Project acronym and title:

SECURe – Subsurface Evaluation of Carbon capture and storage and Unconventional risks

REPORT ON MODELLING AND SIMULATION

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Public introduction

Subsurface Evaluation of CCS and Unconventional Risks (SECURe) is gathering unbiased, impartial scientific evidence for risk mitigation and monitoring for environmental protection to underpin subsurface geo-energy development. The main outputs of SECURe comprise recommendations for best practice for unconventional hydrocarbon production and geological CO2 storage. The project is funded from June 2018–May 2021.

The project is developing monitoring and mitigation strategies for the full geo-energy project lifecycle; by assessing plausible hazards and monitoring associated environmental risks. This is achieved through a program of experimental research and advanced technology development that includes demonstration at commercial and research facilities to formulate best practice. We will meet stakeholder needs; from the design of monitoring and mitigation strategies relevant to operators and regulators, to developing communication strategies to provide a greater level of understanding of the potential impacts.

The SECURe partnership comprises major research and commercial organisations from countries that host shale gas and CCS industries at different stages of operation (from permitted to closed). We are forming a durable international partnership with non-European groups, providing international access to study sites, creating links between projects and increasing our collective capability through exchange of scientific staff.

Executive report summary

This document reports the work done at the University of Nottingham, in relation to Work Package 4, focused on the development of Modelling and Simulation tools, suitable for integration of monitoring data. Available monitoring data for CCS and Shale Gas, and more generally geoenergy applications, are often sparse and heterogeneous in space, type, and time. A systematic assimilation of data into the computational models, to update uncertain parameters and improve its predictive capabilities is often unfeasible due mainly to two reasons: i) the limited availability of open-data and open-simulators and ii) the computational costs of standard reservoir simulation. We address these shortcomings by developing a new open-source set of reservoir multi-physics simulation tools, based on OpenFOAM®, a widely used library for computational fluid dynamics in academic and industrial settings. Building up on OpenFOAM® robustness and flexibility we developed key models and solvers for geoenergy applications including flow and transport solvers, multi-continuum formulations for heterogeneous media, geomechanics, multiphase capabilities, geostatistics tools. To address the computational cost of reservoir simulation, we focus on upscaling methodologies based on the multi-continuum and multi-rate mass-transfer formulations that allow to include heterogeneities in an implicit way while keeping a relatively coarse grid resolution.

Contents

FIGURES

TABLES

1 Introduction

In this document we report the theoretical and computational work carried out at the University of Nottingham to develop an open-source parallel geological simulation suite. This software suite named SECUReFoam - since it is largely based on the open source finite volume library OpenFOAM (The OpenFOAM Fundation, 2020)- is subdivided into interconnected modules that represent different solvers or utilities. Each solver solves the governing equations corresponding to a specific model, while utilities can perform data generation and analysis.

The flow of data through each solver can be grouped into three categories:

- **Input data**: which can be geological model, physical parameters, operating conditions. This is data needed and used in the simulation setup and can be provided externally (for example converting external datasets) or even generated inside SECUReFoam.
- **Output data**: quantities of interest such as leakage prediction. This is data measured by monitoring techniques and/or computed with numerical models.
- **Model discrepancy**: difference between model predictions and monitoring data. This is composed of modelling and experimental error.

This software suite can be integrated with measurements from monitoring devices to detect, for example, the existence of fractures, predict where new fractures can form, and develop proper mitigation techniques. Due to the complexity of the physics involved and the enormous uncertainty in the subsurface properties, we focus on a probabilistic description of the problem. For example, given a large-scale geological characterisation of a site, by studying different scenarios it is possible to identify the set of geological and flow properties that results in the leakage measured by monitoring devices. Once this is completed, it is possible to explore different scenarios (for example, different injection pressures) that may lead to leakage mitigation. These operations would be extremely expensive without an efficient multiscale model that is also able to properly interpret monitoring data.

A proper prediction of dynamical fracture formation requires a local-global modelling technique, which will be the focus of the deliverable 4.5. Here, fracture-prediction is based on a matching between measured and predicted leakage. Simulations are here run on hypothetical scenarios. Examples on how incorporate measured data into this framework using Bayesian inversion or machine learning techniques will be instead the focus of deliverable 3.9 in the SECURe project.

1.1 MODEL REDUCTION FOR MONITORING AND MITIGATION

Monitoring data are often sparse and heterogeneous, which means that it is generally difficult to understand the subsurface dynamics by simply looking at surface measurements. Furthermore, even when a leakage is detected, there is no model able to uniquely describe leakage dynamics and fracture location in the aftermath.

Even when the whole leakage process can be modelled in detail through numerical simulations, a single direct approach is likely to fail, leading to results that are incompatible with observations. Instead, many simulations are run with different geological configurations until the spectrum of geological properties leading to compatible results is narrowed down to a sufficiently small window. As this operation would be prohibitively expensive in terms of computational resources, one must rely on “reduced models” which are able to run faster while maintaining the fundamental physical principles.

A reduced model must satisfy the following interconnected properties:

- ➢ It must be able to run on a much coarser grid than the base model. This means that it should have predictive power at scales larger than the Darcy scale, where the complex conjugate transfer between different rocks and between fracture and matrix becomes more relevant than capillary forces and local thermodynamic processes. It should also be able to honour bulk changes in rock properties at appropriate scales in terms of the main processes being modelled (e.g., flow, composition, storage capacities).

- As a result, the method should lead to an efficient numerical solution, which means that the algorithm should be stable for large time steps. Furthermore, the loss of accuracy due to large time steps should not result in completely erroneous predictions. Therefore, it should be possible to solve the resulting system of equations with implicit discretisation schemes and strong coupling.
- As some physical phenomena become less relevant at larger scales, it is crucial that the reduced model also operates on a reduced physics to allow a formal upscaling procedure to be carried out. Subsequently, model coefficients can be calibrated to account for the missing physics if required, but the core equations to solve should remain relatively simple to keep the computational cost to a minimum.

In order to develop integrated modelling to support monitoring data, it is required to possess interoperable open data that can be connected to different platform and processed. However, a crucial piece of information is represented by the exact position of fractures or “feeders”, i.e., paths where the contaminant can stream faster (for example fractures). Such level of detail is generally not available in open data and, consequently, one must rely on statistical tools able to generate many different configurations to test. Therefore, in the following we will make use of randomly generated statistical fields with physical properties qualitatively similar to the Sleipner (The Open Porous Media, 2020) reservoir model.

Understanding transport phenomena in the reservoir allows to develop further reduced order techniques, based for example on transfer functions, to quickly analyse a wide range of scenarios (Dassargues, 2020).

1.2 OPEN DATA AND INTEROPERABILITY

While in recent years we have witnessed a growing positive attitude of the community towards making geological data publicly available, there are still several issues regarding their actual usability, especially when crossing disciplinary barriers.

This is mostly due to the highly non-standard (or proprietary) data format used in reservoir simulations, which targets specific software like Eclipse (Schlumberger, 2020), while other opensource libraries like MRST (Industries, 2020) and OpenGeoSys (OpenGeoSys, 2020) adapt their internal algorithms to read such formats.

Communication between software employing a similar data format or interoperability is a key characteristic of many established software solutions for computational fluid dynamics like ANSYS (ANSYS, 2020), COMSOL (COMSOL Multiphysics Modelling Package, 2020), and OpenFOAM. Such condition has the advantage to provide flexibility to the user as well as the freedom to implement new models without being bounded to a particular architecture. Scientific software for the numerical simulation of porous media are therefore often composed of many dedicated modules (like for example MRST) or are limited to simulations being performed on relatively simple geometries (like Dumux (Dune for multi flow and transport in porous media, 2020)). Reservoir simulations require a special attention due to the complexity of the grid, which is mostly unsuitable for standard computational fluid dynamics due to the large aspect rations and topological defects. Generally, very specialised discretisation algorithms are required to solve a set of transport equations on such grids.

OpenFOAM is an opensource finite volume library with many users in both academia and industry that can be applied to a wide array of problems. Furthermore, it is continuously updated and maintained on three main branches and can be interfaces with most of the existing datasets. Unfortunately, there is no reader for data formats used in geological simulations.

While there are utilities provided in the Open Porous Media package that can convert GRDECL data into vtk, the resulting vtk grid is not suitable for simulations, since it does not contain a suitable description of the connectivity between cells. Therefore, we developed our own conversion tool based on MRST, which exploits the GRDECL reader in MRST and writes the data directly in polyMesh format (the format natively employed in OpenFOAM). OpenFOAM provides tools for converting these data into proper vtk files or in ANSYS format.

However, data files from reservoir simulations do not obey a unique standard and are likely to be different for different versions of the proprietary (closed source) simulator. Therefore, one must manually account for these changes, and be aware that error messages can simply be due to a slightly different nomenclature. Such problems can only be addressed if the community migrates to standard formats like vtk or msh. This would be desirable since while it is true that in its basic idea corner point geometries are simple, they require adjustment to account for complex topology and faults, eventually making them inefficient compared to polyhedric orthogonal grids (for example grid made of regular polygons).

1.3 DATA SETS AND GEO-STATISTICS

Despite the recent effort and focus (including within EU projects) on open and accessible data, only few large-scale reservoir data sets are openly available. Among the it is worth mentioning the recent CO2Share initiative that has released a large data set of the Sleipner reservoir. While this is and will be of great value to the whole community, the geological model contains significant uncertainties particularly in the position of the “feeders” connecting two permeable layers (Peter Zweigel, 2004) that have been found to be crucial to match the CO2 plume captured by seismic and other monitoring data. This clearly shows how a detailed computationally very costly model can still be poorly predictive.

In this project we have developed data conversion tools to allow standard commercial Petrel/Eclipse data to be loaded into open-source simulators, such as OpenFOAM and our SECUReFoam suite. Below are two examples of geological and petrophysical data imported.

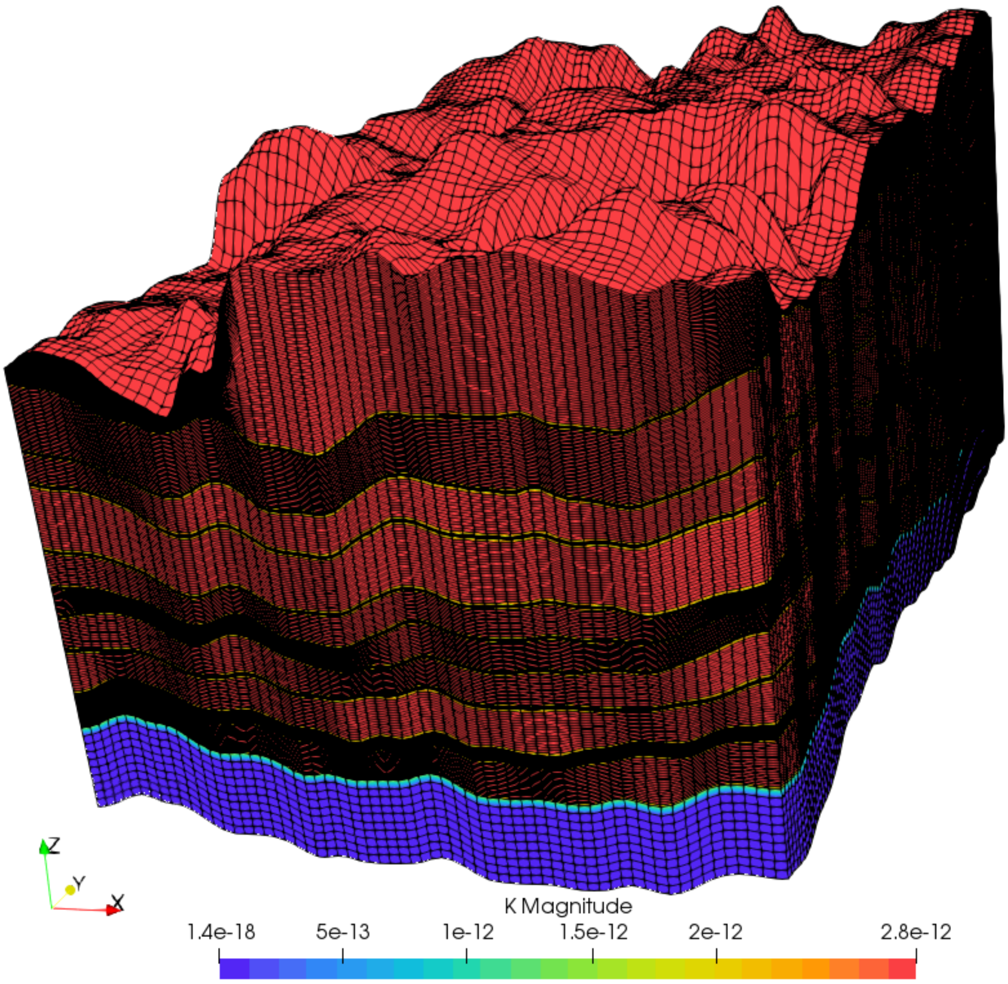


Figure 1: Sleipner reservoir as processed and imported in SECUReFoam

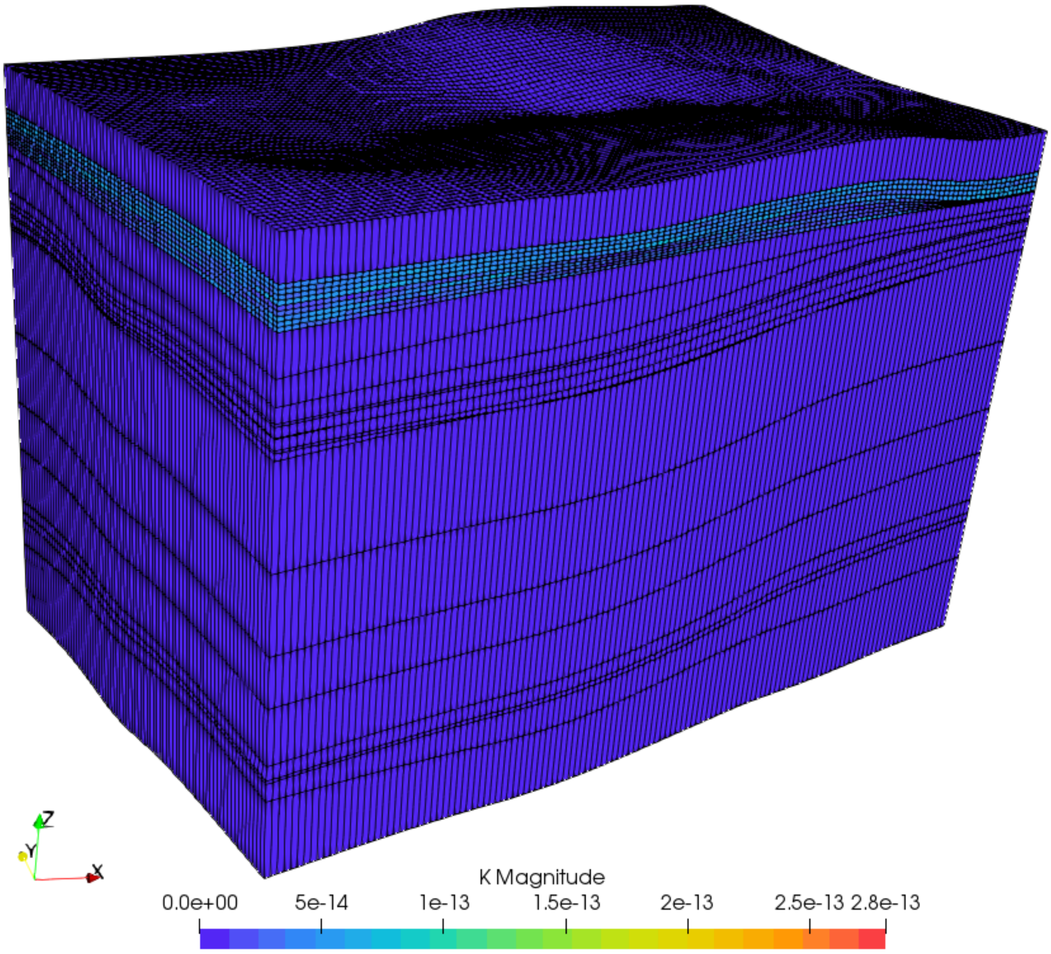


Figure 2: Borzecin reservoir as processed and imported in SECUReFoam

While data sets like Sleipner (and Borzecin) will be considered for the final activities and deliverables of the project, we will limit here to reproduce qualitative properties of the reservoir to synthetically generated heterogeneous reservoirs. These are generated using a Fourier spectral approach to obtain lognormal, truncated and bi-truncated random fields starting from geological information (continuous vs categorical data) and variograms. Examples of random heterogeneous media are presented below. While these are fully random unconditional realisations of random fields, the random generation can be conditioned on known data. Given an initial geological model with an associated degree of (un)certainty, the possibility of generating possible scenarios is crucial to match and assimilate additional monitoring data that are often not directly compatible with the original model.

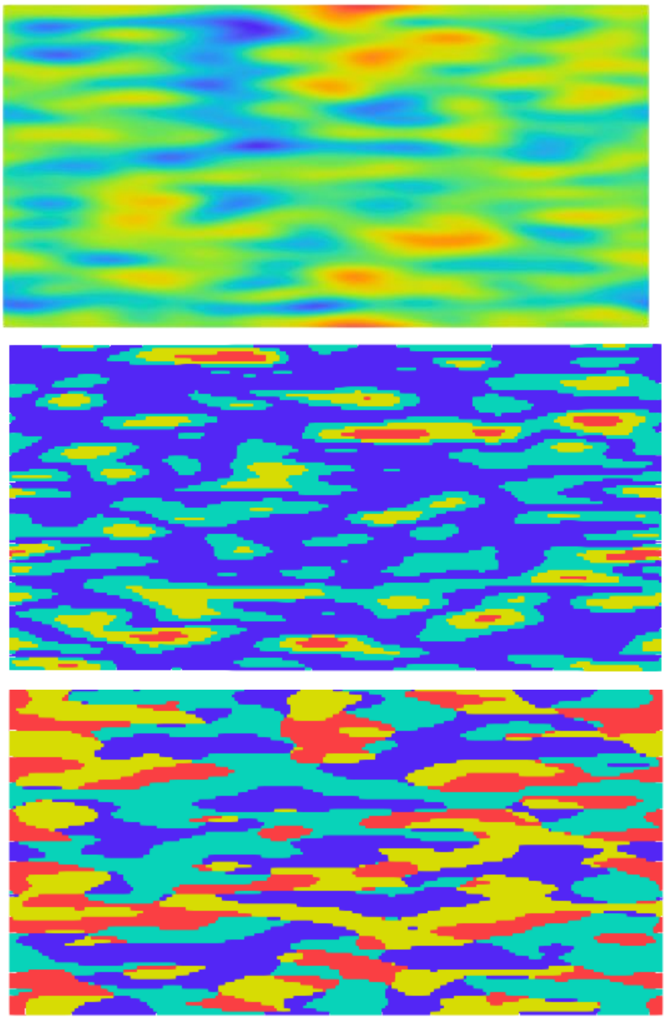


Figure 3: Example of random continuous, truncated, and pluri-truncated random permeability fields

2 SECUReFoam software suite

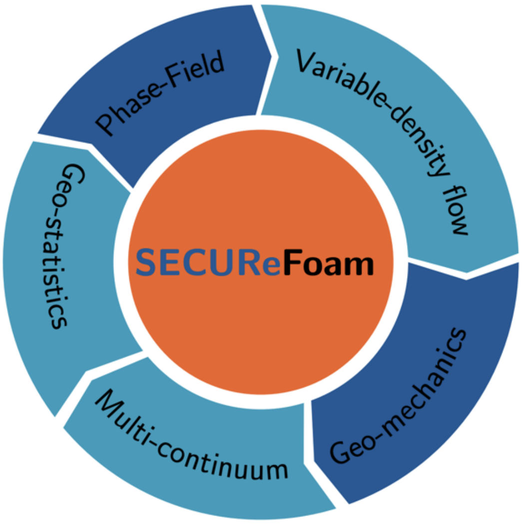


Figure 4: SECUReFoam logo

For the purpose of this document and the SECURe project, we have packaged all the developments into a single online software package which we called SECUReFoam. This includes

- ***mrmtFoam***: a collection of solvers that uses the multi-rate mass transfer model. The main functionalities of this solver are implemented in a dedicated dynamically linked library (shared object), so that they can be easily integrated in other solvers.
- ***upscalingTransportFoam***: a collection of tools to compute the effective dispersion, the effective velocity, and the upscaled reaction properties for heterogeneous systems (both pore- and lab-scale).
- ***poroelasticFoam***: a solver that couples Darcy flow model and with geomechanics.
- ***geoStatFoam***: an application to generate random geological media given some statistical properties.
- ***rhoDarcyFoam***: a Darcy solver with variable density for multiphase flows, with its dual-continuum version named *dualRhoDarcyFoam*
- ***CahnHilliardFoam***: a phase-field solver for partially miscible fluids.

2.1 HETEROGENEOUS MEDIA: THE GENERALISED MULTI-RATE TRANSFER MODEL

Transport in heterogeneous media can be represented by the multi-continuum hypothesis, where variables (pressure, concentration) are described on overlapping media (e.g. fracture network and porous matrix). This construction allows to neglect most small and intermediate scale heterogeneities that are instead implicitly considered by transfer (or "memory") functions between the different "continua". As a motivating example, a highly fractured reservoir will be dominated by the flow and transport within the fracture network. However, it is important (for example, for CO2 trapping) to describe also the surrounding porous matrix. This is achieved by the multi-continuum model, by solving separate equations for matrix and fractures. The key challenge in the development of predictive multi-continuum models is the form and parametrisation of these transfer functions.

Multi-continuum models for concentration fields are often called "multi-rate models" as the transport in the low porosity regions (dominated by diffusion) can be further decomposed into "diffusion modes" that are able to exactly reproduce the transport in arbitrarily complex geometrical structures. In our recent paper we proposed a novel approach to derive the multi-rate mass transfer model that is different from that of the memory function or that of Haggerty & Gorelick (Gorelick, 1995). Our model is derived starting from the underlying physical process and mathematical equations and it is parameter free, i.e., it is possible to directly evaluate all the closure parameters in a unique manner. While our method agrees with previous results obtained by Haggerty & Gorelick, it also contains their multi-rate model as a special case and allows extension to non-equilibrium situations, where the concentration in the mobile region is not uniform. Hence the term “generalised”, that indicates the model offers a broader description of non-asymptotic transfer in porous media.

Especially, when mathematical homogenisation techniques are employed to evaluate the effective transport in the mobile region, our method provides an exact framework for the upscaling of the conjugate transfer problem, the accuracy of which is given by the terms retained from the infinite series. Our model predicts that additional terms arise in the governing equations of the multi-rate mass transfer when accounting for the effect of transport processes in the mobile region on the inter-region exchange. These terms are brought into the framework by the corrector equation resulting from homogenisation, which at the second order have the form of a drift and a diffusive contribution.

Furthermore, under the assumptions of isotropy and homogeneity these terms can be absorbed into the effective diffusivity and effective velocity, thus leaving the form of the governing equations in the mobile region unchanged. However, the concentration in each immobile region will now depend on high order spatial derivatives of the concentration in the mobile region.

Despite the self-consistency of this model (all the parameters can be evaluated from first principles without calibration) and its completeness with respect to the initial hypothesis (we never introduced additional hypothesis or simplifications in the development of our formulation) there are still some significant phenomena that should be accounted for when modelling real systems. While a rigorous derivation is possible therefore only for purely diffusive inclusions (negligible flow and buoyancy), the multi-continuum concept has been also extended for mobile-mobile regions (where flow is not negligible in low-permeability regions) and for a coupled flow-concentration (multiphase) context (see section below).

2.1.1 Mathematical model

The complete set of equations of the generalised multi-rate mass transfer model (GMRT) reads:

$$\text{(GMRT)}\begin{cases}\beta_m \dfrac{\partial \bar{c}_m}{\partial t} + \displaystyle\sum_{i=1}^{N_i} \beta_i \sum_{k=1}^{\infty} \beta_{ik}\lambda_{ik}\left(c_{ik} - \bar{c}_m - \sum_{n=1}^{\infty} \Psi_{ikn}:\right) = -\nabla \cdot J_{m,eff} \\ \dfrac{\partial c_{ik}}{\partial t} = \lambda_{ik}\left(c_{ik} - c_{ik}^{eq}\right) \qquad i = 1,\ldots,N_i;\; k = 1,\ldots,\infty\end{cases}$$

Where the concentration field c is split into a mobile component c_m for which standard fluxes are considered (RHS) and multiple immobile “modes” c_{ik}. The mobile and immobile concentrations interact by linear interactions λ_{ik} that are dependent on the immobile region shapes, as well as their properties (e.g. diffusion/dispersion coefficients). When immobile/slow regions are large, like in the case of large geological formations, additional terms Ψ_{ikn} arise in the transport equation to describe the non-homogeneous transfer.

It is important to notice that the number of terms in the multi-rate expansions can be tuned to the desired accuracy. In practical applications, several modes below 10 result in a significant computational advantage compared to fully resolve all heterogeneities at high resolution.

2.1.2 Implementation

The multi-rate multi-continuum model has been implemented in different forms. The main structure of the user defined multi-continuum variables is however implemented in a general library, called *multiContinuumModel,* applicable to various solvers. As an example, the simplest application to deal with transport in heterogeneous media is *multiRateScalarTransportFoam* which, for a given velocity field, solves a scalar transport equation with the multi-rate mass transfer model. The solver is based on the standard *scalarTransportFoam* available in native OPENFOAM® and employs a special *multiContinuumControl* object (derived from the PIMPLE algorithm in OPENFOAM®) that wraps the *multiContinuumModel* library and checks for convergence. The algorithm representing the *multiRateScalarTransportFoam* is reported In Figure 5.

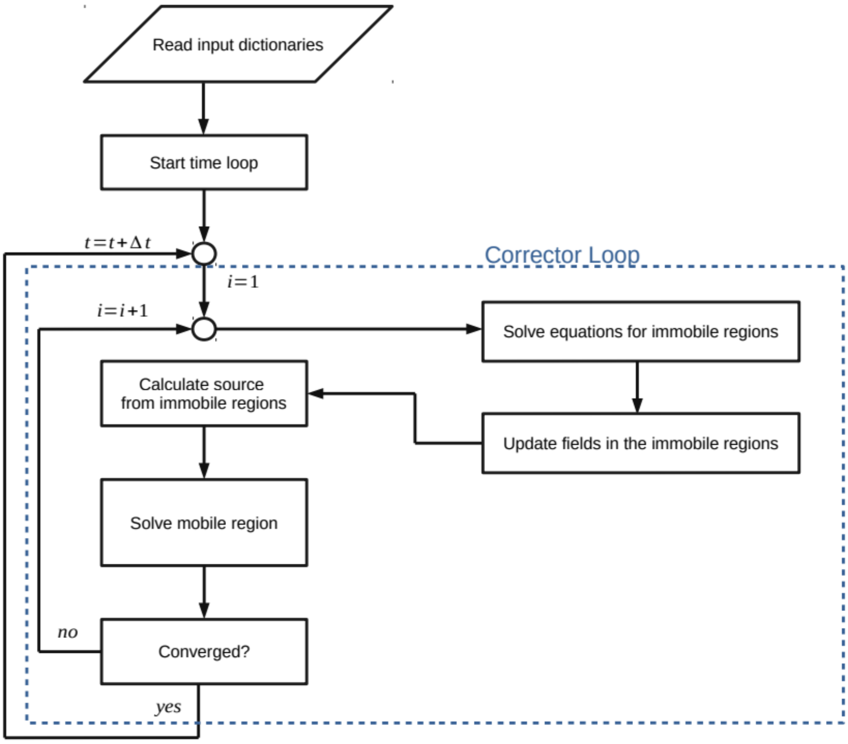


Figure 5: Diagram showing the numerical algorithm for multiRateScalarTransportFoam

While the additional multi-continuum variables add computational costs to the simulator, they are fully parametrised by large-scale parameters (such as porosity, shapes and flow/dispersion properties), therefore making the approach more suitable to be used in history matching and data assimilation.

2.1.3 Simulation results

We tested our model for the transport at different scales:

Field-scale example:

In this section, we apply *multiRateScalarTransportFoam* to solve for solute transport in media characterised by spatially variable properties. The modelling of transport of dissolved substances and energy in heterogeneous porous media is a key issue in a series of applications such as groundwater remediation. The computational domain considered here is a 2D domain of width 200 m and height 100 m. The numerical grid was built in OPENFOAM® using the blockmesh utility, which allows the generation of orthogonal hexahedral meshes. The total number of cells in our computational domain is 20000. The permeability field, representing the flow in the more permeable region, is generated (by means of our geostatistics tool) as a continuous lognormal field with anisotropic variogram (with longer correlation in the longitudinal direction). The immobile inclusions are assumed to be of spherical shape and of different sizes. For CO2 and contaminant applications these can represent areas where micro-porosity diffusion and trapping happens. In this testcase we are therefore neglecting multiphase properties and gravity forces. A “clean” water flow is imposed on the left side of the domain and the solute concentration on the right side is measured as a breakthrough concentration curve in time. The immobile regions are assumed to contain initially no solute, while the reservoir is assumed to be initially fully saturated with the solute. This is an idealised extreme scenario to be able to measure the effect of the heterogeneities in the well extraction data.

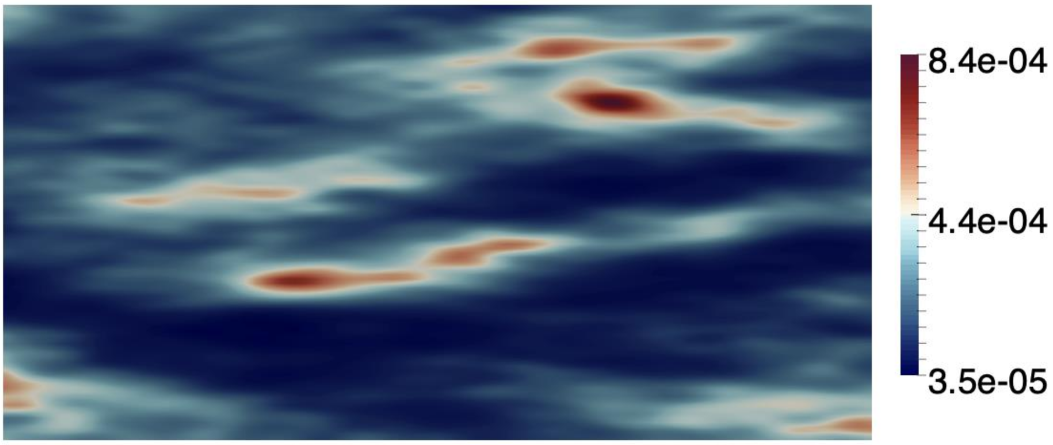


Figure 6: Contour plot of the randomly generated permeability field [Da]

As it can be seen in the figure below, the presence of heterogeneities is significant, causing the solute to be trapped in the immobile regions and then slowly released (blue curve). The tail of the breakthrough curve is fully determined by the multi-rate parameters. In a CO2 storage application, for example, the shape and behaviour of this slow release is crucial to establish the safety of geological storage.

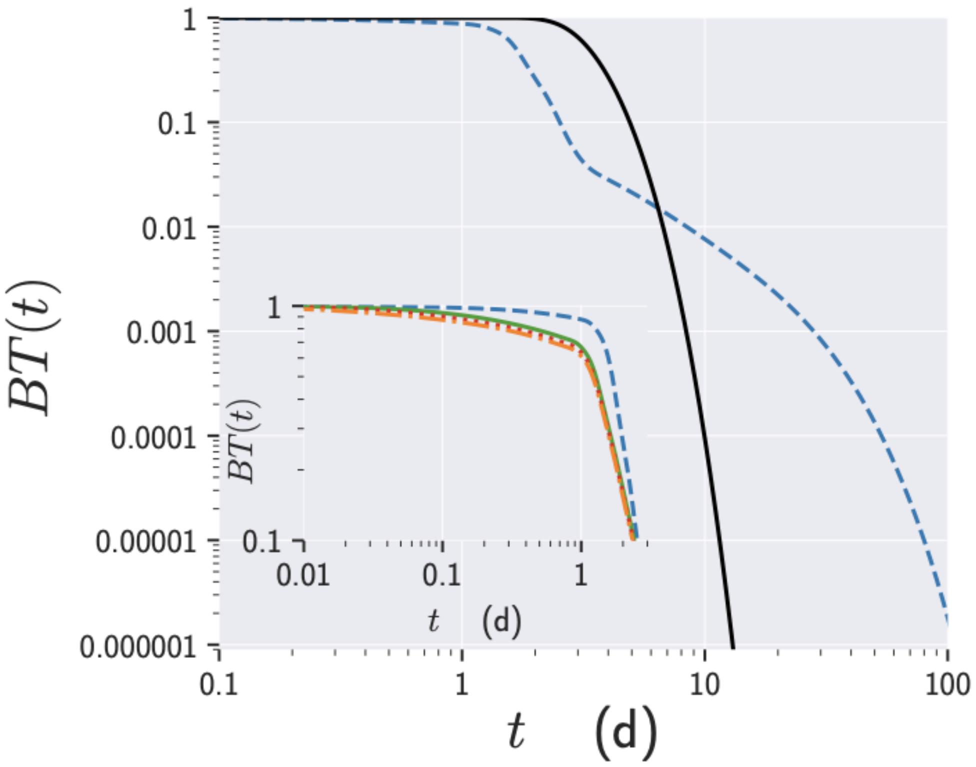


Figure 7: Breakthrough curves and comparison with the case without multi-rate (black continuous curve). In the inset, the results for the first 3 days, with different number of terms M in the multi-rate expansion, are reported: M=2 (dashed blue), M=50 (dashed orange) and intermediate (M=10, M=20) values

Lab-scale example

As a proof of concept for the feasibility of 3D applications, we include the application of *multiRateScalarTransportFoam* to a core-flow test case. Within the MRMT framework, the core, similarly to the field-scale example, is composed of a highly permeable heterogeneous rock. Larger heterogeneities are directly represented by a heterogeneous permeability field, while local micro-porosity region are modelled with the multi-rate multi-continuum hypothesis. A steady-state Darcy equation can be solved on the randomly generated permeability field with the solver named *simpleDarcyFoam*, while the transport in the immobile regions is solved with the MRMT library. Thanks to the C++ efficient solver, this 3D testcase can be solved in a few hours on a standard workstation.

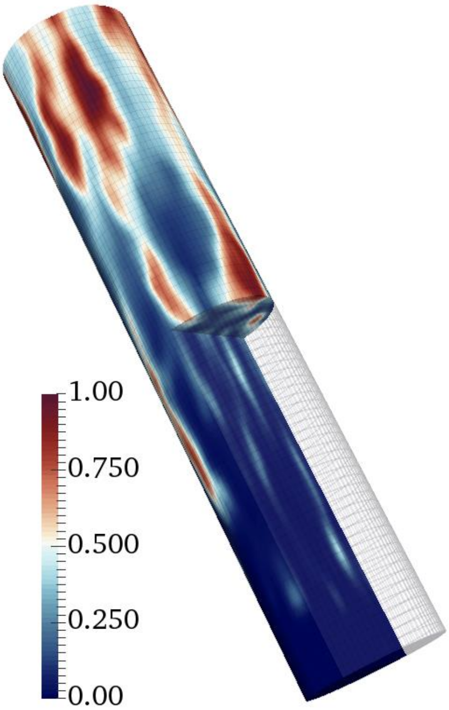


Figure 8: Contour plot of the concentration of the chemical species in (kg/m3) in the mobile zone for the column test.

The simulation initialisation and outputs are similar to the previous testcase and results are again showing the importance of the trapping in the immobile regions, although, in this case, due to the faster flow and the three-dimensional configuration, the effect of this trapping in the breakthrough curve is less pronounced.

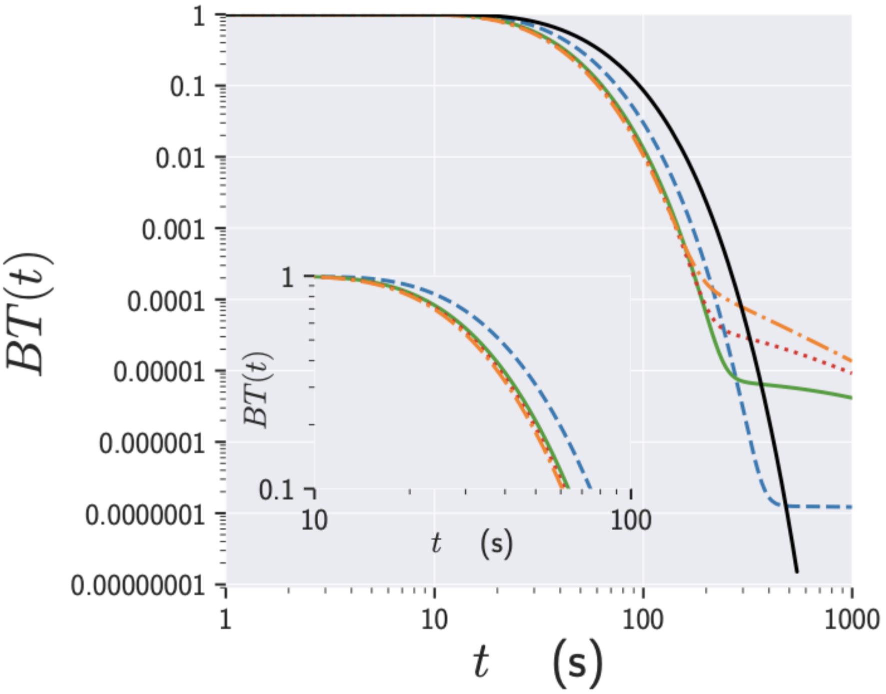


Figure 9: Breakthrough curves predicted by the multi-rate mass transfer (details in the paper)

2.1.4 Dual porosity models

Another similar approach consists on describing the matrix and fracture network using two different pressure fields p_m and p_f which give rise to a source term (mass flux) in the pressure equation:

$$S_p = \beta(p_m - p_f)$$

Where β is an exchange coefficient that depends on the material properties.

Clearly, this model requires the definition of two porosity fields and two permeability fields corresponding to the fracture domain and the matrix domain. A similar source term (volumetric flux) is also present in the governing equations for the concentration fields c_m and c_f:

$$S_c = \frac{S_p}{\rho} c^{>}$$

Where $c^{>}$ is c_f if $p_f > p_m$ or c_m in the other case. Thus, it is the concentration “upstream”, from the region with the largest pressure. Clearly, both S_p and S_c appear with opposite sign in fracture and matrix equations.

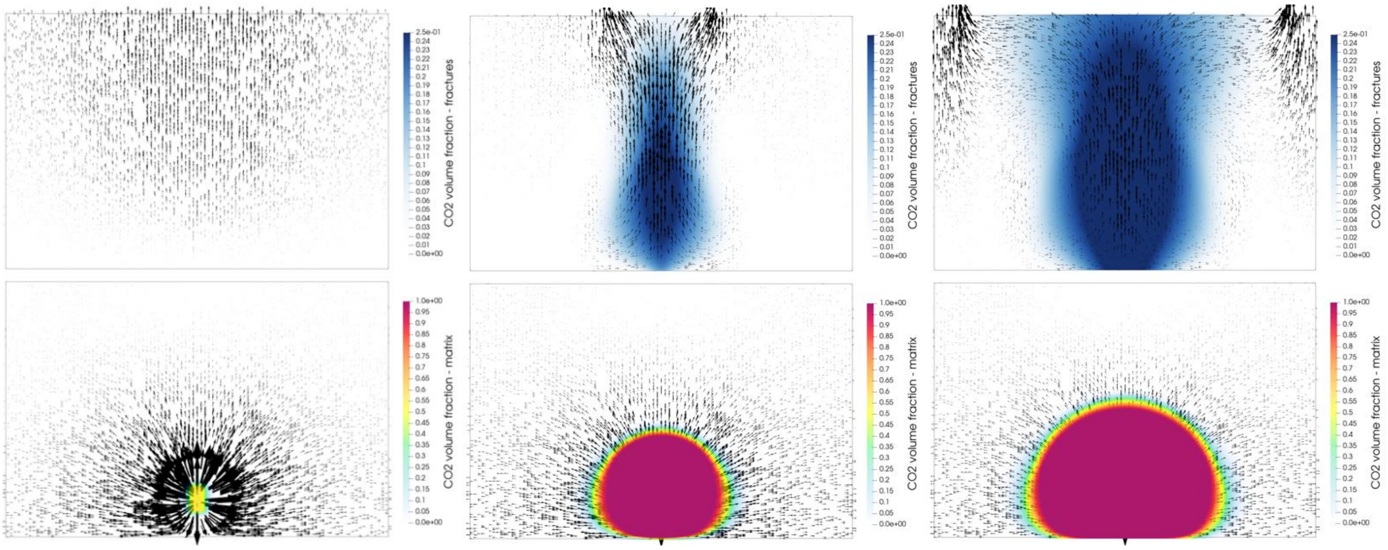


Figure 10 Dual porosity example simulation of CO_2 injection in a fractured isotropic medium. Top: fracture flow velocity field and concentration. Bottom: matrix velocity field and concentration.

In Figure 10 an example to verify the implementation is reported for a reservoir composed of uniform and isotropic medium where the fractures are represented by an overlapping continuum with 100 times higher permeability. The transfer term between matrix and fracture is here assumed linear, and homogeneous. The concentration of CO_2 in the matrix (bottom) and fractures (top) is reported for three different times. Injection occurs in the matrix only, where a radial velocity field is developed. Due to the higher permeability of the fractures, once the gas is transferred to the fractures it quickly reaches the top boundary. This testcase permits to assess the qualitative accuracy, efficiency and mass conservation properties of the implementation and does not constitute a realistic CO_2 injection scenario.

2.2 REACTIVE TRANSPORT: UPSCALING OF FAST REACTION

Heterogeneities and fractures affect even more significantly the reaction (e.g. dissolution or remediation) with the rock. Here the model reduction can be performed by appropriately choosing the upscaled macro- or field-scale model, without explicitly resolving at the reaction scale. However, in presence of fast kinetics (large reaction constants), the reaction has a complex interplay with the flow and dispersion properties, resulting, for example, in an observed slower and more dispersive transport. This can be easily misinterpreted as a modification of permeability and dispersivity properties, while it is instead since heterogeneous reactions (happening locally at the rock surface) significantly alter the concentration profiles. Therefore, the effective properties of the non-reactive problem can be used, and only a combined upscaling to estimate all parameters at once is need.

During the project, we performed an extensive analysis of reactive transport (see publication) and extended the current state-of-the-art techniques employed to derive macroscopic models. The results of theoretical and computational work will be connected to the activities and deliverable in WP5. Specifically, we studied the problem of advection-diffusion of a solute c:

$$\frac{\partial \mathrm{c}}{\partial \mathrm{t}} + \frac{\partial}{\partial x_j}\left(u_j c - D\frac{\partial \mathrm{c}}{\partial x_j}\right) = 0,$$

With boundary conditions at the pore interfaces:

$$D\frac{\partial c}{\partial n} = k(g-c).$$

All symbols are detailed in Table 1. Our approach leads to a macroscopic equation for the average macroscopic concentration $\bar{\mathrm{c}}$

$$\frac{\partial \bar{\mathrm{c}}}{\partial \mathrm{t}} + \frac{\partial}{\partial x_j}\left(u_j^e \bar{\mathrm{c}} - D_{jk}^e \frac{\partial \bar{\mathrm{c}}}{\partial x_k}\right) = \lambda\left(\bar{\psi} - \bar{\mathrm{c}}\right),$$

All the effective macroscopic parameters can be obtained by solving an appropriate cell problem (i.e. a local problem resolving all the scales of the system). This approach has been tested for pore-scale periodic arrangements of spheres with surface reaction, but it can be readily extended to macro- or field-scale heterogeneous problems.

Table 1: Symbols used in the reactive transport analysis

Name	Description	Units
t	Time	[s]
x	Space	[m]
c	Volume concentration of contaminant	[-]
D	Diffusion coefficient	[m^2/s]
D_{jk}^{e}	Effective dispersion tensor	[m^2/s]
u_j	Velocity field	[m/s]
u_j^e	Effective velocity field	[m/s]
k	Reaction speed	[m/s]
λ	Effective reaction rate	[s^{-1}]
g	Inhomogeneous source	[-]
$\overline{\psi}$	Effective inhomogeneous term	[-]

This method can also be applied to the problem of rock dissolution and coupled with phase-field and multiphase models for CO_2 and shale gas applications. For example, it is possible to model flow induced by fast chemical reactions (“blowing” or Stefan effect) through the inhomogeneous boundary condition.

Furthermore, we developed a numerical solver capable of solving the required cell problems using an implicit power iteration method to extract the effective reaction coefficients. Results have been applied to a wide range of porosity in porous geometries. We named this solver *specCellFoam*, since and its workflow is illustrated in Figure 11.

This solver, together with other tools related to upscaling (i.e. deriving appropriate macro- and field-scale parameters based on local physics), such as the computation of permeabilities, are part of the *upscalingTransportFoam library.*

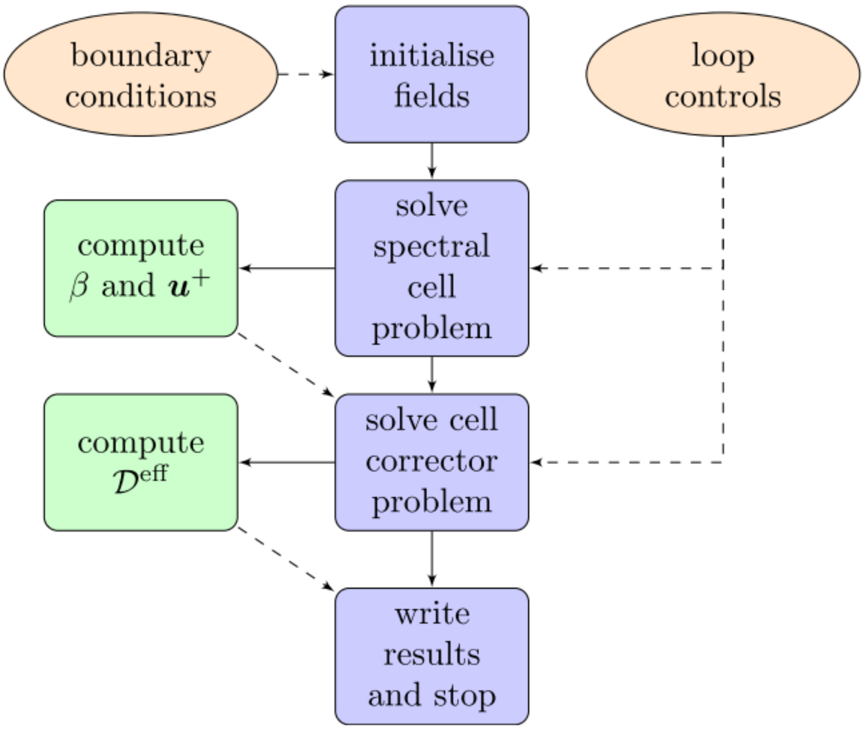


Figure 11: Main structure of specCellFoam.

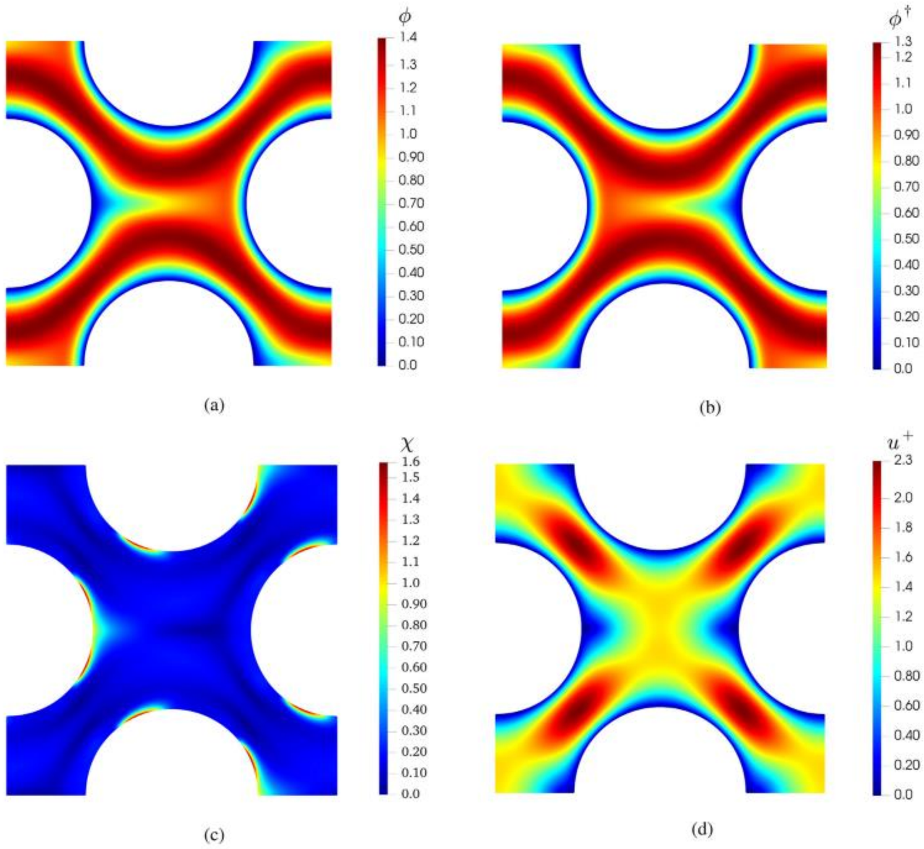


Figure 12: Eigenfunctions, corrector, and modified velocity in the periodic porous geometry.

As a verification testcase, we applied *specCellFoam* to two- and three-dimensional periodic geometries to compute the effective parameters used in large-scale simulations. Comparison between the resulting macroscopic model and direct numerical simulation showed excellent agreement (Figure 13), demonstrating the effectiveness of the proposed methodology.

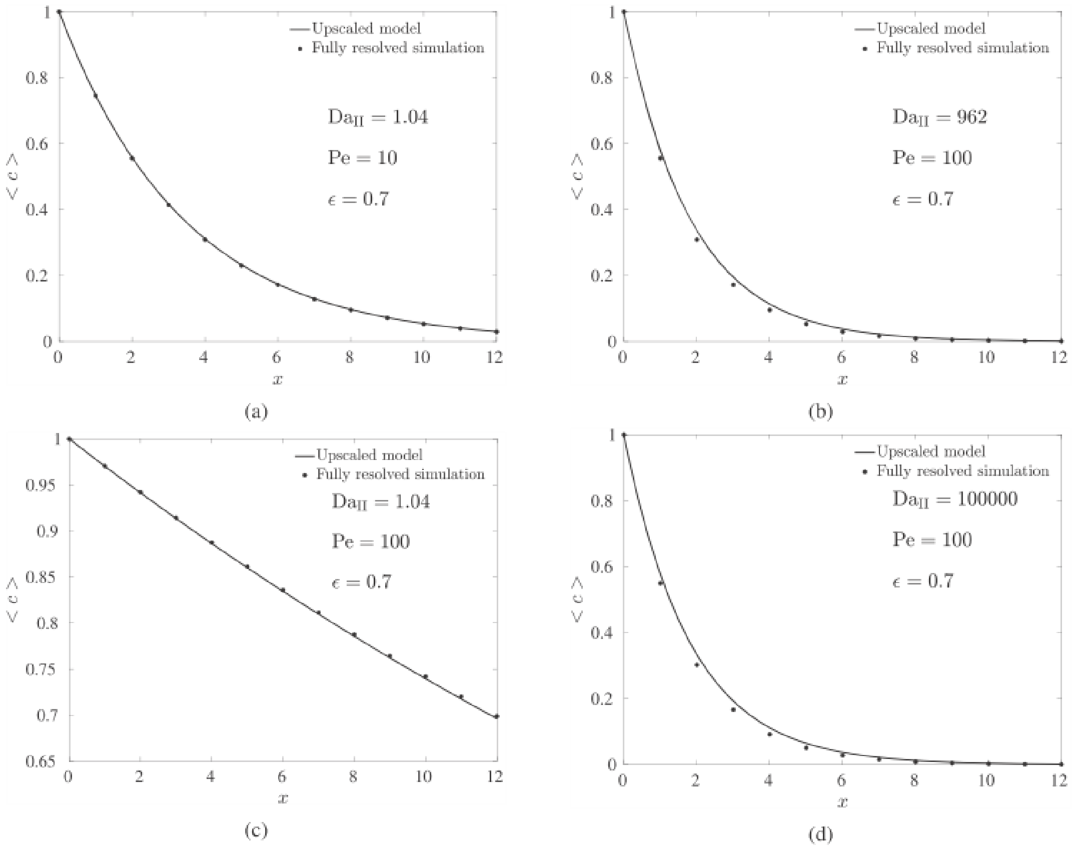
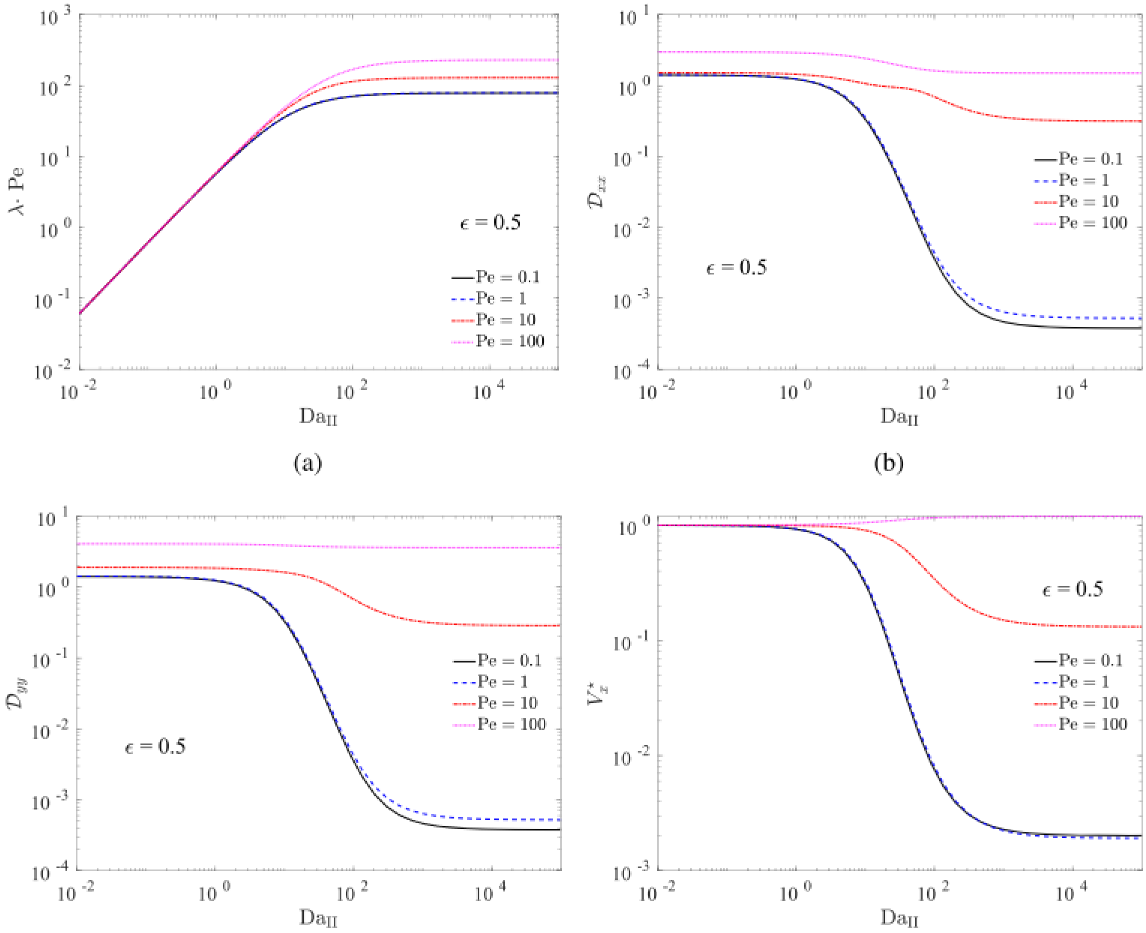


Figure 13: Comparison between results from upscaling and direct numerical simulations.

We then probed the space of parameters extensively to compute the effective parameters on a very wide range of microscopic reaction rates- Figure 14 illustrate the results for a porosity of 0.5.



(a) (b)

(c) (d)

Figure 14: Effective parameters for the porous geometry with porosity 0.5.

These methods we developed have great potential to develop models for shale gas applications, where surface reactions are extremely strong due to dissolution phenomena and large mass transfer.

2.3 GEOMECHANICS AND FLOW COUPLING

We developed an application in OpenFOAM to solve the problem of poroelasticity, involving a system of coupled Darcy and elasticity equations. This application, named *poroelasticFoam*, complement our local-to-global numerical tools to analyse the near-wellbore region. While the constitutive model employed is that of simple Hooke linear elasticity, the deformations occurring in geological media are relatively small if one assumes no fracturing occurs. At the current stage, the application is only suitable for the simulation of standard operations where no significant fracturing is expected to happen. Future work will address the modelling of fractures, for example by decoupling faces where the stress exceeds the limits of the modified Coulomb theory for brittle material failures. We include here a brief description of the model and software to give the complete picture of the *SECUReFoam* package but detailed results on this will be part of a subsequent deliverable.

2.3.1 Mathematical model

A segregated algorithm was employed to solve the following momentum balance equations (written in Einstein notation):

$$\frac{\partial}{\partial \mathrm{t}}(\rho_f s_f p)-\frac{\partial}{\partial \mathrm{x_i}}\left(\frac{1}{\nu_f}\mathrm{K_{ij}}\frac{\partial \mathrm{p}}{\partial \mathrm{x_j}}\right)=\frac{\partial}{\partial \mathrm{x_i}}\left(\frac{1}{\nu_f}\mathrm{K_{ij}}\mathrm{g_j}\right)-\frac{\partial}{\partial \mathrm{t}}\left(\alpha\frac{\partial \mathrm{D_j}}{\partial \mathrm{x_j}}\right),$$

$$\frac{\partial^2}{\partial t^2}(\rho_s D_i)-\frac{\partial}{\partial \mathrm{x_j}}\left(\mu\frac{\partial \mathrm{D_i}}{\partial \mathrm{x_j}}\right)=\frac{\partial}{\partial \mathrm{x_j}}\left(\mu\frac{\partial \mathrm{D_j}}{\partial \mathrm{x_i}}+\lambda\delta_{\mathrm{ij}}\frac{\partial \mathrm{D_k}}{\partial \mathrm{x_k}}\right)+\rho_s \mathrm{g_i}+\alpha\frac{\partial \mathrm{p}}{\partial \mathrm{x_i}}.$$

Refer to Table 2 for an explanation of the symbols employed in equations above. The solver is available in our SECUReFoam repository.

Table 2: Parameters and quantities appearing in the governing equations of poroelasticFoam

Name	Description	Units
t	Time	[s]
x	Space	[m]
ρ_f	Fluid density	[kg/m^3]
ρ_s	Solid density	[kg/m^3]
ν_f	Fluid kinematic viscosity	[m^2/s]
K_{ij}	Permeability tensor	[m^2]
p	Pressure field	[kg/(m s^2)]
g_j	Gravitational acceleration	[m/s^2]
$\mathrm{D_j}$	Displacement field	[m]
α	Biot number	[-]
s_f	Storativity	[(m s^2)]/Kg^2]
μ	First Lamé coefficient (shear modulus)	[kg/(m s^2)]]
λ	Second Lamé coefficient (bulk modulus)	[kg/(m s^2)]]
δ_{ij}	Kronecker delta	[-]

2.3.2 Simulation results

We illustrate the usage of *poroelasticFoam* in a wellbore injection application. The wellbore is represented by a two-dimensional corona, where a pressure difference of 10^4 Pa is applied between the inner and outer cylinders. We employed a sample permeability of 10^{-6} [m^2] (corresponding approximately to 1 Darcy), the fluid considered is water, and the material properties of the rocks are given by $\mu = 2.5 \cdot 10^6$ Pa and $\lambda = 1.15 \cdot 10^6$ Pa are in the range of mechanical properties measured for soft clay.

All simulations are run until a steady state is achieved.

We explored four cases corresponding to different permeability tensors (see Table 3) and we found that the solver produces the expected results in terms of deformation and pressure field.

Figure 15 shows the expected axisymmetric profile for both pressure and displacement, with a uniform radial displacement, from case A.

Figure 16 and Figure 17 correspond to case B and case C respectively and show a non-uniform displacement that warps the geometry into an ellipsoid oriented over the x or y axis. This is expected, since the material is impermeable in one direction, which therefore experiences the maximum pressure gradient at the inner cylinder. Thus, the deformation on the axis normal to the permeability tensor is large in order to balance the larger pressure force.

Figure 18 shows the results from case D, where the permeability tensor is full. Being the tensor symmetric, the flow finds the lowest resistance in the direction $\theta = \pi/4$, where θ is the angular coordinate. Therefore, the maximum deformation occurs in the normal direction at $\theta = 3\pi/4$.

Table 3: Permeability tensors in the wellbore simulations of poroelasticFoam

Case name	Permeability tensor
Case A	$K = \begin{bmatrix} 10^{-6} & 0 \\ 0 & 10^{-6} \end{bmatrix}$
Case B	$K = \begin{bmatrix} 10^{-6} & 0 \\ 0 & 0 \end{bmatrix}$
Case C	$K = \begin{bmatrix} 0 & 0 \\ 0 & 10^{-6} \end{bmatrix}$
Case D	$K = \begin{bmatrix} 10^{-6} & 10^{-6} \\ 10^{-6} & 10^{-6} \end{bmatrix}$

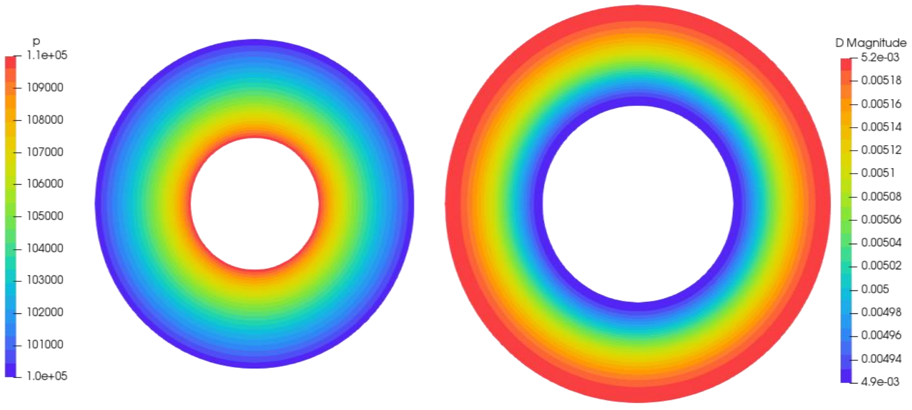


Figure 15: Pressure contours (left) on the original grid and displacement contours (right) on a deformed grid (magnified by a factor of 200) for case A

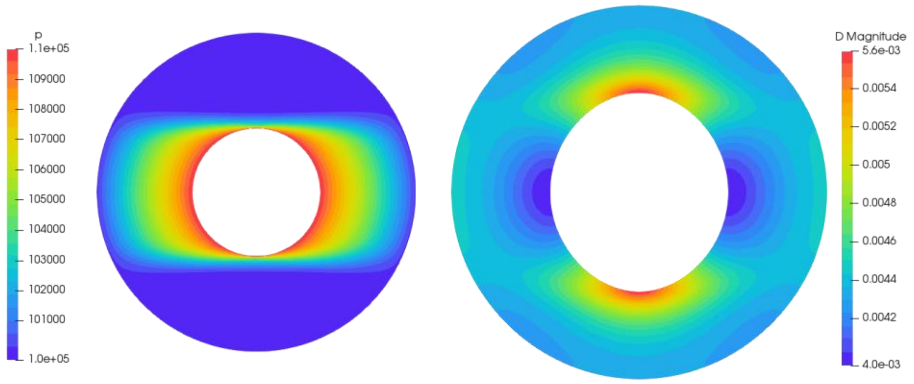


Figure 16: Pressure contours (left) on the original grid and displacement contours (right) on a deformed grid (magnified by a factor of 200) for case B

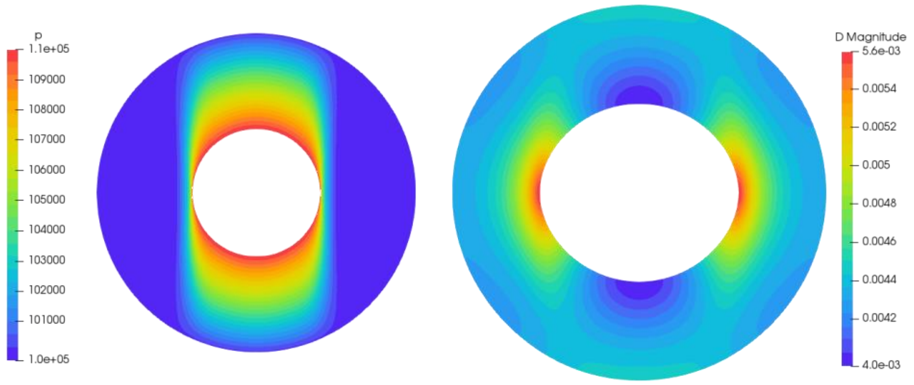


Figure 17: Pressure contours (left) on the original grid and displacement contours (right) on a deformed grid (magnified by a factor of 200) for case C

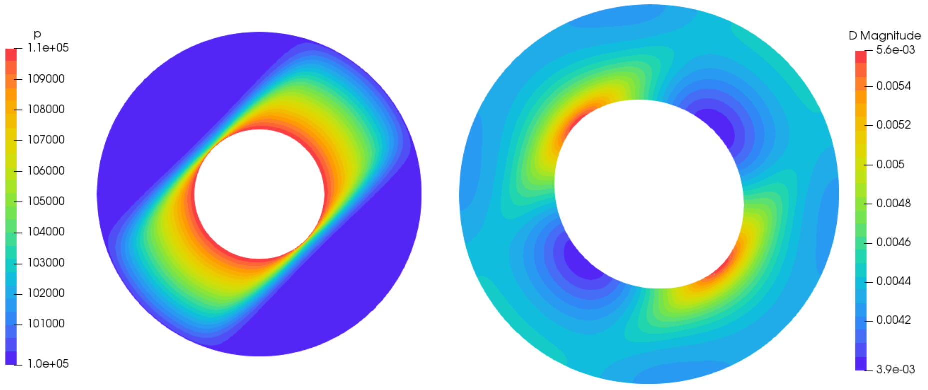


Figure 18: Pressure contours (left) on the original grid and displacement contours (right) on a deformed grid (magnified by a factor of 200) for case D

2.4 MULTIPHASE MODELS

Carbon dioxide transport in porous media is a multiphase process which plays a central role in leakage prediction. In the following, we describe the models we implemented in SECUReFOAM to model multiphase flows.

2.4.1 Variable-density flows

We consider a mixture model where the density field ρ can be expressed as:

$$\rho = \rho_1 \alpha + \rho_2 (1 - \alpha)$$

Where ρ_1 and ρ_2 are the densities of two phases while α is the volume fraction of phase 1.

Our model solves the mass conservation equation for the mixture velocity:

$$u_i^{(m)} = \alpha u_i^{(1)} + (1 - \alpha) u_i^{(2)}$$

Where each velocity satisfies a Darcy equation. This approach is like a two-fluid model, where the phases are inter-compenetrating. The volume fraction field is then evolved using an advection-diffusion equation:

$$\frac{\partial \alpha}{\partial \mathrm{t}} + \frac{\partial}{\partial x_j}\left(u_j^{(m)} \alpha - D \frac{\partial \alpha}{\partial x_j} \right) = 0$$

In Figure 19 we compute the time evolution of the volume fraction field in a 2D randomly generated heterogeneous medium, where a fixed injection located in the lower part of the domain is provided. Furthermore, we manually prescribed a vertical region of low permeability representing a fracture or an anomaly on the permeability field where leaks may occur. In this case, the fracture is modelled by an explicit and localised change of permeability.

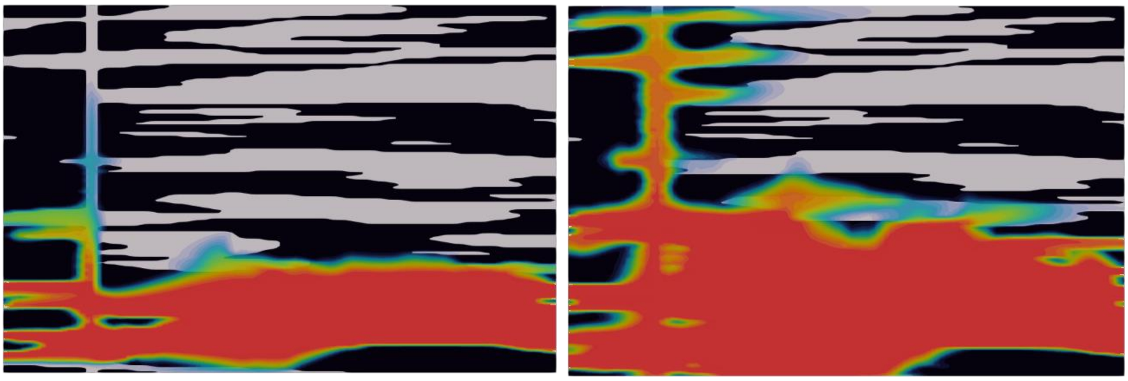


Figure 19: Volume fraction field (blue to red) in a heterogeneous 2D medium at different instants of time. Black and white stripes represent regions of low and high permeability respectively.

2.4.2 Partially miscible fluids: the phase-field formulation

SECUReFOAM also contains a stable implicit phase field solver call CahnHilliardFoam, which solves the Cahn-Hilliard equations for partially miscible fluids, where a surface potential is provided.

The phase field model requires the solution of the following equation for the phase field α:

$$\frac{\partial \alpha}{\partial t} - \nabla \cdot [m \nabla (W' - \epsilon^2 \nabla^2 \alpha)] = 0$$

Where the potential is given by:

$$W(\alpha) = \frac{1}{4}(1 - \alpha^2)^2$$

We denoted with m is the mobility field and ϵ is the interface thickness. The potential has been chosen to correctly predict coarsening phenomena, i.e., the tendency of the system to minimise the interface between phases. However, while this method is often applied to porous media (Xiaojing Fu, 2016), the existence of such sharp interface and the mathematical expression for the minimisation potential (which do not involve any property of the porous medium like permeability or porosity) are still debatable. Therefore, while the solver is included in SECUReFOAM for the sake of completeness and to increase the flexibility and potential of the library for future research, we do not apply it to any specific case within SECURe.

2.5 HETEROGENEOUS FRACTURED MEDIA AND LEAKAGE PATHWAYS

We now combine heterogeneity, dual porosity, and multiphase capabilities of our software platform to illustrate how they can be used to model leakage in realistic reservoirs. The setting is similar to that used in Section 2.4, but with a heterogeneous randomly generated permeability field and realistic material properties.

To this end, we employ a simplified two-dimensional domain with properties akin to those of the Sleipner reservoir have setup a two-dimensional simulation mimicking some parameters and properties of the Sleipner reservoir. As it can be seen in Figure 20, a significant horizontal layering is present with impermeable thin layers. These have been generated randomly preserving statistical properties of the resulting media.

Other than these layers, our model contains regions where fracture networks are present (highlighted by the purple lines) modelled using a dual continuum with linear a transfer term. Due to the presence of these fractures, the CO_2 plume leaks to higher layers up to surface instead of being confined in the lower layers close to the well.

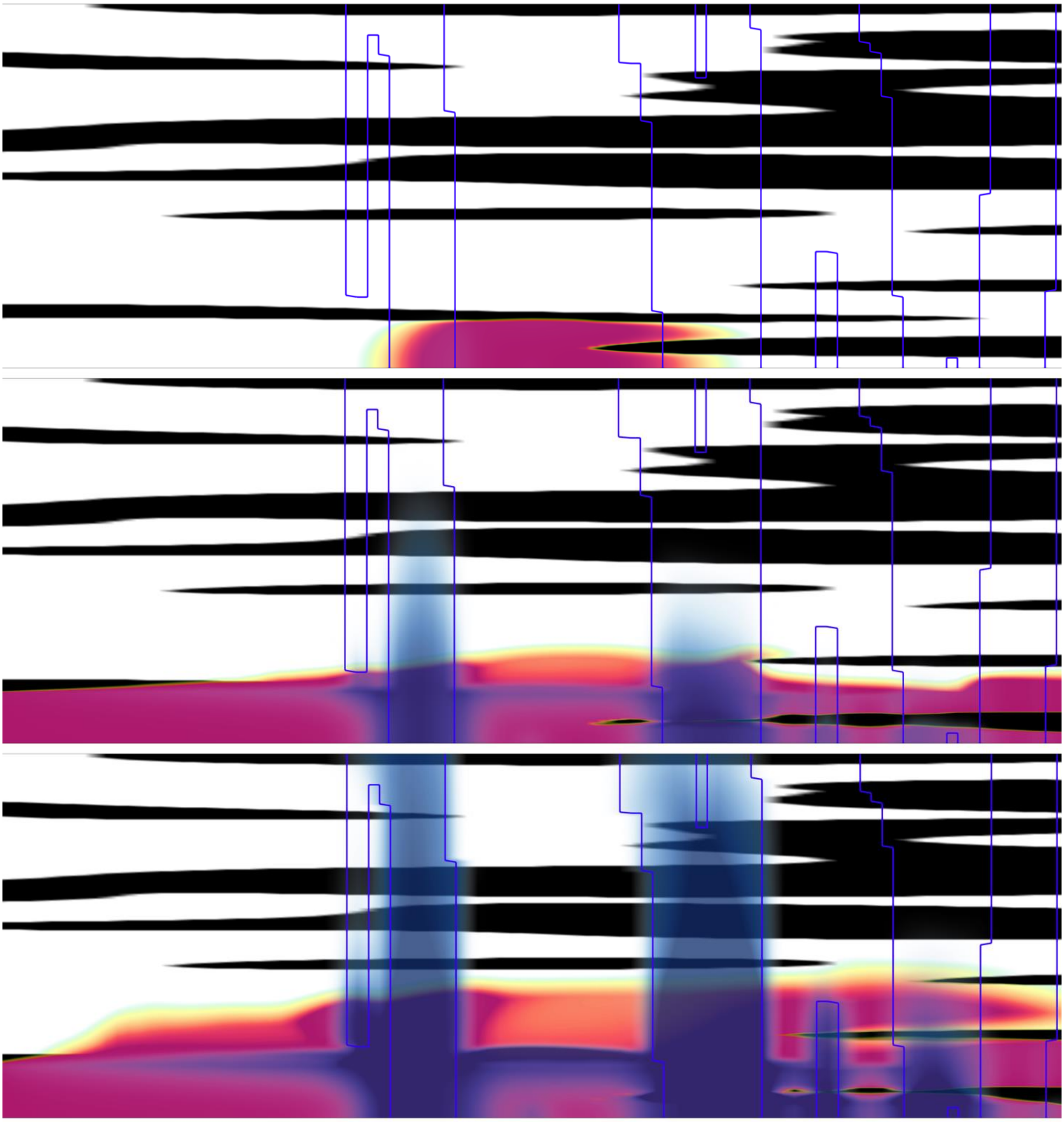


Figure 20 A two-dimensional heterogeneous layered reservoir with regions of vertical fractures. CO_2 in the matrix is represented by the red plume while, when reaching the fractures, it is represented by the blue plume. 1 month from injection (top), 12 months (mid), 36 months (bottom).

3 Dissemination and Knowledge Transfer

3.1 PUBLICATIONS AND SCIENTIFIC TALKS

Here we report the outcomes which are related to the current working package

- Federico Municchi and Matteo Icardi, “Generalized multirate models for conjugate transfer in heterogeneous materials”, Phys. Rev. Research 2, 013041 (2020)
- Federico Municchi, Nicodemo di Pasquale, Marco Dentz, Matteo Icardi, “Heterogeneous Multi-Rate mass transfer models in OpenFOAM”, submitted to Computational Physics Communications, under review, (https://arxiv.org/abs/2006.02704)
- Federico Municchi, Nicodemo di Pasquale, Matteo Icardi, “mrmtFoam”, code repository, https://zenodo.org/record/3938868
- Municchi, F., & Icardi, M. (2020). Macroscopic models for filtration and heterogeneous reactions in porous media. Advances in Water Resources, 141(September 2019), 103605. https://doi.org/10.1016/j.advwatres.2020.103605
- SECUReFoam repository https://github.com/multiform-UoN/SECUReFOAM

Furthermore, the work has been presented at the following international conference:

- APS-DFD, American Physical Society – Division of Fluid Dynamics, Seattle (2019)
- INTERPORE Annual Meeting, May 2019, Valencia
- INTERPORE Annual Meeting, Sept 2020, Online Event

3.2 WORKSHOPS

Two workshops have been organised by the University of Nottingham with the precise scopes of:

1. Gathering experts in fractured geological media operating both within and without SECURe to discuss effective and novel modelling techniques.
2. Providing training sessions and material on the employed software, discussing further technical developments with other experts.

Both these activities where sponsored by SECURe, which was explicitly acknowledged during the sessions.

3.2.1 Modelling, simulation, and risk assessment for fractured geological media workshop

The *Modelling, Simulation and risk assessment for fractured geological media workshop* was held in Nottingham between 27/03/2019 and 29/03/2019. Attendance was between 26 and 23 people per day. The main objective of this workshop was to provide a general view of the state of the arti in fractured geological media modelling to all the SECURe partners, while informing the scientific community in Europe on the aims of the SECURe project.

First day – secure meeting and updates

To introduce SECURe to new and external members, the Work Package 4 meeting was held the first day.

Afterwards, results from a previous EU project (FracRisk) where presented by Prof. Monica Riva (Politecnico of Milano).

Finally, Dr. Marco Dentz (Spanish National Research Council) gave a seminar lecture at the Department of Industrial and Applied Mathematics in Nottingham on the mathematical modelling of fractured media through the study of the first passage behaviour in the flow through 3-dimensional random fracture networks. First passage times are constructed as the sum of transition times over hydrodynamically independent network features and converge toward stable densities with distance from the inlet boundary. Trapping in immobile domains are quantified by a compound Poisson process for the total trapping time. Dr. Marco Dentz presented an analysis of the pre-asymptotic first passage behaviours and the evolution toward stable distributions, which are quantified in a systematic way by an unsteady continuous time random walk approach.

Second day - talks

A series of talks on different topics not necessarily exclusive to fractured geological media (but still strongly connected) were given in the second day, giving a broader overview of the state of the art. The day was scheduled in the following sessions:

I. Model reduction and multiscale technologies
II. Early career session: Reactive transport
III. Geomechanics
IV. Risk Assessment and Data Assimilation

Model Reduction and Multiscale Technologies

The following talks were given:

- Dr. Florian Doster (Heriot-Watt University) on the widely used multi-continuum models for fractured media. He discussed recent achievements with respect to the development of transfer functions and criteria to identify optimal representations of fractures. Such developments are based on detailed fine-scaled simulations as well as analytical and quasi-analytical representations. Furthermore, he discussed approaches to incorporate additional physics such as poro-elasticity.
- Dr. Gianluca Boccardo (Politecnico of Torino) on reactive transport in porous media. He showed an approach clearly separating pore-scale and surface processes, valid when colloidal particles are small enough, and presented a study on Brownian and gravity-driven deposition on a fcc arrangement of spherical grains, to define a robust upscaling based on a linear effective reaction rate.
- Dr. Reuben O'Dea (University of Nottingham) on multiphase and morpho-elastic multiscale models of growing porous media. He showed how the restrictive assumptions typically made on the underlying model to permit a more straightforward multiscale analysis can be relaxed, by considering finite growth and deformation at the pore scale.

Early career sessions: Reactive Transport

In this session, two Phd students presented their ongoing and previous work in the field of fractured porous media.

- Eugenio Pescimoro (University of Nottingham) presented his work on the effect of sediment heterogeneity on nutrient cycling in streambeds. He showed that streambeds with a higher volume proportion of silt exhibit lower hyporheic exchange rates but more efficient nitrate removal along flow paths compared to predominantly sandy streambeds. The implication is that hyporheic zones with a mixture of inorganic sands and organic silts have a high capacity to remove nitrate, despite their moderate permeabilities.
- Christopher Zahasky (Imperial College London) presented a comparison of imaging techniques for experimental fracture characterization in geologic materials. Specifically, he showed that a large amount of information on flow field and dispersion in porous media can be achieved by mean of positron emission tomography.

Geomechanics

- Dr. Chris McDermott (University of Edinburgh) presented several case study examples including HM coupling at an experimental scale through to reservoir scale, numerical modelling and field data for the KTB site in Germany, and the use of statistical and novel modelling approaches to solve HM(C) problems under laboratory conditions. The relevance of these approaches in terms of risk assessment using FEP approach & surrogate surface concept is demonstrated on hand of a case study for THM stability analysis of CO2 Storage in the Captain Aquifer, North Sea. This leads to the consideration that the right balance of information is required to improve confidence building in models. Finally, he presented new unique state of the art experimental equipment for the investigation of coupled processes under reservoir conditions, with a focus on fluid driven hydraulic fracturing, shear and permeability changes under true triaxial conditions.
- Dr. Xavier Rainaud (SINTEF Digital) presented geomechanical simulations coupled with realistic reservoir flow simulations and filtering processes in fractured porous media. The discretization method of the geomechanical equations is based on Virtual Element Methods (VEM) to handle directly the polyhedral grids that are common in subsurface models. After a short presentation of SINTEF's modelling approach for filtering processes and fractured media flow, he gave some details about the

implementation framework that has been used in MRST in this context and showed 2D and 3D examples on simplified geometries.

- Dr. Piotr Letkowski (Oil and Gas Institute, Poland) provided a general overview on the use of geomechanical-flow coupling to model the impact of geomechanical effects on the reservoir behavior. He gave a general outline on theoretical remarks, coupling implementation procedure on the example of selected commercial software, preparation of flow and geomechanical models, case study discussion.
- Dr. Hossein Fazeli (University of Nottingham) presented a set of microfluidic experiments studying the effect of CO2 phase states on Halite precipitation and how they can lead to clogs in the fractures.

Risk Assessment and Data Assimilation

- Prof. Monica Riva (Politecnico of Milano) focused on concepts of Sensitivity Analysis and the ensuing characterization of the way model parameter uncertainties which propagates to outputs in the context of hydrogeological modelling. This uncertainty stems from incomplete knowledge of the physics controlling the evolution of a real subsurface system and their transposition into mathematical formulations, as well as from difficulties of properly defining and characterizing input parameters embedded in such mathematical models. In this broad context, identifying priorities for the characterization of model parameters and optimizing data acquisition during sampling campaigns for model application should be considered as key elements associated with modern model developments and engineering within an application-oriented framework. She presented the implementation of a variety of sensitivity analysis tools (local and global) that can assist quantification of (a) the relative importance of uncertain model parameters and (b) the ensuing uncertainty of model outputs in the context of relevant environmental scenarios was evaluated.
- Dr. Marco Iglesias (University of Nottingham) introduced the Ensemble Kalman filter (EnKF) developed by Evensen and co-workers in the 1990s, which has had enormous impact in the geosciences and various engineering disciplines. He discussed recent parametrisations of EKI which enable to infer geometric features of the underlying (unknown) field. He showed the potential advantages of these parameterisations for new application areas which include the non-destructive evaluation of composite materials, the thermal characterisation of building walls, as well as the geological characterisation of the subsurface from geodetic data.

Third day – hands on workshop

This last day was totally devoted to the practical usage of reservoir simulation tools.

Specifically, Dr. Federico Municchi (University of Nottingham) showed how to quickly implement an efficient multi-rate mass transfer model in the finite volume library *OpenFOAM*, while Dr. Halvor Nilsen and Xavier Raynaud (SINTEF Digital) gave a training on the *MATLAB Reservoir Simulation Toolbox / MDEM*.

Both trainings followed a step-by-step approach, starting from installation of the required software on different architecture to the usage and modification of the source code.

3.2.2 First Nottingham OpenFOAM Workshop

The *Nottingham OpenFOAM Workshop* was held in Nottingham on Monday 22nd July and Tuesday 23rd July 2019. The overall scope was to provide basic-to-advanced OpenFOAM training to possible beneficiaries of the code developed within SECURe and to discuss future development with experts.

Hands-on training was provided during each day and pre-installed packages were provided when needed. The first day consisted in a tutorial session organised by Dr. Mirco Magnini (University of Nottingham) on basic usage of OpenFOAM and multiphase solvers, to make the participants familiar with the library.

The second day was split in two parts. In the first part, a set of research talks were given illustrating the versatility of OpenFOAM:

I. Dr. Andrea Ferrari (Swiss Federal Laboratories for Material Science and Technology) illustrated ho OpenFOAM can be applied to urban climate modelling and the large number of equations that can solve at the same time (one of the reason why it is employed in SECURe).
II. Dr. Federico Municchi (University of Nottingham) gave a talk on the use of runtime C++ in OpenFOAM for a wide range of applications: from pre-processing to post-processing and customised terms in the governing equations.

III. Andrew Nicoli (Gas Turbine and Transmission Research Centre, Nottingham) showed how to model sprays in OpenFOAM.
IV. Dr. Mirco Magnini (University of Nottingham) provided an extensive description of the volume of fluid solvers in OpenFOAM.

Finally, the remaining time was dedicated to solving problems proposed by the participants using the techniques presented in the previous talks.

4 Conclusions and best practices

This document reports the work done at the University of Nottingham, in relation to Work Package 4, focused on the development of Modelling and Simulation tools, suitable for integration of monitoring data.

We developed a multi-physics software platform for leakage prediction in subsurface flows using the opensource library OpenFOAM and presented some relevant applications to illustrate its usage.

We found significant issues with the current approach to data in the community of reservoir simulations. These can be summarised as follows:

- Numerical grids employed in reservoir simulations are often not suitable for standard algorithms in computational fluid dynamics due to the presence of invalid primitive geometries (e.g., faces and cells). Therefore, appropriate mesh quality checks should be performed before releasing any data.
- Thanks to the enormous improvement in computing hardware during the past decade, large files and memory usage is far less concerning. Therefore, it would be in the interest of the wider modelling community that the corner point format be substituted with a more standard format (e.g., vtk or msh), which has wider usage and it is therefore better documented and maintained.
- Related to the point above, data formats are still too influenced by the proprietary software employed in the community. Even in the Open Porous Media, open data are not easily understandable by someone not familiar with proprietary software like Eclipse, despite reservoir simulations being, in their essence, standard computational continuum mechanics. Also, there is a surprising lack of documentation regarding the usage of these data.

It is our opinion that the use of opensource software and standard data formats would allow the community to widen significantly.

Another significant point concerns the amount of information needed to predict leakage. As it can be noticed, many of the parameters of our models, like matrix and fracture network permeability, are mostly unknown in real applications. The correct usage of the methods described in this report requires integration with field data to find possible values for these parameters through calibration (i.e., inverse problem). Once a set of parameters generating the measured data is found, one can proceed to explore different operating conditions like, for example, the injection rate.

References

ANSYS. (2020). Retrieved from https://www.ansys.com/

COMSOL Multiphysics Modelling Package. (2020). Retrieved from https://www.comsol.com/

Dassargues, R. H. (2020). Continuous Dissolved Gas Tracing of Fracture-Matrix Exchanges. *Geophysical Research Letters*.

Dune for multi flow and transport in porous media. (2020). Retrieved from https://dumux.org/

Gorelick, R. H. (1995). Multiple-Rate Mass Transfer for Modeling Diffusion and Surface Reactions in Media with Pore-Scale Heterogeneity. *Water Resources Research, 10*(31), 2383-2400.

Industries, S. (2020). Retrieved from https://www.sintef.no/projectweb/mrst/

OpenGeoSys. (2020). Retrieved from https://www.opengeosys.org/

Peter Zweigel, R. A. (2004). Reservoir geology of the Utsira Formation at the first industrial-scale underground CO2 storage site (Sleipner area, North Sea). *Geological Society of London Publications*(233), 165-180.

Schlumberger. (2020). Retrieved from https://www.software.slb.com/products/eclipse

The Open Porous Media. (2020). Retrieved from https://opm-project.org/

The OpenFOAM Fundation. (2020). Retrieved from https://openfoam.org/

Xiaojing Fu, L. C.-F. (2016). Thermodynamic coarsening arrested by viscous fingering in partially miscible binary mixtures. *Physical Review E, 94*(033111).