG, Tzyy-Leng
Feng Chia University.
tlhorng123@gmail.com

ICARDI, Matteo
University of Nottingham.
Matteo.icardi@nottingham.ac.uk

JABBARI, Amira
ajh@lgpc.cpe.fr

JAKABCIN, Lukas
University of Orléans.
lukas.jakabcin@univ-orleans.fr

JOHANSSON, Peter
pjohansson@univ-pau.fr

JONVAL, Maxime
maxime.jonval@inria.fr

KEILEGAVLEN, Eirik
Department of Mathematics, University of Bergen.
Eirik.Keilegavlen@uib.no

KERKACHE, Halla
halla.kerkache@univ-pau.fr

KERN, Michel
INRIA Paris, SERENA.
michel.kern@inria.fr

KHELIDJ, Abdelhafid
abdelhafid.khelidj@univ-nantes.fr

LANDA MARBAN, David
dmar@norceresearch.no

LANNABI, Ibtissem
ilannabi@univ-pau.fr

LEBAIGUE, Olivier
olivier.lebaigue@cea.fr

LE POTIER, Christophe
christophe.le.potier@gmail.com

LIPOVAC, Veljko
University of Bergen, Department of Mathematics.
veljko.lipovac@uib.no

LOCATELLI, Francesca
University of Pavia.
francesca.locatelli03@universitadipavia.it

LOENARTZ, Mara
Forschungszentrum Juelich.
m.loenartz@fz-juelich.de

MAHE, François
francois.mahe@ec-nantes.fr

MERTEN, Julie
j.y.merten@rug.nl

MICHAUD, Maïté
mmi@lgpc.cpe.fr

NAFIRI, Salem
nafiri@ehtp.ac.ma

OKUMBO, Victor
okumko.victor@univ-pau.fr

OUCHTOUT, SALIH
Salih.Ouchtout@univ-nantes.fr

PANFILOV, MICHEL
Institut Elie Cartan, Université de Lorraine &
CNRS, Nancy.
michel.panfilov@univ-lorraine.fr

PAUTARD, MATTHIAS
matthias.pautard@thalesgroup.co

PAVULURI, SAIDEEP
University of Orléans.
saideep.pavuluri@univ-orleans.fr

PESCIMORO, EUGENIO
University of Nottingham.
meugenio.pescimoro@nottingham.ac.uk

PILLARDOU, NICOLAS
LMAP & CNRS, University of Pau, France.
nicolas.pillardou@univ-pau.fr

POONOOSAMY, JENNA
Forschungszentrum Juelich.
j.poonoosamy@fz-juelich.de

POP, IULI SORIN
sorin.pop@uhasselt.be

RIPAMONTI, SIMONE
Politecnico di Milano.
simone2.ripamonti@mail.polimi.it

ROKNIAN, ARASH ANDREA
Politecnico di Milano.
arashandrea.roknian@mail.polimi.it

SAYET, THOMAS
University of Orléans.
thomas.sayet@univ-orleans.fr

SERIN, JEAN-PAUL
jean-paul.serin@univ-pau.fr

SIN, IRINA
MINES ParisTech, PSL University.
irina.sin@mines-paristech.fr

SOCIE, ADRIEN
EOAS, University of British Columbia,
Vancouver, BC, Canada.
asocie@eoas.ubc.ca

TAAKILI, ABDELAZIZ
ENSAM-Meknés.
ataakili@gmail.com

TABRIZINEJADAS, SARA
University of Strasbourg.
tabrizinejadas@unistra.fr

TAJANI, CHAKIR
chakir_tajani@hotmail.fr

TALALI, KHADIJA
talali.khadija@gmail.com

TAMBUE, ANTOINE
antonio@aims.ac.za

TÓTH, MICHAL
Heidelberg University.
michal.toth@iwr.uni-heidelberg.de

TRABELSI, ABDELKRIM
UCBL.
abdelkrim.trabelsi@univ-lyon1.fr

VOSKOV, DENIS
TU Delft, Delft, The Netherlands.
D.V.Voskov@tudelft.nl

WANG, YUE
Institute for Modelling Hydraulic and
Environmental Systems, University of Stuttgart
yue.wang@iws.uni-stuttgart.de

YANG, YUANKAI
Forschungszentrum Juelich.
y.yang@fz-juelich.de

ZAIM, MOHAMED
mohammed.zaim@ec-nantes.fr

ZANOTA, MARIE-LINE
mlz@lgpc.cpe.fr

FULLY IMPLICIT SCHEME FOR MULTIPHASE REACTIVE FLOWS IN POROUS MEDIA: APPLICATION TO A BENCHMARK FOR GEOLOGICAL SEQUESTRATION OF CO_2

E. Ahusborde, B. Amaziane and M. Kern

Keywords: Reactive Transport Modeling, Fully implicit scheme, finite volume, DuMu^X.

Reactive multiphase flows play a significant role for many applications in geological and reservoir engineering processes. They are modeled by a set of highly nonlinear degenerate partial differential equations (mass conservation laws governing a compositional two-phase flow model) coupled to ordinary and/or algebraic differential equations (modeling kinetic and equilibrium chemical reactions respectively).
In this talk, we present a parallel, fully coupled, fully implicit, finite volume scheme for modeling isothermal reactive multiphase flow based on a Direct Substitution Approach (DSA). The DSA formulation consists in incorporating the mass actions laws directly in the mass conservation laws above-mentioned [1]. The method has been implemented in the DuMu^X platform [2], using High Performance Computing. The nonlinear system are solved using an appropriate Newton's method with variable time stepping. The linear systems are solved by solvers provided by DUNE [3]. The method has been validated by numerous 1D, 2D and 3D test cases. Here, we will focus on a recently proposed benchmark that models scenarios of CO_2 geological storage into a deep saline aquifer. Our results will be compared with those obtained by other participants for 1D and 2D configurations and preliminary results on a more complex chemical system will be proposed.

References

[1] E. Ahusborde, B. Amaziane, M. Id Moulay, High Performance Computing of 3D reactive multiphase flow in porous media: application to geological storage of CO_2, 25, 2131-2147 (2021).

[2] T. Koch *et al*, DuMu^X 3 - an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling, *Computers & Mathematics with Applications*, 81, 423-443 (2021)

[3] P. Bastian, M. Blatt, A. Dedner, N.A. Dreier, C. Engwer, R. Fritze, C. Gräser, D. Kempf, R. Klöfkorn, M. Ohlberger, O. Sander. The DUNE framework: Basic concepts and recent developments. *Computers & Mathematics with Applications*, 81, 75-12 (2021).

E. Ahusborde and B. Amaziane
Universite de Pau et des Pays de l'Adour, E2S UPPA, CNRS, LMAP, Pau, France.
etienne.ahusborde@univ-pau.fr; brahim.amaziane@univ-pau.fr

M. Kern
INRIA, Paris, France & ENPC, Univ. Paris–Est,
France
michel.kern@inria.fr

DERIVATION OF REACTIVE TRANSPORT PARAMETERS FOR THE SANDY OPALINUS CLAY FACIES

N. Ait-Mouheb, M. Henkes, Z. Paparigas, G. Deissmann and D. Bosbach

Keywords: Ra-226 migration, reactive transport modelling, Opalinus clay, solid solution formation..

Opalinus clay (OPA) is proposed as host rock formation for a geological disposal facility for radioactive waste in Switzerland and is also considered in the newly started site selection procedure for a high-level radioactive waste repository in Germany. In this context, we evaluate the effect of the natural heterogeneity of the sandy facies in the Opalinus clay formation (OPA-SF) on radionuclide transport. Therefore, this work provides chemical and mineralogical characteristics as well as sorption and transport parameters of Ra-226, determined on different drill core samples from the OPA-SF extracted from the Mont Terri underground rock laboratory in Switzerland.

Through-diffusion experiments parallel to the bedding are conducted with a cylindrical diffusion cell to derive the Ra-226 reactive transport parameters [1]. Three different samples representative of the heterogeneity of the drill core are being used in these experiments. The setup consists of a thin OPA-SF sample of 10 mm thickness sealed and mounted between two compartments filled with artificial clay water. A concentration gradient is maintained with a constant Ra-226 concentration of $1.86 \cdot 10^{-8}$ M in the upstream compartment and zero concentration in the downstream compartment. The preliminary experimental results are supported by reactive transport modelling utilising iCP version 2.0 [2], which couples the chemistry provided by PHREEQC v3.5.0 [3] and the physics of COMSOL version 5.5 [4]. The model is implemented in 1D and considers the uptake of Ra-226 via cation exchange, surface complexation reactions [5] and formation of solid solutions of Ra-bearing carbonates and sulphates.

References

[1] Ait-Mouheb, N., Joseph, C., Schäfer, T., Montoya, V. *Multi-method approach for studying HTO and 36Cl⁻ migration through "low-pH" cement pastes and mortars*. Cement and Concrete Research (under review).

[2] Nardi, A., Idiart, A., Trinchero, P., de Vries, L.M., Molinero, J., 2014. *Interface COMSOL-PHREEQC (iCP), an efficient numerical framework for the solution of coupled multiphysics and geochemistry*. Computers & Geosciences 69, 10-21.

[3] Parkhurst, D.L., Appelo, C.A.J., 2013. U.S. Geological Survey Techniques and Methods, book 6, chap. A43, 497 p.

[4] COMSOL 2019. Multiphysics 5.5. Finite-element software package. COMSOL AB, Stockholm.

[5] Bradbury, M.H., Baeyens, B., 2011. *Predictive sorption modelling of Ni(II), Co(II), Eu(IIII), Th(IV) and U(VI) on MX-80 bentonite and Opalinus Clay: A "bottom-up" approach*. Applied Clay Science 52, 27-33.

N. Ait-Mouheb
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
n.ait.mouheb@fz-juelich.de

M. Henkes
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
m.henkes@fz-juelich.de

Z. Paparigas
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
z.paparigas@fz-juelich.de

G. Deissmann
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
g.deissmann@juelich.de

D. Bosbach
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
d.bosbach@juelich.de

CONVERGENCE ACCELERATION OF ITERATIVE SEQUENCES FOR EQUILIBRIUM CHEMISTRY COMPUTATIONS

S. Al Nazer, M. Jazar and C. Rosier

Keywords: Nonlinear systems, Thermodynamic chemistry, Anderson acceleration, Polynomial vector extrapolation..

The modeling of thermodynamic equilibria leads to complex nonlinear chemical systems which are often solved with the Newton-Raphson method. But this resolution can lead to a non convergence or an excessive number of iterations due to the very ill-conditioned nature of the problem. In this work, we combine a particular formulation of the equilibrium system called the Positive Continuous Fraction method with two iterative methods, Anderson Acceleration method and Vector extrapolation methods (namely the reduced rank extrapolation and the minimal polynomial extrapolation). The main advantage of this approach is to avoid forming the Jacobian matrix. In addition, a strategy is used to improve the robustness of the Anderson acceleration method which consists in reducing the condition number of matrix of the least squares problem in the implementation of the Anderson acceleration so that the numerical stability can be guaranteed. We compare our numerical results with those obtained with the Newton-Raphson method on the Acid Gallic test and the $1D$ MoMas benchmark test case and we show the high efficiency of our approach.

References

[1] Carrayrou, J., Mosé, R., Behra, P., *New efficient algorithm for solving thermodynamic chemistry*. AIChE J. 48(4), 894-904 (2002).

[2] Anderson, D. G., *Iterative procedures for nonlinear integral equations*. Journal of the ACM, 12 (1965), pp. 547-560.

[3] Sidi, A., *Vector Extrapolation methods with applications to solution of large systems of equations and to PageRank computations*. Computer science department, Technion - Israel institute of technology, Haifa 32000, Israel.

S. Al Nazer
Université du Littoral Côte d'Opale, LMPA & CNRS - Université Libanaise, LaMA-Liban.
safaa_nazer@hotmail.com

M. Jazar
Université Libanaise, LaMA-Liban.
mjazar@laser-lb.org

C. Rosier
Université du Littoral Côte d'Opale, LMPA.
rosier@univ-littoral.fr

Simulation of reactive transport in heterogenous porous media with a Newton-Krylov method

L. Amir and M. Kern

Keywords: Reactive transport, porous media, nonlinear systems, Newton-Krylov method, preconditioning, precipitation and dissolution reactions.

Reactive transport modeling in porous media involves the simulation of several physic-ochemical processes: flow of fluid phases, transport of species, chemical reactions between species. It leads to a highly nonlinear system of partial differential for transport, coupled to algebraic equations for chemistry.
In [1], we have presented a globally coupled approach, where transport and chemistry are solved in a fully coupled manner, but that keeps the transport and chemistry modules separate. The method uses the same fixed point formulation than the Standard Iterative Approach, but, at each time step the nonlinear system of algebraic equations that couples all chemical species at all mesh points is solved by a Newton-Krylov method. The linear system at each Newton step is solved by the GMRES method, with a Jacobian free implementation where the required matrix by vector product may be approximated by a finite difference quotient or computed exactly. Linear and nonlinear preconditioners give a method where the number of both Newton and GMRES iterations do not grow when the mesh is refined [2].
In this talk, we recall the main features of the method, and we present an extension to handle mineral precipitation and dissolution reactions using an interior point Newton method [3]. We also study the performance of the method on 2D heterogeneous geometries.

References

[1] L. and M. Kern, *A global method for coupling transport with chemistry in heterogeneous porous media*, Computat. Geosci., 14 :465–481, 2010.

[2] L. Amir and M. Kern, *Preconditioning a coupled model for reactive transport in porous media* Int. J. Numer. Anal. Model., 16(1) :18–48, 2019.

[3] L. Amir and M. Kern, *Jacobian free methods for coupling transport with chemistry in heterogenous porous media* Water (13), 370, 2021.

L. Amir
L2IS, Faculté des sciences et techniques, Université Cadi Ayyad, Marrakech, Maroc
l.amir@uca.ma

M. Kern
INRIA, Paris, France & ENPC, Univ. Paris–Est,
France
michel.kern@inria.fr

Error estimate of a gradient discretization method on a linear poroelasticity system

A. Béguinet, L. Goudenège and D. Hilhorst

Keywords: Error Estimate, Porous media.

n this paper, we study a linear system for flow in porous media coupled to small mechanical deformations of the ground proposed by Mikelic, Wheeler and Whang. We apply gradient discretization methods which include numerical methods such as finite element methods and generalized finite volume methods. We prove the existence of the discrete solution by means of an iteration scheme and then present error estimates.

References

[1] A. Mikelic, B. Whang, M. Wheeler Numerical convergence study of iterative coupling for coupled flow and geomechanics, Computational Geosciences, 18, pp. 325-341, 2014.

[2] J. Droniou, R. Eymard, T. Gallouët, C. Guichard, R. Herbin. The gradient discretisation method . 2018. hal-01382358v6.

[3] . Bonaldi, K. Brenner, J. Droniou, R. Masson. Gradient discretization of two-phase flows coupled with mechanical deformation in fractured porous media. 2020. hal-02549111.

A. Béguinet
LMO & CentraleSupelec, Université Paris-Saclay
adrien.beguinet@universite-paris-saclay.fr

L. Goudenège
LMO & CentraleSupelec, Université Paris-Saclay
ludovic.goudenege@centralesupelec.fr

D. Hilhorst
LMO & CentraleSupelec, Université Paris-Saclay
danielle.hilhorst@gmail.com

A TWO-SCALE PHASE-FIELD MODEL FOR REACTIVE TRANSPORT IN POROUS MEDIA WITH EVOLVING PORE-SCALE GEOMETRY

M. Bastidas-Olivares, C. Bringedal, I. S. Pop and L. von Wolff

Keywords: Reactive transport, evolving microstructure, pase field modelling, upscaling, two-scale numerical scheme, linear iterations.

We consider a two-scale model for reactive transport in a porous medium. At the pore scale, a micro-structural evolution can be encountered due to processes like precipitation and dissolution, which can impact the fluid flow. One encounters free boundaries separating the space available for flow from the solid, impermeable part in the medium. To avoid difficulties related to the micro-scale free boundaries, we consider a phase-field pore-scale model [1]. Employing formal homogenization, a two-scale phase-field model is derived, in which the pore-scale and the Darcy-scale model components are coupled through the cell problems providing the effective parameters. For the resulting model, we discuss an adaptive two-scale scheme [2]. It involves iterations between the two scales, linear iterations for solving the nonlinear cell problems, an adaptive selection of the elements wherein the effective parameters are computed, and adaptive mesh refinement.

References

[1] M. Bastidas, C. Bringedal, and I.S. Pop, *A two-scale iterative scheme for a phase-field model for precipitation and dissolution in porous media*, Applied Mathematics and Computation, 396, 125933, 2021.

[2] C. Bringedal, L. von Wolff, I.S. Pop, *Phase field modeling of precipitation and dissolution processes in porous media: Upscaling and numerical experiments*, Multiscale Modelling and Simulation, 18, pp. 1076-1112, 2020.

M. Bastidas Olivares
INRIA Paris
manuela.bastidas-olivares@inria.fr

C. Bringedal
University of Stuttgart
Carina.Bringedal@iws.uni-stuttgart.de

I. S. Pop
Hasselt University
sorin.pop@uhasselt.be

L. von Wolff
University of Stuttgart
lars.von-wolff@mathematik.uni-stuttgart.de

Multiphase Reactive Transport Benchmark and a Connection With Outcrop Observations

S. de Hoop and D. Voskov

Keywords: Multiphase flow, finite volume method, OBL, LiDAR, fractures..

This talk presents the preliminary results of the proposed multiphase reactive transport benchmark. These results consist of both 1D and 2D test cases with equilibrium and kinetic chemistry. Furthermore, we link reactive transport simulations to outcrop observations obtained through a fieldwork expedition in several caves in Bahia, Brazil. The outcrop observations consist of a high-resolution LiDAR dataset of the interior of the caves. Slices are made through the surveys after which a projection of the point cloud on these planes results in a comprehensive shape-analysis. The link between fractures and other sources of heterogeneity on the dissolution patterns are discussed. One of the main applications of these systems is the production of geothermal energy, hence, an uncertainty quantification workflow is presented in which we apply a fracture simplification algorithm to reduce computational complexity while keeping the main characteristics of the fracture network. Finally, we show some recent results related to a Carbon Capture Storage project where dissolution occurs in a carbonate rock layer due to large concentrations in CO_2.

References

[1] D. Voskov, *Operator-based linearization approach for modeling of multiphase multi-component flow in porous media*, Journal of Computational Physics, 337, pp. 275–288, 2017.

[2] Delft Advanced Research Terra Simulator (DARTS)

[3] S. de Hoop, D. Voskov, and G. Bertotti, *Studying the Effects of Heterogeneity on Dissolution Processes Using Operator Based Linearization and High-Resolution LiDAR Data*, ECMOR XVII, European Association of Geoscientists & Engineers, 2020.

S. de Hoop
Delft University of Technology
S.dehoop-1@tudelft.nl

D. Voskov
Delft University of Technology
D.V.Voskov@tudelft.nl

Numerical Simulation of Coupled Multiphase Flow and Kinetic Reaction in Porous Media using IFPEN Code CooresFlow: Application to the 1D and 2D Benchmark test cases

E. Flauraud, T. Faney and A. Michel

Keywords: Multi-phase flow, phase equilibrium, chemical kinetic reaction, finite volume, CooresFlow..

In this talk, we will present the formulation used in CooresFlow to simulate multiphase flow coupled with kinetic reactions. This formulation, known as the Coats formulation, consists in solving a system of conservation equations coupled with phase equilibrium equations and kinetic reaction equations. The resulting nonlinear system is discretized by a fully implicit Finite Volume scheme and is solved using Newton's method. One of the particularities of CooresFlow is that new physical laws can be defined directly in the dataset without the need to make additional developments in the code. In this presentation, we will also illustrate the application of this concept on the two cases of the benchmark which simulate a two-phase flow with a single kinetic reaction on 1D and 2D geometries. The results are analyzed and can be compared with those obtained by the other participants.

E. Flauraud
IFP Energies nouvelles, Rueil-Malmaison (France).
eric.flauraud@ifpen.fr

T. Faney
IFP Energies nouvelles, Rueil-Malmaison (France).
thibault.faney@ifpen.fr

A. Michel
IFP Energies nouvelles, Rueil-Malmaison (France).
anthony.michel@ifpen.fr

UNCERTAINTY QUANTIFICATION FOR NUMERICAL SIMULATIONS IN CARBON MINERALIZATION

A. Fumagalli, S. Ripamonti, A. A. Roknian and A. Scotti

Keywords: Reactive transport, CO_2 sequestration, uncertainty quantification, sparse grids, fractured porous media.

CO_2 sequestration is one of the promising technology to mitigate the climate change in the next decades, by using depleted wells it is injected into the underground and there long term stored thanks to reliable cap rocks. In [1], it is reported that it is very likely that 99% of CO_2 is retained for the next 100 years in selected and well managed geological reservoirs. To enhance the security of the system, following [2], the CO_2 can be injected in favourable rocks, rich of $CaSiO_3$ that react with the CO_2 creating pore-filling precipitates and thus enhance the sealing of the system, quite important process especially in presence of permeable fractures [3].

In the underground uncertainty is ubiquitous and can compromise the predictive properties of numerical simulations, moreover the measurement of some of the physical parameters may be rather challenging. In this study, we consider an uncertainty quantification analysis on the previous system of chemical reactions to estimate, with the Sobol indices, the most important parameters on the sealing mechanism. To speed up the process, we have employed the sparse grid technique that substantially decrease the computational burden.

References

[1] Metz, B., Davidson, O., d. Coninck, H., Loos, M., and Meyer, L. IPCC special report on carbon dioxide capture and storage. (2005).

[2] Ling, F., Plattenberger, D., Peters, C. & Clarens, A. Sealing Porous Media through Calcium Silicate Reactions with CO2 to Enhance the Security of Geologic Carbon Sequestration. *Environmental Engineering Science*. **38**, 127-142 (2021)

[3] Fumagalli, A. & Scotti, A. A mathematical model for thermal single-phase flow and reactive transport in fractured porous media. *Journal Of Computational Physics*. **434** (2021)

A. Fumagalli
MOX Laboratory, Politecnico di Milano
alessio.fumagalli@polimi.it

S. Ripamonti
Politecnico di Milano
simone2.ripamonti@mail.polimi.it

A. A. Roknian
Politecnico di Milano
arashandrea.roknian@mail.polimi.it

A. Scotti
MOX Laboratory, Politecnico di Milano
anna.scotti@polimi.it

OPEN-SOURCE SOLUTIONS FOR REACTIVE TRANSPORT PROBLEMS: FROM PORE- TO FIELD-SCALE

M. Icardi, E. Pescimoro, F. Municchi and J. J. Hidalgo

Keywords: Reactive transport simulation, OpenFOAM, Homogenization..

In this talk, we will present our recent work on the development of a flexible open-source simulator for reactive transport problems in porous media. We will first describe the mathematical models and the upscaling techniques recently developed [1] that allow to derive continuous models for arbitrary large reaction kinetics. Extensions to non-linear kinetics and evolving porous media will be discussed. I will then present some features of the macro-scale solvers and models in SECUReFoam, the suite of open-source OpenFOAM-based porous media simulators.

References

[1] F. Municchi, M. Icardi. Macroscopic models for filtration and heterogeneous reactions in porous media. *Advances in Water Resources* (2020).

[2] M. Icardi, E. Pescimoro, F. Municchi, J. J. Hidalgo, Computational framework for complex flow and transport in heterogeneous porous media, In preparation.

M. Icardi
School of Mathematical Sciences, University of Nottingham, UK

F. Municchi
Colorado School of Mines, Golden, Colorado, USA

E. Pescimoro
School of Mathematical Sciences, University of Nottingham, UK

J. J. Hidalgo
IDAEA, CSIC, Barcelona, Spain

A FULLY COUPLED SIMULATION TOOL FOR REACTIVE MULTIPHASE FLOW WITH CAPACITY FOR HANDLING MIXED-DIMENSIONAL GEOMETRIES

E. Keilegavlen

Keywords: Reactive transport, multiphase flow, finite volume methods, fractured porous media..

We are interested in including multiphase and geochemical effects into a simulation tool which is primarily developed for fractured and deformable porous media, motivated by application areas such as geothermal energy and CO2 storage. Our starting point is the modeling and simulation framework PorePy [1], which is based on a mixed-dimensional representation of fracture networks, and we discuss the implementation of reactive multiphase flow within the framework. The equations are solved fully coupled, using finite volume methods for spatial terms and a unified treatment of phase transitions and chemical effects presented in [2]. We discuss application of our simulation tool to the SITRAM benchmark, and also discuss likely challenges in extending the methodology to mixed-dimensional geometries.

References

[1] E. Keilegavlen, R. Berge, A. Fumagalli, M. Starnoni, I. Stefansson, J. Varela and I. Berre, Porepy: An open-source software for simulation of multiphysics processes in fractured porous media, *Computational Geosciences*, 25, 243-265 (2021).

[2] K. Kala and D. Voskov, Element balance formulation in reactive compositional flow and transport with parameterization technique,*Computational Geosciences*, 24, 609-624 (2020).

E. Keilegavlen
Department of Mathematics, University of Bergen.
Eirik.Keilegavlen@uib.no

Multiphase Flow with Reactive Transport: Description of the Benchmark Proposal

M. Kern, E. Ahusborde, B. Amaziane, S. de Hoop and D. Voskov

Keywords: Reactive transport, numerical simulation, benchmark.

Coupling chemical reactions with multiphase flow has become an important topic in subsurface simulations, with applications to CO_2 sequestration, nuclear waste storage or enhanced oil recovery.

This talk will describe a proposal for a benchmark problem addressing the numerical difficulties in the simulation of coupled flow with chemical reactions. Such benchmarks exist for one phase flow with reactions, and several models have been presented in the literature, though non is fully suitable as a benchmark. In such a benchmark it is important that the model be fully specified, so as to ensure that the same problem is simulated by all participants. This precludes the use of black box models, both for the flow simulations (equations of state, behavior laws for the fluids) and for the chemistry (all reactions must be explicitly given, which makes the use of chemical database problematic).

The proposed benchmark starts with a single reaction involving mineral dissolution, either at equilibrium or kinetic, and addresses the feedback of chemistry on the porosity. Both a 1D model and a 2D model are proposed. Taking into account more chemical reactions, such as a complex aqueous phase, will be part of a second stage. Software and network elements that enable participants to share their results will be presented. This talk will describe the benchmark so that the following presentations in the session can focus on solutions methods and discuss their results.

M. Kern
Inria, France
michel.kern@inria.fr

E. Ahusborde
Universite de Pau et des Pays de l'Adour, France
etienne.ahusborde@univ-pau.fr

B. Amaziane
Universite de Pau et des Pays de l'Adour, France
brahim.amaziane@univ-pau.fr

S. de Hoop
TU Delft, Netherlands
S.deHoop-1@tudelft.nl

D. Voskov
TU Delft, Netherlands and Stanford University, USA
D.V.Voskov@tudelft.nl

Coherent diffusion-reaction waves in bioreactive transport through double-porosity media: example of underground hydrogen

M. Panfilov and S. Zaleski

The object of research is a system of equations describing diffusion with chemical reactions caused by microorganisms in a periodically heterogeneous medium (double porosity). The medium is considered at the macrolevel as two continua interacting with each other. The reaction kinetics is determined by the kinetics of population growth, which is nonlinear and non-monotonic in the general case. A typical example of such a system concerns natural hydrogen reservoirs or underground hydrogen storages, in which the microorganisms consume hydrogen for their respiration and initiate several reactions between hydrogen and other species, converting them into other species (CH_4 or H_2S).

The objective was to find various classes of limit solutions at large times (patterns).

The mass transfer term in the equations of double porosity imposes a qualitative difference on the types of patterns compared to the classical reaction-diffusion system. Along with steady-state patterns determined by Turing's instability (diffusion-reaction instability), and permanent quasi-periodic temporal oscillations caused by the Hopf-Andronov bifurcation, we have revealed joint temporal and spatial periodic patterns formed by **coherent waves**, the frequency of which is determined by the medium heterogeneity (the higher the heterogeneity degree, the lower the frequency). Coherent waves differ from standing waves that exist in homogeneous media.

Along with theoretical analysis, the system was analysed numerically both on the macro- and micro-scales. The results for the microscale case show the occurrence of an additional pattern in the form of travelling flashes. They correspond to the Hopf-Andronov temporal oscillations in the blocks and to Turing's spatial fluctuations in the fractures.

There results were used to analyse the behaviour of an underground storage of hydrogen. We show various scenarios of the evolution of such a storage and discuss the optimal regime.

M. Panfilov
Institut Jean le Rond d'Alembert - Sorbonne Université/CNRS, Paris
Institut Elie Cartan - Université de Lorraine/CNRS, Nancy.
michel.panfilov@univ-lorraine.fr

S. Zaleski
Institut Jean le Rond d'Alembert - Sorbonne Université/CNRS, Paris
Institut Universitaire de France
stephane.zaleski@upmc.fr

NUMERICAL SIMULATION OF MULTIPHASE THERMO-HYDRO-CHEMICAL COUPLING IN POROUS MEDIA

N. Pillardou, E. Ahusborde and F. Croccolo

Keywords: Finite Volume, HPC, Nonisothermal multiphase flow, Reactive transport.

Reactive multiphase flows in porous media appear in diverse energetic and environmental problematics such as geological gas storage (CO_2, natural gas and H_2), nuclear waste management, petroleum engineering or geothermal energy production. In this talk, we will mainly focus on the application of CO_2 storage that appears as a promising way to reduce greenhouse gas emissions. Such storage problems are studied thanks to numerical simulations because of their flexibility to treat large size of reservoirs and span a wide range of time scales for investigating the behaviour of the injected fluid. Despite the large effort of the scientific community, simulations of Thermo-Hydro-Chemical (THC) processes in complex porous media remains a challenge.

Reactive multiphase flows are governed by a non-linear system of degenerated partial differential equations (flow is modelled by mass conservation laws and an energy balance equation to take into account temperatures effects), coupled with algebraic or ordinary differential equations (provided by chemical reactions). Finally, the system is closed by equations of state and solubility laws characterizing each phase equilibrium.

In this talk, we propose an extension to nonisothermal flows of the fully coupled, fully implicit scheme developed in [1] for isothermal reactive multiphase multicomponent flows. Spatial discretization is carried out using a cell-centered finite volume scheme and time discretization is done by using a Backward Differentiation Formula 2 (BDF2). This THC model has been implemented in the DuMu^{X}platform [2] and some preliminary results will be presented. We also investigated the difference between isothermal and nonisothermal simulations in order to highlight temperature effects on the dissolution of supercritical/gaseous CO_2 in liquid phase.

References

[1] Ahusborde, E., Amaziane, B., Id Moulay, M., High performance computing of 3D reactive multiphase flow in porous media: application to geological storage of CO_2, *Computational Geosciences*, 25, 2131–2147 (2021).

[2] Koch, T., Gläser, D., Weishaupt, K. et al., DuMu^{X}3 - an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling, *Computers & Mathematics with Applications*, 81, 423-443 (2021).

Pillardou Nicolas
UPPA, E2S UPPA, CNRS, LMAP & LFCR, Pau
nicolas.pillardou@univ-pau.fr

Ahusborde Etienne
UPPA, E2S UPPA, CNRS, LMAP, Pau
etienne.ahusborde@univ-pau.fr

Croccolo Fabrizio
UPPA, E2S UPPA, CNRS, Total, LFCR, Anglet
fabrizio.croccolo@univ-pau.fr

Experimental benchmarks for the development of conceptual approaches in reactive transport modelling

J. Poonoosamy, M. Loenartz, Y. Yang, G. Deissmann and D. Bosbach

Keywords: Coupled processes, upscaling, porous media, multiphase flow..

The construction of underground repositories for nuclear wastes and the emplacement of waste packages will create perturbations in the subsurface induced by chemical, thermal and pressure gradients at the interfaces of different components of the multi barrier system, leading to mineral dissolution and precipitation to achieve re-equilibration. Reactive transport modeling (RTM) can be applied to investigate these perturbations and processes across temporal and spatial scales, from the micro-scale at interfaces via the repository near field to the entire repository system – information not accessible through experiments alone. Although RTM is capable of addressing highly complex hydrogeochemical phenomena, the application of RTM codes to real systems is impeded by the often simplified description of coupled processes. To enhance the predictive capabilities of reactive transport models and to gain fundamental insights into the coupling between solute and radionuclide transport properties (e.g.,permeability and diffusivity) of porous media and dissolution/precipitation processes, we conducted experiments on "simplified" chemical systems combined with pore-scale and continuum-scale reactive transport modelling to study processes in isolation; the final aim is to improve conceptual approaches for process couplings implemented in reactive transport codes. In this context, we investigated the effects of coupled mineral dissolution and precipitation in porous media on changes in permeability using flow-through experiments conducted in a magnetic resonance imaging scanner, which enabled the in situ investigation of porosity evolution in combination with monitoring changes in permeability and mineralogy. Our observations showed that classical implementations in reactive transport codes such as the Kozeny–Carman equation (Carman, 1937) failed to reproduce the changes in permeability and that more sophisticated approaches are required [1, 2]. Moreover, we developed a novel "lab-on-a-chip" setup, i.e., micronized counter diffusion reactors with in operando 3D Raman tomography [3, 4], which enables evaluating the alteration in pore architecture and studying of the effects of coupled mineral dissolution and precipitation on the diffusive transport of solutes and radionuclides in porous media. Our diffusion experiments show that despite a negative molar volume change involved in a mineral replacement reaction, the accessible porosity and diffusion properties of the matrix decreases. This questions current implementations in reactive transport models to account for porosity and diffusivity changes as a result of coupled mineral dissolution precipitation processes. Currently, we focus on the development of 2D reactive transport experiments involving coupled mineral-dissolution and precipitation with gas generation to test the conceptual approach for describing multiphase flow. Our approach enables the development of process-based theoretical models which allow for improvements in RTM codes and for predicting the evolution of perturbed interfaces in waste repositories, thus building confidence in the predictive capabilities of reactive transport models and reducing uncertainties with respect to future repository evolution.

References

[1] Poonoosamy, J., Klinkenberg, M., Deissmann, G., Brandt, F., Bosbach, D., Mäder, U., Kosakowski, G *Effects of solution supersaturation on barite precipitation in porous media and consequences on permeability: Experiments and modelling*, Geochimica et Cosmochimica Acta, 270, 2020.

[2] Poonoosamy, J., Haber-Pohlmeier, S., Deng, H., Deissmann, G., Klinkenberg, M., Gizatullin, B., Stapf, S., Brandt, F., Bosbach, D., Pohlmeier, A. *Combination of MRI and SEM to assess changes in the chemical properties and permeability of porous media due to barite precipitation*, Minerals,10(3), 2020.

[3] Poonoosamy, J., Westerwalbesloh, C., Deissmann, G., Mahrous, M., Curti, E., Churakov, S.V., Klinkenberg, M., Kohlheyer, D., von Lieres, E., Bosbach, D., Prasianakis, N.I. *A microfluidic experiment and pore scale modelling diagnostics for assessing mineral precipitation and dissolution in confined spaces*, Chemical Geology,528, 2019.

[4] Poonoosamy, J., Soulaine, C., Burmeister, A., Deissmann, G., Bosbach, D., Roman, S. *Microfluidic flow-through reactor and 3D Raman imaging for: In situ assessment of mineral reactivity in porous and fractured porous media*, Lab on a Chip,20 (14), 2020.

J. Poonoosamy
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
j.poonoosamy@juelich.de

M. Loenartz
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
m.loenartz@juelich.de

Y. Yang
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
y.yang@juelich.de

G. Deissmann
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
g.deissmann@juelich.de

D. Bosbach
Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany
d.bosbach@juelich.de

MULTIPHASE REACTIVE TRANSPORT BENCHMARK RESULTS OF HYTEC

I. Sin

Keywords: Reactive transport, multiphase flow, coupled processes, gas storage.

Multiphase reactive transport addresses variable natural and engineered systems covering complex geochemical processes in evolving porous medium. Various methods of coupling have been proposed over the last several decades. The reactive transport HYTEC [1] provides a general multi-purpose flexible framework for solving complex hydrogeochemical problems both with cell-centered and vertex-centered finite volume schemes. A multiphase flow coupling integrated in HYTEC is based on an operator-splitting approach applying appropriate equations of state facilitated precise descriptions of the compressible multicomponent phases, their thermodynamic properties and relevant fluxes [2]. The coupling was verified and validated [3]. The proposed benchmark on multiphase reactive transport consists of gas injection in saturated porous medium inducing mineral precipitation and dissolution. This work presents numerical results of HYTEC.

References

[1] van der Lee, J., de Windt, L., Lagneau, V., and Goblet, P. *Module-oriented modeling of reactive transport with HYTEC.* Computers & Geosciences 29, 3 (2003), 265–275.

[2] Sin, I., Lagneau, V., and Corvisier, J. *Integrating a compressible multicomponent two-phase flow into an existing reactive transport simulator.* Advances in Water Resources 100 (2017), 62–77.

[3] Sin, I., and Corvisier, J. *Chapter 6 Multiphase multicomponent reactive transport and flow modeling.* Mineralogical society of America ed. Reviews in Mineralogy and Geochemistry 85, 1 (2019), 143–195.

I. Sin
Mines ParisTech, PSL Research University, Centre de Géosciences
irina.sin@mines-paristech.fr

MULTIBODY APPROACH FOR REACTIVE TRANSPORT AND POROMECHANICAL MODELING IN DISCONTINUOUS POROUS MEDIA

A. Socié, F. Dubois, M. Neji, Y. Monerie and F. Perales

Keywords: Reactive Transport Modeling, Zero-thickness interface, Poromechanics.

In the context of long-term degradation of porous media, the coupling between fracture mechanics and reactive transport is investigated. To capture the effect of the discontinuities into the reactive transport kinetics and the expansion induced by solid precipitation, a reactive transport model has been developed into the IRSN numerical platform XPER [1, 2]. The fracture is studied through micromechanical modeling based on a multibody concept and Frictional Cohesive Zone Model (FCZM). Each mesh of a finite element modeling is considered as an independent body and the overall behavior is obtained by the coupling of a volume behavior and a surface behavior respectively inside and between the finite elements. The volume behavior takes into account the poromechanics and the geochemical behavior of a porous medium without any damage. The surface behavior describes the fracture mechanics and the species transport across and along the discontinuities. The first application is dedicated to chemical attack in a pre-cracked concrete where the crack path has been computed by the mechanical solver [2]. The second application focuses on the expansion of concrete induced by strong solid precipitation [3].

References

[1] F. Perales, F. Dubois, Y. Monerie, B. Piar, and L. Stainier, *A NonSmooth Contact Dynamics-based multi-domain solver. Code coupling (Xper) and application to fracture.*, European Journal of Computational Mechanics, 19, pp 389– 417, 2010

[2] A. Socié, F. Dubois, Y. Monerie, and F. Perales, *Multibody approach for reactive transport modeling in discontinuous-heterogeneous porous media.*, Computational Geosciences, 5, pp 1473 – 1491, 2021

[3] A. Socié, *Modélisation chimiomécanique de la fissuration de matériaux cimentaires : vieillissement et tenue des enceintes de confinement des centrales nucléaires*, Université de Montpellier, 2019

A. Socié
EOAS, University of British Columbia, Vancouver, Canada.
asocie@eoas.ubc.ca

Y. Monerie and F. Dubois
LMGC, CNRS, Univ Montpellier and MIST Laboratory, IRSN-CNRS-UM.
yann.monerie@umontpellier.fr, frederic.dubois@umontpellier.fr

F. Perales
Institut de Radioprotection et de Sûreté Nucléaire and MIST Laboratory, IRSN-CNRS-UM.
frederic.perales@irsn.fr

M. Neji
Institut de Radioprotection et de Sûreté Nucléaire
mejdi.neji@irsn.fr

BENCHMARK SIMULATIONS OF CO_2 INJECTION INTO A REACTIVE POROUS MEDIUM WITH THE COMPOSITIONAL FLOW AND REACTIVE TRANSPORT SIMULATOR MIN3P

A. Socié and K.U. Mayer

Keywords: Reactive Transport Modeling, Multiphase multicomponent flow, Fully implicit, Global implicit approach.

This talk presents the results for a benchmark on two-phase flow with reactive transport in porous media applied to CO_2 storage. The injection of carbon dioxide both induces the desaturation of the porous medium and the precipitation of calcite, requiring the simulation of the complex coupling behavior between multiphase flow and geochemical reactions. The problem is tackled through a compositional approach integrated into the existing flow and reactive transport simulator MIN3P [1]. In this approach, water is considered as a chemical component and its mass conservation equation is included in the reactive transport framework. The method is built on the traditional reactive transport equations (concentration-dependent), but utilizes molar fractions, liquid phase pressure, and phase saturation as primary unknowns. The overall system is solved by a fully implicit scheme using a Newton semi-smooth method to handle the local gas phase appearance/disappearance without a discontinuous switch of primary variables. The model has been validated for several coupled solute-solvent systems against the sequential groundwater flow-reactive transport solver previously developed [2]. Current results highlight the ability of the new development to model gas appearance and the influence of an advancing gas saturation front on calcite precipitation. It is anticipated that the model will allow considering complex geochemical systems and is particularly suitable for problems involving strong coupling between multiphase flow and multicomponent reactive transport processes.

References

[1] K.U. Mayer, E. O. Frind, and D. W. Blowes,*Multicomponent reactive transport modeling in variably saturated porous media using a generalized formulation for kinetically controlled reactions*, Water Resources Research, 38 (9), pp 1 – 21, 2002

[2] T.H. Henderson, K.U. Mayer, B.L. Parker, and T.A. Al, *Three-dimensional density-dependent flow and multicomponent reactive transport modeling of chlorinated solvent oxidation by potassium permanganate*, Journal of Contaminant Hydrology, 106, pp 195 – 211, 2009

A. Socié
EOAS, University of British Columbia, Vancouver, BC, Canada.
asocie@eoas.ubc.ca
K. U. Mayer
EOAS, University of British Columbia,
Vancouver, BC, Canada.
umayer@eos.ubc.ca

Robust numerical model for reactive-thermohaline convection of CO_2 in brine saturated reservoirs

S.Tabrizinejadas, M.Fahs, H.Hoteit, A.Younes, B.Ataie-Ashtiani, CT. Simmons and J.Carrayrou

Keywords: CO_2 sequestration, Reactive Thermohaline Convection, Arrhenius equation..

Geological CO_2 sequestration (GCS) remains the main promising solution to mitigate global warming. GCS occurs as a Reactive THermohaline Convection (RTHC) process involving fluid flow, and mass and heat transfer coupled to geochemical dissolution/precipitation reactions. RTHC involves multi-physical processes taking place at different time and space scales. The numerical models dealing with RTHC play an essential role in the simulations of GCS, for several purposes, such as the evaluation of reservoir storage capacity, the analysis of leakage risks, and for predicting the effect of CO_2 on in-situ fluids in the reservoirs. Despite extensive efforts to develop numerical models, current models face deficiencies in accurately and efficiently simulating this multli-physical problem at relevant scales. Thus, the development of advanced numerical schemes for improving the applicability, efficiency, and accuracy of models is of great interest. We develop an advanced RTHC numerical model based on the combination of the most updated numerical techniques for time and space discretization. The mixed hybrid finite element method (MHFE) is used for groundwater flow, the discontinuous Galerkin finite element (DGFE) method for the advective and convective term of mass and heat transfer, and MultiPoint Flux Approximation (MPFA) for dispersive and conductive term of mass and heat transfer. The reaction processes are considered with the sequential non-iterative approach. An adaptive time-stepping approach based on error control is implemented to manage the intrinsic errors related to operator splitting. The novelty of this work is the application of the combination of these advanced schemes to RTHC. The advantages of the newly developed model are highlighted by comparison against a standard Finite Element model (COMSOL), based on common benchmarks. Existing studies on RTHC of CO_2 do not consider the dependency of the dissolution reaction rates on temperature. We address this gap by taking advantage of the newly developed model. The model is applied to the Viking field in the North Sea, and the effect of reaction rate-temperature dependency on reservoirs storage capacity and total flux of CO_2 is investigated. Results show that neglecting the temperature effects on reaction rates leads to an overestimation of the reservoir storage capacity.

S. Tabrizinejadas
University of Strasbourg
tabrizinejadas@unistra.fr

M. Fahs
University of Strasbourg
fahs@unistra.fr

A. Younes
University of Strasbourg
Younes@unistra.fr

H. Hoteit
King Abdullah University
hussein.hoteit@kaust.edu.sa

B. Ataie-Ashtiani
Flinders University
behzad.ataieashtiani@flinders.edu.au

CT. Simmons
Flinders University
craig.simmons@flinders.edu.au

J. Carrayrou
University of Strasbourg
jerome.carrayrou@unistra.fr

APPLICATION OF THE PROJECTED LINE SEARCH STEP IN SOLVING THE PROBLEM OF LEACHING AND ACCELERATED CARBONATION OF THE CONCRETE

M. Tóth and P. Bastian

Keywords: Reactive multiphase flow, porous media, finite volume method, projected Newton method..

We present a simplified model of accelerated carbonation of concrete. It encompasses two-phase flow in the porous medium, transport of calcium and carbon dioxide, and two reactions affecting the porosity: leaching and carbonation. The mineral composition of the concrete changes as it degrades, but this model does not track the mineral concentrations directly -they are assumed to be in chemical equilibrium with the pore solution. As a result, the leaching reaction releases different amounts of water and calcium at different levels of calcium concentration. The biggest challenge is the progression of the sharp carbonation front. The position of the front relative to the mesh strongly affects the convergence, though this issue is addressed through the addition of the projection step into the line search method of the nonlinear solver.

Additionally, we implement the SiTraM benchmark problem. Both models use a fully implicit finite volume scheme implemented in the PDELab module of the DUNE project.

References

[1] B. Bary, and A. Sellier, *Coupled moisture-carbon dioxide-calcium transfer model for carbonation of concrete*, Cement and Concrete Research, 34, 2014.

[2] DUNE project web-page: https://dune-project.org

M. Tóth
Heidelberg University
michal.toth@iwr.uni-heidelberg.de

P. Bastian
Heidelberg University
peter.bastian@iwr.uni-heidelberg.de

HYDRAULIC AND POROMECHANICAL EFFECTS OF INDUCED CALCITE PRECIPITATION

Y. Wang and H. Class

Keywords: Poroelasticity, Geomechanics, Precipitation.

This talk presents the preliminary results of a study investigating the hydraulic and poromechanical effects of Enzymatically or Microbially Induced Calcite Precipitation(E/MICP). At the moment, we focus on subsurface gas-injection scenarios on an E/MICP treated site, where two-phase (water and CO_2) transient flow occurs in a heterogeneous deformable porous medium under isothermal conditions. A linear poroelasticity model [1, 2] is implemented to account for the matrix deformation as well as the porosity changes. Additional constitutive relationships determined by digitial rock physics [3] are tested and applied to estimate the soil's improved mechanical properties due to porosity reduction. The numerical model for simulating the geomechanical hydraulic processes is developed in the Open-Source numerical simulator DuMu$^{\text{X}}$ [4].

References

[1] Beck, Martin. *Conceptual Approaches for the Analysis of Coupled Hydraulic and Geomechanical Processes.* Universität Stuttgart, 17 June 2019, doi:10.18419/OPUS-10418.

[2] Cheng, Alexander H. D. *"Poroelasticity." Theory and Applications of Transport in Porous Media*, Springer International Publishing, 2016. Crossref, doi:10.1007/978-3-319-25202-5.

[3] Wetzel, Maria. *Pore space alterations and their impact on hydraulic and mechanical rock properties quantified by numerical simulations*. Diss. Universität Potsdam, 2021.

[4] Koch, Timo, et al. *DuMux 3–an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling.* Computers & Mathematics with Applications 81 (2021): 423-443.

Y. Wang
Institute for Modelling Hydraulic and
Environmental Systems, University of Stuttgart
yue.wang@iws.uni-stuttgart.de

H. Class
Institute for Modelling Hydraulic and
Environmental Systems, University of Stuttgart
holger.class@iws.uni-stuttgart.de

A HYBRID PORE-SCALE AND CONTINUUM-SCALE MODEL FOR SOLUTE TRANSPORT AND LOCAL PRECIPITATION IN POROUS MEDIA

Y. Yang, R. Lu, J. Poonoosamy, G. Deissmann, H. Shao and D. Bosbach

Keywords: Hybrid model, precipitation, reactive transport, lattice Boltzmann method, OpenGeoSys.

Precipitation of minerals and solute transport are involved in many geological and technical processes. Mineral precipitation changes the solid structures of porous media and thus affects the transport pathways of solutes. When the rate of precipitation is much faster than the rate of transport, the chemical heterogeneity becomes significant and the continuous medium assumption fails. In this work, a hybrid pore-scale and continuum-scale model has been recently developed to consider the reactive solute transport with local precipitation in porous media. In the region with high chemical heterogeneity, a pore-scale reactive transport model based on the lattice Boltzmann method (LBM) is employed in order to accurately capture the dynamics of liquid-solid interfacial reactions; in the other regions, it is adequate to apply continuum-scale standard simulations by using OpenGeoSys (OGS-6). Examples of solute diffusion in a straight channel with local precipitation are designed to indicate the differences between a continuum-scale model and the hybrid model. These comparisons are helpful to understand and improve the applicability of macroscopic reactive transport simulations with local precipitation/dissolution.

References

[1] M. Tartakovsky, G. Redden, P. Lichtner, T. Scheibe and P. Meakin, *Mixing-induced precipitation: Experimental study and multiscale numerical analysis*, Water Resources Research, 44, pp. W06S04, 2008.

[2] OpenGeoSys web-page https://www.opengeosys.org/.

Y. Yang
Forschungszentrum Jülich GmbH
y.yang@fz-juelich.de

R. Lu
Helmholtz-Zentrum Umweltforschung GmbH
renchao.lu@ufz.de

J. Poonoosamy
Forschungszentrum Jülich GmbH
j.poonoosamy@fz-juelich.de

G. Deissmann
Forschungszentrum Jülich GmbH
g.deissmann@fz-juelich.de

H. Shao
Helmholtz-Zentrum Umweltforschung GmbH
haibing.shao@ufz.de

D. Bosbach
Forschungszentrum Jülich GmbH
d.bosbach@fz-juelich.de