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Mathematical analysis and numerical simulation of multi-phase multi-component flow in heterogeneous porous media

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ABSTRACT

Multi-phase multi-component flow processes are fundamental to engineering applications in hydrocarbon and geothermal reservoirs but also to many classical geological processes. This review will highlight recent developments in the mathematical modelling and numerical simulations of the underlying physical processes from the pore- to the reservoir scale. Many modern approaches now rely on integrating numerical and analytical methods and incorporate results across the different length scales. This provides new insights into the fundamental properties of multi-phase multi-component flow and helps to mitigate some of the inherent difficulties in quantifying them in subsurface reservoirs.

1. Introduction

The transport of dissolved chemical components (e.g., CO_2, NaCl, CH_4) in different fluid phases (e.g., water, oil, gas) occupying the pore space of geological formations underground (see Fig. 1 for an example of a geological formation) is of fundamental importance to a large number of geological and reservoir engineering processes. These include, but are not limited to, storing greenhouse gases such as CO_2 in saline aquifers and oil fields [7], enhancing the recovery of oil and gas from hydrocarbon reservoirs through the injection of chemicals [4] or viscosifying polymers [81], heat flow in high-enthalpy geothermal and volcanic systems [39], flow in the vicinity of radioactive waste repositories [88], remediation of toxic contaminants in groundwater aquifers [62], or the formation of hydrothermal ore deposits [30].

All these applications have in common that they are modelled, in various degrees of complexity, by the governing equations for multi-phase multi-component flow at the reservoir scale. In the most general form, transport of a chemical component c in fluid phase α is given by

$$\frac{\partial M_c}{\partial t} + \nabla \cdot F_c = \mathcal{R}_c, \tag{1}$$

where R_c is a general source/sink term, describing, for example, the rate at which a chemical component is consumed by a mineral reaction or injected at a well into a hydrocarbon reservoir. The mass of component c, M_c, is given by

$$M_c = \varphi \sum_{\alpha=o,a,g} S_\alpha \rho_\alpha \chi^c_\alpha, \tag{2}$$

where φ is the rock porosity, S and ρ are the saturation (fluid volume fraction) and density of phase α, respectively. Note that $S_o + S_w + S_g = 1$. $\chi^c{}_\alpha$ is the mass fraction of component c in phase α. The subscripts o, a, and g denote the oelic, aqueous, and gaseous phase, respectively. The flux vector $\mathbf{F}_c$ describing the advective and dispersive component c is defined as

$$F_c = \sum_{\alpha=o,\alpha,g} \left(\underbrace{v_\alpha \rho_\alpha \chi^c_\alpha}_{\text{Advection}} - \underbrace{S_\alpha \mathcal{D}_\alpha \nabla (\rho_\alpha \chi^c_\alpha)}_{\text{Dispersion}} \right), \tag{3}$$

where $\boldsymbol{D}_\alpha$ is the dispersion tensor, which is a function of the phase velocity $\boldsymbol{v}_\alpha$ and molecular diffusivity of $\chi^c{}_\alpha$. $\boldsymbol{v}_\alpha$ is given by the extended Darcy's law

$$v_\alpha = -\frac{k_\alpha \mathbf{k}}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g). \tag{4}$$

Here, $\boldsymbol{k}$ is the permeability (a tensor) of the rock, k_α is the relative permeability, μ_α is the viscosity, p_α the pressure in phase α, and $\mathbf{g}$ the vector of gravitational acceleration, i.e. $\mathbf{g} = [0, 0, -g]^T$.

The set of governing equations (Eq. (1) to (4)) gives rise to a complex flow behaviour with multiple displacement fronts. To illustrate this, consider the simplified case where a wetting phase displaces a

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Fig. 1. Folded carbonate rocks in Oman with vertical fractures. Similar rocks like these, but buried underground in approximately 1 to 4 km depth, contain the world's largest oil reservoirs in the Middle East. Fluid phases (e.g., oil, gas and water) and dissolved chemical components (e.g., CO_2, NaCl, CH_4) flow through tiny connected pores contained in these geological formations (Fig. 4). Image courtesy of Prof. Patrick Corbett, International Centre for Carbonate Reservoirs, Edinburgh.

non-wetting phase while carrying a dissolved chemical component at high concentration (Fig. 2). In this two-phase one-component scenario, one front develops where the two fluid phases displace each other ("saturation front") and another front develops, usually trailing the former one, where the wetting phase at high concentration mixes with the wetting phase at low concentration ("concentration front"). The shape of the two fronts depends on the flow conditions, i.e. if advective processes dominate over diffusive processes or vice versa. The shape of the saturation front always influences the shape of the component front. The shape of the component front only impacts the shape of the saturation front if the chemical components affect the relative permeability k_α or phase pressure p_α [78••,79].

Solving these equations is non-trivial for the following reasons: (1) Porosity φ and permeability $\boldsymbol{k}$ vary spatially and possibly temporally if chemical reactions (e.g., mineral scale formation) alter the pore-space geometry (Fig. 3). (2) Permeability coefficients can readily vary over orders of magnitude, giving rise to large variations in flow velocities (Eq. (4)) and localised flow (Fig. 3). (3) The distribution of permeability and porosity coefficients is unknown and multiple distributions must be generated stochastically to evaluate uncertainties in flow and transport. (4) Relative permeability k_α and phase pressure p_α are non-linear functions of the phase saturation S_α and, possibly, the mass fraction of a dissolved chemical component $\chi^c{}_\alpha$, for example if chemical reactions change the wettability of the rock surface (Fig. 2). (5) Phase density ρ_α and phase viscosity μ_α typically depend on the mass fraction of a dissolved chemical component (e.g., the density of brine increases with increasing NaCl concentration). (6) The phase saturation can change as a function of phase pressure and mass fraction of a dissolved chemical component (e.g., the amount of CO_2 that can be dissolved in the water phase depends on the phase pressure and the amount of free CO_2 determines the saturation of the water and gas phase).

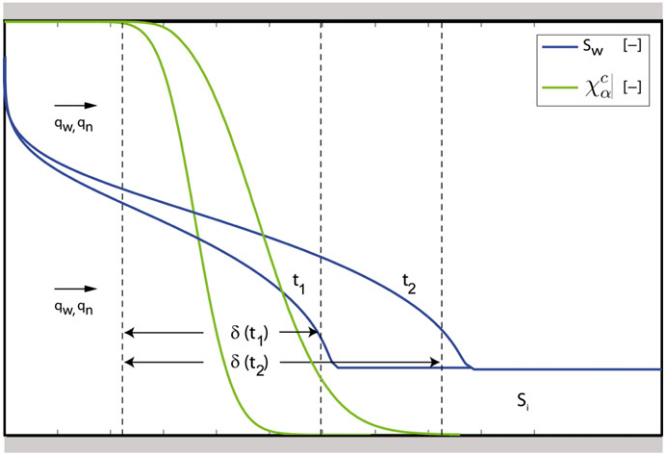

Fig. 2. Schematic representation of two-phase displacement of a non-wetting phase by a wetting phase with an initial wetting saturation S_i at two different times t_1 and t_2. Behind the wetting front, a mixing zone of length $\delta(t)$ develops between the "old" composition of the wetting phase and the "new" one with composition $\chi^c{}_\alpha > 0$. In most cases, the solute front trails the saturation front [78••,79]. Figure adapted from [79].

The aim of this paper is to review the state-of-the-art solution approaches for the above equations using numerical methods at the pore and continuum scale and (semi-)analytical methods. While our review focuses mostly on recent advances with respect to oil and gas production from hydrocarbon reservoirs, it immediately carries over to other disciplines because of the generality of the governing equations. In the next section we will discuss analytical solutions which are imperative for the simulation and understanding of the fundamental scaling of multi-component transport during multi-phase flow. This is followed by two sections discussing recent advances in the numerical simulation of multi-component transport and multi-phase flow at the pore- and continuum scale, respectively. We close by highlighting some of the outstanding questions and future challenges in this field.

2. Analytical solutions

Analytical solutions for Eq. (1) to (4) play an important role for three reasons. The first and most obvious reason consists in benchmarking of new numerical methods (see Section 4). Second, analytical solutions can be used as parts of a numerical code as grid-free methods that significantly speed up the calculations [43•,24••,25]. Finally, analytical solutions can shed light onto the often complicated interactions of some of the non-linearities included in Eq. (1) to (4) [45,16], and help in interpreting experimental results [52]. However, due to the complexity of the governing equations, to date no solutions are known that resolve all the dependencies that are possible in a multi-phase multi-component system, and most likely never will be. Instead, analytical solutions are derived for homogeneous domains, and certain limiting cases that are particularly important in practical applications. Often self-similarity is heavily exploited. This makes the governing partial differential equations mathematically tractable, but excludes the investigation of important non-self-similar effects like flow instabilities [41].

2.1. Analytical solutions for CO_2 storage

Many recently proposed solutions investigate key problems that arise in connection with the modeling and simulation of CO_2 capture and storage. Often, the researchers active in this field have developed a sequence of increasingly complex solutions in separate publications, and we will only focus on the most recent ones. CO_2 storage involves its injection into deep saline aquifers. Since these aquifers can be penetrated by many abandoned oil wells, leakage rates of CO_2 through these wells are a major concern, and [67] derived analytical solutions for this scenario. The pressure buildup during CO_2 injection is another major concern [58•], since during CO_2 injection, the pressure near the well increases which can lead to excessive formation damage. [58•] give analytical solutions for pressure buildup that account for partial miscibility of CO_2 and brine, and for volume change on mixing. Another impact of CO_2 injection on the formation are changes in porosity and permeability, and [94] derive analytical solutions that describe porosity and permeability reduction due to salt precipitation. Since the injected CO_2 is lighter than the reservoir brine, the extent of the CO_2 plume is governed by buoyancy while a significant fraction of the CO_2 in the plume's tail will be disconnected from the tail and thus be trapped. [31•] derive closed-form analytical solutions for gravity currents and residual trapping. [45] consider the same

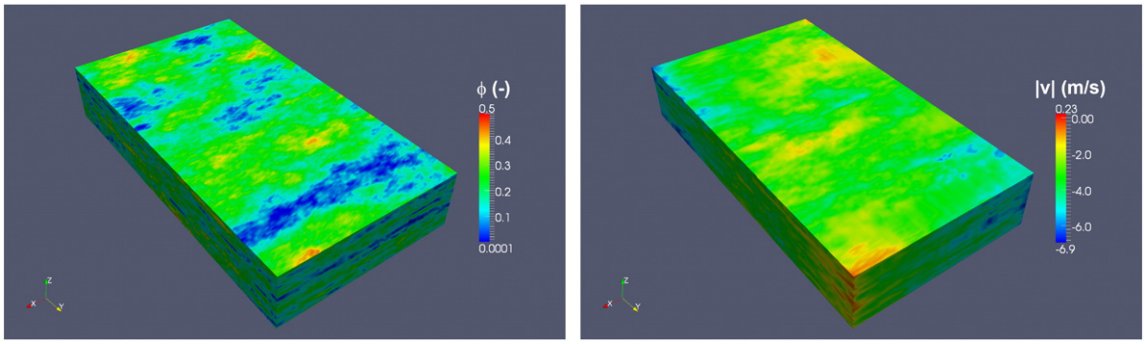

Fig. 3. Porosity distribution in a synthetic hydrocarbon reservoir [10] (left) and magnitude of the corresponding velocity field in $\log_{10}$ scale computed for a vertical injection and production well located at two opposite corners in the reservoir (right). Model dimensions are $680 \times 365 \times 12$ m. The model is discretised by finite volumes and the size of each finite volume grid cell is $6 \times 3 \times 0.6$ m. Porosity and permeability distributions are generated stochastically to represent the flow behaviour of the actual geological formation, for example the one shown in Fig. 1. Note that the vertical dimension is exaggerated tenfold. Modified after [27••].

situation and additionally take the effect of regional groundwater flow into account. In all these contributions, the vertical-equilibrium, sharp-interface assumption is evoked. For the vertical-equilibrium it is assumed that the large aspect ratio of the plume (length to height $\gg 1$) justifies neglecting vertical flow, and the assumption of hydrostatic pressure. The sharp-interface assumption requires that capillary effects between both phases are negligible.

2.2. Analytical solutions for dispersive effects: imbibition and hydrodynamic dispersion

All the studies in the previous two sections ignore the influence of capillary and hydrodynamic dispersion on flow and transport since both effects lead to highly non-linear parabolic terms where the analytical techniques used in the above works are either difficult to apply or fail altogether.

However, both capillarity and dispersion give rise to effects of central importance. For example, capillary pressure and spontaneous imbibition are one of the main driving mechanisms to recover oil from fractured hydrocarbon reservoirs (Fig. 1), which contain approximately 60% of the world's remaining oil reserves. If more than one component is present, and both miscible and immiscible displacement occur (Fig. 2), dispersion governs how well the miscible fluids mix [15••,41,78••], and thus limits fast chemical reactions [15••]. In the case of CO_2 injection, for example, neglecting dispersion leads to highly erroneous estimation of dissolution [32].

While the analytical solution to the hyperbolic (i.e., advection-only) two-phase system has long been known – the well-known Buckley–Leverett solution – and has been extended to far more complex cases [52], an analytical solution even for the simple case of immiscible two-phase flow without components but honouring capillary pressure effects was the matter of intensive research until recently: [78••] derived analytical solutions for the case where both hydrodynamic effects and capillary pressure act. The solutions [78••,79] describe immiscible flow and transport of a component. They also account for the important case of spontaneous imbibition (Fig. 2). The analytical description of the saturation and the capillary flow field is exact, and valid for arbitrary capillary-hydraulic properties. Thus, they form the capillary counterpart to the Buckley–Leverett solution. The solutions furthermore reveal how the mixing zone in two phases depends on whether viscous or capillary flow occur, and that sorption decreases the extent of the mixing zone [79].

3. Pore-scale modelling

Flow and transport processes in geological formations occur within the tiny pores comprising the formation (Fig. 4). Here they are modelled by a set of equations different from Eq. (1) to (4), the

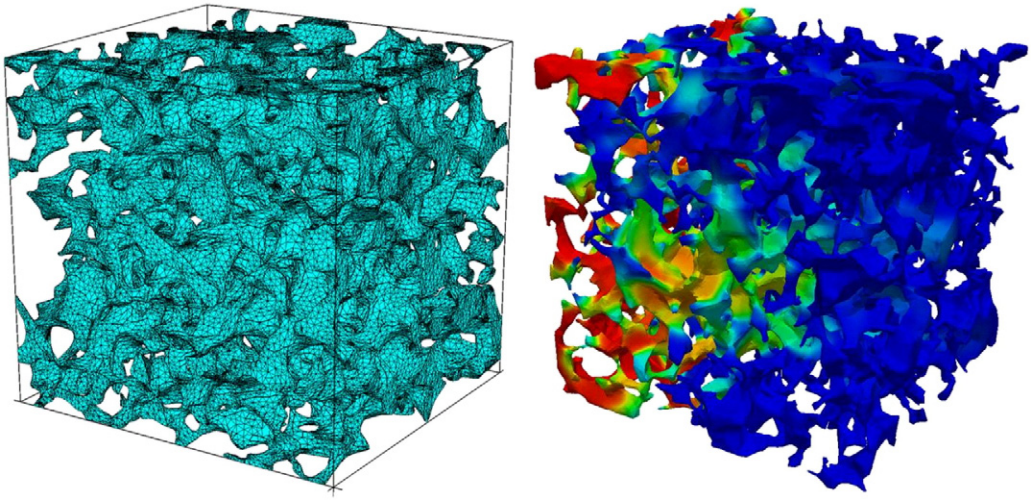

Fig. 4. Triangulated surface of a pore-space geometry (left) and simulated concentration distribution (right) where red colours show the highest and blue colours the lowest concentrations values. A chemical component (e.g., CO_2, NaCl, CH_4) enters the pore-space through the left boundary and flows through the pore-space due to advection and diffusion. Note how the flow is channeled in a small number of pores, causing the concentration to spread due to mechanical dispersion. These small-scale spreading and mixing effects can have a noticeable impact on the flow behaviour at the reservoir scale (Fig. 3) and hence must be modelled correctly. The size of the sample is 1.5 mm in each direction. Modified after [93•].

Navier–Stokes equation. The Navier–Stokes equation resolves flow in the pores explicitly while Eq. (1) to (4) are the corresponding averaged equations for the reservoir scale.

Pore-scale modelling offers three key advantages: First, the analysis and quantification of complex laboratory experiments, which study, for example, trapping of super-critical CO_2 in pores [38••], can be leveraged by pore-scale simulations. Second, complex flow processes such as the simultaneous flow of oil, gas, and water or the transport of reactive species can be quantified at the pore-scale and upscaled to model these processes more robustly at the continuum, that is reservoir, scale [33•,3•]. Lastly, new approaches emerge that directly couple pore- and continuum-scale simulations to model reservoir scale processes more reliably [74,6••]. Incorporating results from pore-scale simulations in reservoir scale simulations is driven by the knowledge that small-scale heterogeneities affect the large-scale flow behaviour, both for component transport [15••] and multi-phase flow [1•].

Several comprehensive reviews have been published in the last decade, the most recent ones focusing on a discussion of the latest numerical methods for pore-scale modelling [59••] and the general limitations of pore-scale modelling [82••]. It is hence not our aim to provide another detailed review but to highlight how pore-scale modelling techniques are currently being expanded to provide further insights into multi-phase multi-component processes, although to this date published solutions of multi-phase multi-component problems at the pore-scale are very few. Instead, research often concentrates on just one aspect of the problem – either multi-phase flow or single-phase multi-component transport. Nevertheless, there is great potential for pore-scale modelling techniques to provide exciting new insights into multi-phase multi-component flow and important research progress is currently being made.

3.1. Multi-phase flow

The use of pore-networks to represent multi-phase flow can be dated back to the middle of the previous century. Pore-network modelling is a rule-based method that deals with idealized pore space representation, simplified flow equations and does not require explicit fluid-fluid interface tracking. Therefore it is currently the only pore scale technique that can be applied to numerical rocks with hundreds of thousands of pores. As such it currently has the best predictive capabilities and very good agreement between experimental and numerical results can be obtained for two- and three-phase flow in relatively homogeneous porous media [57,1•]. High-resolution and multi-scale pore-network geometries can now be constructed to model flow and transport processes in realistic but challenging geometries [9•,54]. Despite the large success of using pore-networks as a modelling tool, this approach has some limitations which are currently being overcome. This is an important progress in the context of multi-phase multi-component transport. Most network models are restricted to capillary dominated conditions and assume that the influence of viscous forces leading to advective displacement of fluid phases can be neglected. To overcome this limitation, dynamic pore network models are being developed, and first promising results show that the classical Buckley–Leverett profile can be recovered directly from the pore-scale [37•]. Another way to include viscous forces and advective displacement is to simulate the multi-phase fluid dynamics directly on images of the pore structure. This can be achieved using either conventional simulation techniques adapted from computational fluid dynamics (CFD) or particle-based methods, among which Lattice Boltzmann (LB) method, an approximation of the Navier–Stokes equation, remains the most popular one. LB methods can be extended to two-phase flows more straightforwardly than CFD methods because no interface tracking is required. [73] show the comparison between LB calculations of relative permeabilities and experimental measurements and corroborate that the method has predictive capabilities, at least for homogeneous sandstone geometries. Nevertheless, care should be taken when using LB methods as it was also demonstrated that permeability calculations in 3D sandstone samples result in a strong unphysical sensitivity to fluid viscosity through the variation of relaxation time [63]. This sensitivity can be reduced, but not eliminated, by using a multi-relaxation time (MRT) scheme. Similar can be said about LB multi-phase modelling: The most popular multi-phase model, the Shan-Chen model, is not thermodynamically consistent and the resulting surface tension term in the Shan-Chen model has a different form from the one in the two-phase Navier–Stokes equation. [51,50] show how Shan-Chen model can be improved using MRT method. Another complication of the LB method is its high computational costs. Although LB schemes are straightforward to parallelise, they still require a large number of computational nodes if a calculation is to be conducted on a reasonably large domain. For example, [70] used the mature open source code Palabos on 2000 processors with run times of up to 60 hours to model reactive transport processes on relatively small samples of $200\times200\times300$ lattice nodes. Interestingly, computational load is often cited as a drawback of CFD-based methods. However, it it our belief that if properly implemented, multi-phase simulations based on CFD techniques such as finite element or finite volume methods would not require more time and resources than the example above. In fact, it was suggested to speed-up two-phase LB calculations with level-set techniques, a classical CFD method to track interfaces [86•].

Like any simulation approach that aims to model complex non-linear and multi-scale physical processes, pore-scale simulations will probably never be truly predictive in the sense that they can be run without any calibration to experimental data and still provide accurate forecasts of the flow behaviour [82••]. This is, in part, caused by our understanding that even physical processes within individual pores, for example the formation and collapse of oil layers in the corner of a pore or the representation of the cross-sectional pore-shape, already impact large-scale flow behaviour [76•]. Resolving such small-scale physics with LB methods may be intractable for the years to come. Furthermore, it was also demonstrated that the shape of the surface area separating two phases within the pore-space [42] or the presence of small clusters of different fluid phases within the pore-space [1•] influence large-scale the flow behaviour. Without being able to parameterise these processes and/or resolving them numerically, pore-network simulations will not be truly predictive. This applies to both, two-phase flow and three-phase flow processes. Additional complexities are encountered if the network of connected pores contain pore-networks at different scales because the flow through the entire multi-scale network cannot be expressed by an average of the flow behaviour through the individual pore-networks [91•,87].

3.2. Single- and multi-component transport

Since it is well understood that the mechanical spreading and diffusive mixing at the pore-scale affects the large-scale transport of chemical components [6••,15••,74••], analysing single-phase component transport from a pore-scale perspective continues to be a topic of active research, especially as modern hardware are now powerful enough to model transient transport directly on the 3D rock images. [93•] used CFD methods to develop an efficient finite element – finite volume algorithm to model Stokes flow and single-phase transport directly on the pore-space geometry. They further extended the model to account for the presence of a trapped second fluid phase during component transport [92]. Other successful approaches to model transport processes at the pore-scale are Lagrangian moving particle semi-implicit methods [68] and streamline-based random walks [8•]. These simulation approaches allow us to analyse the range validity of classical continuum descriptions, i.e. Fick's law. It is

usually found that available continuum descriptions for transport and chemical reactions break down when they are upscaled from the pore- to the continuum scale [5•,8•].

A key motivation for studying chemical reactions during component transport at the pore-scale is subsurface CO_2 storage; models now include kinetic dissolution/precipitation reactions for CO_2-rich brines [21] and resultant changes in pore-space geometry [3•]. LB methods have also been applied to this scenario [46], which allows for a straightforward incorporation of local changes in pore-space geometry due to dissolution and precipitation. However, so far this approach was only used on artificial 2D geometries, prohibiting an experimental validation.

4. Continuum-scale modelling

While the development of analytical equations and pore-scale modelling techniques for multi-phase multi-component processes progresses continuously (see Sections 2 and 3), oil recovery from hydrocarbon reservoirs or CO_2 migration in saline aquifers must be predicted for complex geological structures (Fig. 1) comprising heterogeneous permeability and porosity fields (Fig. 3), usually with time-varying boundary conditions such as fluctuations of well flow rates or even new wells being drilled over the life-time of an oil reservoir. This cannot be modelled with analytical solutions or at the pore-scale. Robust and efficient numerical solutions to solve the governing equations (Eq. (1) to (4)) are needed instead.

4.1. Discretisation of complex geological structures

Many geological formations comprising subsurface reservoirs contain non-orthogonal and geometrically complex geological structures such as faults, fractures, or folded sedimentary layers (Fig. 1). The classical approach, and current industry-standard, in reservoir simulation is to discretise Eq. (1) to (4) using finite volume methods on Cartesian grids. Gradients in pressure (Eq. (4)) are computed using the pressures at two neighbouring grid cells along each main grid axis. Fluxes (Eq. (3)) are computed using the coefficients (e.g., S_α or $\chi^c{}_\alpha$) from the upstream grid cell. It is well-established that this method gives inaccurate results, for example spurious non-physical oscillations and loss of mass balance, if the grid is skewed to accommodate non-orthogonal geological structures and the permeability tensor varies strongly. Hence significant research efforts continue to be devoted to develop locally conservative and flux-continuous finite volume discretisations that produce physical solutions (i.e. without spurious oscillations) when applied to grids containing anisotropic and discontinuous full-tensor permeability fields as well as non-orthogonal geological structures. Since many multi-phase multi-component transport processes represent inherently unstably physical processes, for example enhanced oil recovery processes involving the injection of a miscible gas phase, numerical errors trigger these instabilities [41]. The need for using grids that can represent complex geological structures is, in part, driven by the increasing need to produce oil and gas from structurally complex hydrocarbon reservoirs using recovery methods that give rise to instable flow processes.

Flux-continuous methods for finite volume discretisations on complex grids with realistic permeability fields were recently made available through a mature open source code [56••]. New families of flux-continuous and locally mass conserving finite volume schemes and control-volume distributed multi-point flux approximation schemes with improved numerical convergence rates for general grids with anisotropic with discontinuous permeability fields were developed by [22,69]. Advective transport of fluid phases or chemical components shows significantly less cross diffusion if multi-dimensional upwinding is used such that it occurs in the direction along which the saturation or concentration waves have travelled instead of along the main grid axes [19,49], or if upwinding can be avoided altogether [18•]. Higher-order methods can be used to reduce numerical diffusion along the main grid axes, providing significantly sharper concentration and saturation fronts [53]. Mixed finite element methods and discontinuous Galerkin methods provide an alternative to finite volume discretisations to model multi-phase multi-component processes on complex grids while ensuring flux continuity and local mass conservation [40,85•]. Like finite volume methods, these discretisation approaches can also be parallelised to provide computational speedup [14]. While these methods may not be readily adapted in commercial simulators, a key advantage is that finite element methods are amenable to combine challenging coupled flow and geomechanical simulations [29].

Direct simulation of multi-phase multi-component problems in fractured rock masses pose a particular gridding challenge if the fractures are to be discretised explicitly because a fracture has a vary narrow width (Fig. 1) but must be represented in models that are tens to hundreds of metres in size. Fractures are often more permeable than the rock matrix and are main flow conduits. It is common to represent the fractures as lower-order entities, for example 2D surfaces in 3D reservoir models. This discretisation approach is robust but care must be taken to model the processes at the interface between fracture and matrix correctly [65]. [28,26] developed a parallelised combined finite element – finite volume method to simulate three-phase – three-component flow including a modified equation of state for gas-oil-water systems in fractured rock masses; higher-order flux approximations were used to preserve sharp concentration fronts. [36] showed that it is important to model diffusive processes of multiple chemical species in fractured rock masses accurately because diffusive exchange of chemical components between fractures and matrix can significantly retard the transport. [80] demonstrated how different time-stepping approaches and higher-order flux approximations can be used to model advection combined with (non-linear) diffusion processes due to mechanical and capillary dispersion accurately in fractured rock masses. Higher-order discontinuous Galerkin methods were also found to be suitable to model flow and transport processes efficiently in fractured rock masses with limited numerical diffusion perpendicular and parallel to the main grid axes [34•]. They can readily be modified to handle discontinuos capillary pressures, a problem that is notoriously difficult to simulate if fractures are represented as lower-dimensional entities [35]. The discontinuous Galerkin approach can also be extended to model three-phase – multi-component oil-gas-water flows with higher-order flux approximations [60•,61].

4.2. Reduced physics approaches

A key challenge often encountered in multi-phase multi-component simulations is the high computational cost, particularly if complex equations of state need to be evaluated to compute how chemical components partition among the different phases. Hence it is often impossible to run a large number of simulations to evaluate how uncertainties in the geological model, expressed in different realisations of the permeability and porosity fields (Fig. 3), may affect, for example, the volume of CO_2 sequestered in the subsurface or the breakthrough of a toxic groundwater contaminant. An obvious way to increase computational efficiency of multi-phase multi-component simulations is to make use of multi-core hardware architectures and run simulations in parallel, capabilities many of the latest multi-phase multi-component flow simulation codes have.

A different approach, and area of strong research activity, is to develop multi-phase multi-component simulations which simplify the physical processes but still give reasonably accurate results. Reduced physics simulations can be used, also in conjunction with parallelisation, to evaluate a large number of geological models and subsequently rank and prioritise them for further “full-physics” simulations that are computationally more costly but yield the most accurate results. This is particularly advantageous for numerical simulations of CO_2

storage in saline aquifers because saline aquifers are larger than hydrocarbon reservoirs and usually less well characterised.

Streamline simulations are a well-established and widely used approach to efficiently simulate flow and transport processes on large and complex geological models, although at reduced physical accuracy [13]. Streamline simulations decouple the computation of the flow field and the transport process: First, the pressure and velocities are calculated in the entire reservoir using conventional finite volume techniques. Streamlines are then traced along the velocity field and transport of fluid phases or chemical components can be computed along the streamlines. Periodically, new concentration and saturation distributions are mapped back from the streamlines onto the finite volume grid and the pressure and velocity fields are updated. In the context of multi-phase multi-component simulations, the work by [72••] presents an important milestone for streamline simulation because it describes a new model for the transport of CO_2, water, oil, and salt in an aqueous and hydrocarbon phase while also accounting for the precipitation of salt as halite and CO_2 as a carbonate mineral. The simulator was successfully applied to evaluate smart CO_2 injections strategies that are capable of trapping large volumes of CO_2 safely in geological formations [71••]. It since has been improved to model the phase behaviour of CO_2-water systems along the streamlines, which provides significantly more accurate results [55]. Other important advances for streamline simulation of multi-phase multi-component processes are the modelling of non-Newtonian polymer floods with physically realistic rheological models for the non-Newtonian fluid [2] and computationally efficient front-tracking schemes that use analytical Riemann solvers along the streamlines to model miscible gas injection processes [43•,44•].

Another important class of reduced physics simulation approaches, which have started to gain traction in CO_2 storage simulations, are vertically integrated models. These models solve vertically averaged flow equations that are discretised with finite volume approaches and use analytical solutions to account for the small-scale physical process that are no longer resolved in the numerical discretisation, such as buoyancy effects and leakage of CO_2 along wellbores [24••] or dissolution and trapping of CO_2 [25]. Since the vertical averaged flow equations reduce a 3D problem to 2D, simulations can be run much more efficiently.

A third approach to reduce computational time of multi-component multi-phase flow simulations are so-called multi-physics methods [12•,66,23•]. They utilise the fact that not all phases and components are present in the reservoir – for example, when injecting CO_2 or a chemical component into a geological formation, it is initially only present in the vicinity of the injection well and then migrates along the high-permeability flow channels such that low-permeability regions of the reservoir maintain low CO_2 concentrations for a long time. A multi-physics approach requires that the regions where certain physical processes occur can grow or shrink automatically during the simulation and that regions of different physical processes are coupled adequately. While this is challenging to implement, it can lead to significant computational gains because superfluous evaluations of flow and transport equations and calls to computationally costly equations of state are minimised. However, results from multi-physics approaches are of comparable accuracy to results from numerical solutions where all physical processes are simulated everywhere in the reservoir [12•,66,23•].

4.3. Incorporating small-scale heterogeneities

As noted in Section 3, it is well known that heterogeneities as small as the pore-scale can significantly impact the large-scale flow and transport predictions. This is particularly important if chemical reactions, e.g. the rate at which CO_2 precipitates as a carbonate mineral, are to be predicted because small-scale heterogeneities impact the rate at which reaction zones grow in a way that is difficult to model with classical continuum descriptions, i.e. Fick's law, as confirmed by numerous theoretical analyses [15••] and combined experimental–numerical studies [47••,17•,77].

While it is theoretically possible to generate reservoir simulation grids with very fine resolution to capture all small-scale heterogeneities, it is practically impossible because this would lead to prohibitively large reservoir models and computing times. Hence, in practice, there will always be geological structures that are not represented explicitly in a large-scale reservoir simulation model because they are smaller than the size of a finite volume grid cell. Since these small-scale heterogeneities can affect the large-scale transport behaviour, they should be treated accurately in large-scale reservoir simulations. A very promising approach is to describe the resulting "sub-grid" fluctuations in the flow field by adding a stochastic forcing term to Eq. (3). This was pioneered by [84•,83••] for modelling miscible single-phase transport with chemical reactions and [90,89••] to model the trapping of fluid phases during two-phase flow. [27••] have used a stochastic partial equation with multiplicative noise to model sub-grid fluctuations and uncertainties in chemical reaction rates during miscible single-phase flow. [64•] used the mean-field theory to estimate effective parameters for small-scale heterogeneities during two-phase flow. A slightly different approach was used by [74••] who used continuum time random walks to model the small-scale transition times in large-scale reservoir simulations of miscible single-phase flow and also discussed how this approach could be extended to multi-phase flow. Another possibility of incorporating challenging flow behaviours due to small-scale heterogeneities is to explicitly couple pore-scale simulations with continuum-scale simulations in regions where continuum-scale descriptions of the transport processes are invalid, which yields more accurate predictions at the continuum-scale [6••,75].

While the idea of stochastic methods to describe small-scale heterogeneities and uncertainties in the flow and transport behaviour is promising, there are to date no methods available that can deal with both, multi-phase flow and multi-component transport.

4.4. Open source codes and benchmark studies

Very recently, general-purpose simulators have been published that are released under the GNU General Public License.[1] These allow the scientific community to utilise existing source code and publish truly reproducible science. These open source codes are often developed, tested, and applied by a large user base. Hence the code infrastructure is mature, which allows for straightforward implementation of new numerical methods for multi-phase multi-component flow simulations. An important open source codes is DuMu^X [20••], which can deal with multi-phase and multi-component transport for multi-physics simulations. It also offers multi-scale simulation techniques. The MATLAB Reservoir Simulation Toolbox (MRST) [56••] offers advanced flux-continuous discretisation approaches for unstructured grids, including corner-point grids, Cartesian, rectilinear and curvilinear grids, Delaunay triangulations and Voronoi grids. It also provides multi-scale simulation techniques and can be be applied to single- and multi-phase flow problems. OpenGeoSys is based on finite element discretisations and allows multi-physics simulations for coupled thermal, hydraulic, mechanical, and chemical processes [48••]. Open source codes, research codes, and industrial simulators for multi-phase multi-component simulations are often subjected to inter-code benchmark comparisons. Benchmark studies for multi-phase multi-component flow have a long-standing history and recent work focused on simulating scenarios related to subsurface CO_2 storage with a variety of realistic flow scenarios [11••]. Key lessons learned were that all simulators show reasonably good agreement in predicting the flow processes

[1] http://www.gnu.org/licenses/gpl-2.0.html

but results can deviate if errors are introduced in the gridding process, model parameters are assigned wrongly, or due to different interpretations of simulation problems.

5. Concluding remarks and future challenges

The mathematical and numerical modelling of multi-phase and multi-component processes will continue to receive major research interest, largely driven by the need to securely store CO_2 and other greenhouse gases underground, improve oil and gas recovery from depleting hydrocarbon reservoirs, and assessing clean-up schemes for contaminated groundwater aquifers. Today's numerical discretisation methods are increasingly capable of modelling flow and transport processes reliably in complex geological structures; varying the degrees of physical complexity allows to speed up numerical simulations if needed. This applies to the reservoir as well as the pore-scale. Here it is particularly exciting that many advanced numerical methods are currently being made available through open source codes.

It is now well understood that flow and transport processes must be studied across multiple scales and reservoir scale simulations need to account for impact of small-scale heterogeneity. In this context, first promising attempts are being made to directly incorporate pore-scale simulation results and other small-scale stochastic processes in simulations at the reservoir scale. However, these still tend to focus on the complex behaviour component transport alone – an area that is challenging enough in its own right – and future research will need to focus on understanding how the small-scale interplay of phase and component transport affects reservoir-scale flow behaviours. Analytical solutions will continue to be of importance as they provide key insights into the fundamental properties of this interplay but are also increasingly used as building blocks for advanced numerical simulations.

However, numerical simulation experiments and analytical solutions are only one way to study the interactions of component transport and chemical reactions in multiple fluid phases; well-designed and carefully monitored laboratory experiments of multi-phase and multi-component processes remain a key requirement as they provide the much-needed validation data for the numerical and analytical models.

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References and recommended readings[2,3]

[1] Al-Dhahli A, Geiger S, van Dijke MIJ. Three-phase pore-network modelling for mixed-wet carbonate reservoirs. . SPE-147991SPE Reservoir Characterization and Simulation Conference. Abu Dhabi, U.A.E. 9-11 October., 2011; 2011. The paper demonstrates how multiple displacement chains during three-phase flow impact predicted residual oil saturations and compares predicted oil recovery in a hydrocarbon reservoir using pore-scale derived and classical relative permeability curves for three-phase gas injection.

[2] Al-Sofi AM, Blunt MJ. Streamline-based simulation of non-newtonian polymer flooding. SPE J 2010;15(4):901–11.

[3] Algive L, Bekri S, Vizika O. Pore-network modeling dedicated to the determination of the petrophysical-property changes in the presence of reactive fluid. SPE J 2010;15(3):618–33. The paper develops a reactive pore network model that accounts for the dynamic modification of pore throat radii due to dissolution/precipitation.

[4] Austad T, Strand S, Madland MV, Puntervold T, Korsnes RI. Seawater in chalk: an EOR and compaction fluid. SPE Reservoir Eval Eng 2008;11(4):648–54.

[5] Battiato I, Tartakovsky DM, Tartakovsky AM, Scheibe TD. On breakdown of macroscopic models of mixing-controlled heterogeneous reactions in porous media. Adv Water Resour 2009;32(11):1664–73. The paper maps out a phase diagram in Peclet number – Damkohler number space to quantify where macroscopic models for reactive transport simulations break down.

[6] Battiato I, Tartakovsky DM, Tartakovsky AM, Scheibe TD. Hybrid models of reactive transport in porous and fractured media. Adv Water Resour 2011;34(9):1140–50. The paper describes the direct coupling of pore-scale and continuum-scale simulation techniques to better model reactive transport processes in regions where continuum-scale descriptions break down.

[7] Bickle M. Geological carbon storage. Nat Geosci 2009;2(12):815–8.

[8] Bijeljic B, Mostaghimi P, Blunt MJ. Signature of non-Fickian solute transport in complex heterogeneous porous media. Phys Rev Lett 2011;107(20):204502. The paper uses a streamline-based random-walk simulator on 3D images of carbonate rocks to demonstrate that Fickian description of dispersion is not valid for heterogeneous porous media.

[9] Biswal B, Øren PE, Held RJ, Hilfer R. Modeling of multiscale porous media. Image Anal Stereol 2009;28:23–34. The paper describes a novel method to combine micro- and macro pore scales in a single pore-network model.

[10] Christie MA, Blunt MJ. Tenth SPE comparative solution project: a comparison of upscaling techniques. SPE Reservoir Eval Eng 2001;4(4):308–17.

[11] Class H, Ebigbo A, Helmig R, Dahle HK, Nordbotten JM, Celia MA, et al. A benchmark study on problems related to CO_2 storage in geologic formations: summary and discussion of the results. Comput Geosci 2009;13(4):409–34. The paper describes a very comprehensive benchmarking study analysing the performance of all state-of-the-art multi-phase multi-component simulators for simulating a wide range of challenging and realistic subsurface CO_2 storage problems.

[12] Class H, Helmig R, Neuweiler I. Sequential coupling of models for contaminant spreading in the vadose zone. Vadose Zone J 2008;7(2):721–31. The paper describes how different physical processes, occurring in small sub-regions of a large-scale groundater reservoir, can be simulated with different mathematical models to increase simulation time.

[13] Datta-Gupta A, King M. *Streamline Simulation: Theory and Practice*, volume 11 of *SPE Textbook Series*. Richardson, Texas, USA: Society of Petroleum Engineers; 2007.

[14] Delshad M, Thomas SG, Wheeler MF. Parallel numerical reservoir simulations of nonisothermal compositional flow and chemistry. SPE J 2011;16(2):239–48.

[15] Dentz M, Le Borgne T, Englert A, Bijeljic B. Mixing, spreading, and reactions in heterogeneous media: a brief review. J Contam Hydrol 2011;120–121:1–17. The paper provides an excellent and concise review of the current state-of-the art on modelling solute transport and chemical reactions in heterogeneous porous media.

[16] DiCarlo DA, Mirzaei M, Aminzadeh B, Dehghanpour H. Fractional flow approach to saturation overshoot. Transp Porous Media 2012;91(3):955–71 doi:10.1007/s11242-011-9885-8.

[17] Edery Y, Scher H, Berkowitz B. Dissolution and precipitation dynamics during dedolomitization. Water Resour Res 2011;47:W08535. The paper analyses and quantifies dedolomitization, a very important chemical reaction problem in the world's largest oil reservoirs, through carefully conducted laboratory experiments and numerical simulations.

[18] Edwards MG. Global and local central non-upwind finite volume schemes for hyperbolic conservation laws in porous media. Int J Numer Methods Fluids 2010;64(7):793–811. The paper describes an interesting discretisation approach that avoids upwinding altogether but still increases the numerical accuracy of advection-dominated transport problems.

[19] Edwards MG. Multi-dimensional wave-oriented upwind schemes with reduced cross-wind diffusion for flow in porous media. Int J Numer Methods Fluids 2011;67(1):33–57.

[20] Flemisch B, Darcis M, Erbertseder K, Faigle B, Lauser A, Mosthaf K, Müthing S, Nuske P, Tatomir A, Wolff M, Helmig R. $DuMu^x$: DUNE for multi-{phase, component, scale, physics, …} flow and transport in porous media. Adv Water Resour 2011;34(9):1102–12. doi:10.1016/j.advwatres.2011.03.007. The paper reviews one of the leading open source codes, written in C++, for multi-phase multi-component transport problems.

[21] Flukiger F, Bernard D. A new numerical model for pore scale dissolution of calcite due to CO_2 saturated water flow in 3D realistic geometry: principles and first results. Chem Geol 2009;265(1):171–80.

[22] Friis HA, Edwards MG. A family of MPFA finite-volume schemes with full pressure support for the general tensor pressure equation on cell-centered triangular grids. J Comput Phys 2011;230(1):205–31.

[23] Fritz J, Flemisch B, Helmig R. Decoupled and multiphysics models for non-isothermal compositional two-phase flow in porous media. Int J Numer Anal Model 2011;9(1):17–28. The paper describes a numerical approach where different physical processes are simulated in different regions of the reservoir and the model sub-regions grow or shrink as the physical processes change.

[24] Gasda SE, Nordbotten JM, Celia MA. Vertical equilibrium with sub-scale analytical methods for geological CO_2 sequestration. Comput Geosci 2009;13(4):469–81. The paper provides the first application of vertically-averaged simulation approaches that model buoyancy effects using analytical equations to CO_2 storage problems.

[25] Gasda SE, Nordbotten JM, Celia MA. Vertically averaged approaches for CO_2 migration with solubility trapping. Water Resour Res 2011;47:W05528.

[26] Geiger S, Huangfu Q, Reid F, Matthäi SK, Coumou D, Belayneh M, et al. Massively parallel sector scale discrete fracture and matrix simulations. . SPE-118924SPE Reservoir Simulation Symposium. The Woodlands, Texas, 2 - 4 February, 2009; 2009.

[27] Geiger S, Lord G, Tambue A. Exponential time integrators for stochastic partial differential equations in 3D reservoir simulation. Comput Geosci in press. doi:10.1007/s10596-011-9273-z. The paper describes the first proof-of-concept study that models fluctuations in small-scale chemical reactions using stochastic partial differential equations in 3D reservoir simulations, including a novel time-integration scheme based on exponential integrators.

[2] • of special interest.

[3] •• of outstanding interest.

[28] Geiger S, Matthäi S, Niessner J, Helmig R. Black-oil simulations for three-component–three-phase flow in fractured porous media. SPE J 2009;14(2):338–54.
[29] Girault V, Pencheva G, Wheeler MF, Widley T. Domain decomposition for poroelasticity and elasticity with DG jumps and mortars. Math Models Methods Appl Sci 2011;21(1):169–213.
[30] Heinrich CA. Fluid-fluid interactions in magmatic-hydrothermal ore formation. In: Liebscher A, Heinrich CA, editors. Fluid-fluid interactions, volume 65 of Reviews in Mineralogy and Geochemistry; 2007. p. 363–87.
[31] Hesse MA, Orr F, Tchelepi HA. Gravity currents with residual trapping. J Fluid Mech 2008;611(1):35–60. The paper derives analytical solutions for the important scenario of migration of gravity currents and trapping during CO_2 injection in a sloping aquifer.
[32] Hidalgo J, Carrera J. Effect of dispersion on the onset of convection during CO_2 sequestration. J Fluid Mech 2009;640:441–52.
[33] Holm R, van Dijke MIJ, Geiger S. Three-phase flow modelling using pore-scale capillary pressure and relative permeabilities for mixed-wet media at the continuum scale. Transp Porous Media 2010;81(3):423–42. The paper studies the impact of wettability, analysed from a pore-scale perspective, on continuum-scale three-phase flow processes during gas injection into hydrocarbon reservoirs.
[34] Hoteit H, Firoozabadi A. An efficient numerical model for incompressible two-phase flow in fractured media. Adv Water Resour 2008;31(6):891–905. The paper discusses the first application of discontinuous Galerkin finite element method to multi-phase flow simulations in complex 2D and 3D reservoirs where fractures are represented explicitly.
[35] Hoteit H, Firoozabadi A. Numerical modeling of two-phase flow in heterogeneous permeable media with different capillarity pressures. Adv Water Resour 2008;31(1):56–73.
[36] Hoteit H, Firoozabadi A. Numerical modeling of diffusion in fractured media for gas-injection and -recycling schemes. SPE J 2009;14(2):323–37.
[37] Idowu NA, Blunt MJ. Pore-scale modelling of rate effects in waterflooding. Transp Porous Media 2010;83(1):151–69. The paper develops a rate-dependent network model that takes viscous forces into account and is the first pore-scale study to reproduce a Buckley–Leverett profile on a model with 100,000 of pores.
[38] Iglauer S, Paluszny A, Pentland CH, Blunt MJ. Residual CO_2 imaged with X-ray micro-tomography. Geophys Res Lett 2011;38:L21403. The paper shows the first-ever direct observation of pore-scale trapping of a super-critical CO_2 phase using high-resolution X-ray CT measurements. These observations confirm predictions made by pore-network models.
[39] Ingebritsen SE, Geiger S, Hurwitz S, Driesner T. Numerical simulation of magmatic hydrothermal systems. Rev Geophys 2010;48:RG1002.
[40] Ingram R, Wheeler MF, Yotov I. A multipoint flux mixed finite element method on hexahedra. SIAM J Numer Anal 2010;48(4):1281–312.
[41] Jha B, Cueto-Felgueroso L, Juanes R. Fluid mixing from viscous fingering. Phys Rev Lett 2011;106:194502.
[42] Joekar-Niasar V, Hassanizadeh SM, Dahle HK. Non-equilibrium effects in capillarity and interfacial area in two-phase flow: dynamic pore-network modelling. J Fluid Mech 2010;655(1):38–71.
[43] Juanes R, Lie KA. Numerical modeling of multiphase first-contact miscible flows. part 1. analytical Riemann solver. Transp Porous Media 2007;67(3):375–93. The paper describes how analytical methods can be used in conjunction with streamline simulations to provide accurate and computationally efficient reservoir simulation techniques for miscible gas injection.
[44] Juanes R, Lie KA. Numerical modeling of multiphase first-contact miscible flows. part 2. front-tracking/streamline simulation. Transp Porous Media 2008;72(1):97–120. The paper demonstrates how the combined analytical-numerical streamline approach to miscible gas flood modelling can be applied to highly heterogeneous 2D and 3D reservoirs. Simulation results show that water-alternating-gas injections are more effective in producing oil than gas or water injection alone.
[45] Juanes R, MacMinn C, Szulczewski M. The footprint of the CO_2 plume during carbon dioxide storage in saline aquifers: storage efficiency for capillary trapping at the basin scale. Transp Porous Media 2010;82(1):19–30.
[46] Kang QJ, Lichtner PC, Viswanathan HS, Abdel-Fattah AI. Pore scale modeling of reactive transport involved in geologic CO_2 sequestration. Transp Porous Media 2010;82(1):197–213.
[47] Katz GE, Berkowitz B, Guadagnini A, Saaltink MW. Experimental and modeling investigation of multicomponent reactive transport in porous media. J Contam Hydrol 2011;120–121:27–44. The paper discusses the application of carefully conducted, quasi-2D flow cell experiments for multi-component reactive transport to examine the performance of high-resolution reactive transport codes that aim to model the spatial evolution of the reaction zone.
[48] Kolditz O, Delfs J, Burger C, Beinhorn M, Park C. Numerical analysis of coupled hydrosystems based on an object-oriented compartment approach. J Hydroinf 2008;10:227–44. The paper introduces another important open source code, written in C++, which is particularly capable of modelling reactive transport processes and mechanical deformation.
[49] Kozdon JE, Mallison BT, Gerritsen MG. Multidimensional upstream weighting for multiphase transport in porous media. Comput Geosci 2011;15(3):399–419.
[50] Kuzmin A, Mohamad A. Multirange multi-relaxation time Shan-Chen model with extended equilibrium. Comput Math Appl 2010;59(7):2260–70.
[51] Kuzmin A, Mohamad A, Succi S. Multi-relaxation time Lattice Boltzmann model for multiphase flows. Int J Mod Phys C 2008;19(6):875–902.
[52] LaForce T, Jessen K. Analytical and numerical investigation of multicomponent multiphase WAG displacements. Comput Geosci 2010;14(4):745–54.
[53] Lamine S, Edwards MG. Higher order multidimensional upwind convection schemes for flow in porous media on structured and unstructured quadrilateral grids. SIAM J Sci Comput 2010;32(3):1119–39.
[54] Latief FDE, Biswal B, Fauzi U, Hilfer R. Continuum reconstruction of the pore scale microstructure for Fontainebleau sandstone. Phys A Stat Mech Appl 2010;389(8):1607–18.
[55] Lazaro-Vallejo L, Leahy M, Dance T, LaForce T. New phase behavior algorithm for simulation of CO_2 storage. . SPE-Paper 141734SPE Reservoir Simulation Symposium. The Woodlands, Texas. 21–23 February., 2011; 2011.
[56] Lie KA, Krogstad S, Ligaarden IS, Natvig RJ, Nilsen HM, Skafelstad M. Open-source MATLAB implementation of consistent discretization on complex grids. Comput Geosci in press. doi:10.1007/s10596-011-9244-4. The paper introduces a mature open source code with a wide range of flux-continuous discretisation methods for complex grids. Capable of modelling single and multi-phase processes. The code is easy to use as it heavily capitalises on the functionality available in MATLAB.
[57] Lopez O, Mock A, Skretting J, Petersen Jr E, Øren P, Rustad A. Investigation into the reliability of predictive pore-scale modeling for siliciclastic reservoir rocks. . Paper SCA2010-4Society of Core Analysts Symposium; 2010.
[58] Mathias SA, Gluyas JG, Gonzalez Martinez de Miguel GJ, Hosseini SA. Role of partial miscibility on pressure buildup due to constant rate injection of CO_2 into closed and open brine aquifers. Water Resour Res 2011;47:W12525. The paper provides so far the most general analytical solutions for estimating the pressure buildup during CO_2 injection. Their solutions can account for the partial miscibility of CO_2 and brine and for the effects of volume change on mixing.
[59] Meakin P, Tartakovsky AM. Modeling and simulation of pore-scale multiphase fluid flow and reactive transport in fractured and porous media. Rev Geophys 2009;47(3):RG3002. The paper provides a comprehensive review that discusses the advantages and disadvantages of a wide range of numerical methods for pore-scale simulations. Mostly focuses on single-phase transport and reaction applications.
[60] Moortgat J, Firoozabadi A. Higher-order compositional modeling with Fickian diffusion in unstructured and anisotropic media. Adv Water Resour 2010;33(9):951–68. The paper extends the discontinuous Galerkin finite element method to the simulation of three-phase multi-component processes in structurally complex geological media.
[61] Moortgat J, Sun S, Firoozabadi A. Compositional modeling of three-phase flow with gravity using higher-order finite element methods. Water Resour Res 2011;47:W05511.
[62] Mulligan C, Yong R, Gibbs B. Surfactant-enhanced remediation of contaminated soil: a review. Eng Geol 2001;60(1–4):371–80.
[63] Narváez A, Zauner T, Raischel F, Hilfer R, Harting J. Quantitative analysis of numerical estimates for the permeability of porous media from Lattice–Boltzmann simulations. J Stat Mech Theory Exp 2010;2010:P11026.
[64] Neuweiler I, Papafotiou A, Class H, Helmig R. Estimation of effective parameters for a two-phase flow problem in non-gaussian heterogeneous porous media. J Contam Hydrol 2011;120–121:141–56. The paper describes an interesting approach to use the mean-field theory to accurately average two-phase flow processes occurring in small-scale heterogeneous media for large-scale two-phase flow simulations.
[65] Nick HM, Matthäi SK. Comparison of three FE-FV numerical schemes for single- and two-phase flow simulation of fractured porous media. Transp Porous Media 2011;90:421–44.
[66] Niessner J, Helmig R. Multi-physics modeling of flow and transport in porous media using a downscaling approach. Adv Water Resour 2009;32(6):845–50.
[67] Nordbotten JM, Kavetski D, Celia MA, Bachu S. Model for CO_2 leakage including multiple geological layers and multiple leaky wells. Environ Sci Technol 2009;43(3):743–9.
[68] Ovaysi S, Piri M. Pore-scale modeling of dispersion in disordered porous media. J Contam Hydrol 2011;124(1–4):68–81.
[69] Pal M, Edwards MG. Anisotropy favoring triangulation CVD (MPFA) finite-volume approximations. Int J Numer Methods Fluids 2011;67(10):1247–63.
[70] Parmigiani A, Huber C, Bachmann O, Chopard B. Pore-scale mass and reactant transport in multiphase porous media flows. J Fluid Mech 2011;686(1):40–76.
[71] Qi R, LaForce T, Blunt MJ. Design of carbon dioxide storage in aquifers. Int J Greenhouse Gas Control 2009;3(2):195–205. The paper evaluates a smart injection scheme where the CO_2 injection is followed by a brine injection to increase the residual trapping of CO_2 in saline reservoirs and depleted oil fields.
[72] Qi R, LaForce T, Blunt MJ. A three-phase four-component streamline-based simulator to study carbon dioxide storage. Comput Geosci 2009;13(4):493–509. The paper extends a research-grade streamline simulator to simulate subsurface CO_2 storage processes in large-scale geological models of depleted oil fields and saline aquifers more accurately. It can account for precipitation of halite and carbonate minerals.
[73] Ramstad T, Idowu N, Nardi C, Øren PE. Relative permeability calculations from two-phase flow simulations directly on digital images of porous rocks. Transp Porous Media 2011:1–18.
[74] Rhodes ME, Bijeljic B, Blunt MJ. Pore-to-field simulation of single-phase transport using continuous time random walks. Adv Water Resour 2008;31(12):1527–39. The paper discusses an interesting approach where continuous time random walks are used in a multi-stage upscaling approach to model miscible flow processes at the reservoir scale including pore-, core-, and outcrop-scale heterogeneities.
[75] Ryan EM, Tartakovsky AM. A hybrid micro-scale model for transport in connected macro-pores in porous media. J Contam Hydrol 2011;126(1–2):61–71.
[76] Ryazanov A, van Dijke MIJ, Sorbie KS. Two-phase pore-network modelling: existence of oil layers during water invasion. Transp Porous Media 2009;80(1):

79–9. The paper demonstrates that a new thermodynamic criterion for the formation and collapse of oil layers and accounting for the cross-sectional pore-space geometry leads to more accurate predictions of residual oil saturation in rocks of arbitrary wettability.
[77] Sanchez-Vila X, Fernandez-Garcia D, Guadagnini A. Interpretation of column experiments of transport of solutes undergoing an irreversible bimolecular reaction using a continuum approximation. Water Resour Res 2010;46:W12510.
[78] Schmid KS, Geiger S, Sorbie KS. Semi-analytical solutions for co- and counter-current imbibition and dispersion of solutes in immiscible two-phase flow. Water Resour Res 2011;47:W02550. The paper derives the first set of analytical solutions where both capillary pressure and dispersion are fully taken into account and investigates their influence on mixing. It contains exact solutions for the case of spontaneous imbibition for arbitrary flow parameters and thus the capillary counterpart to the Buckley–Leverett solutions.
[79] Schmid KS, Geiger S, Sorbie KS. Analytical solutions for co- and counter-current imbibition of sorbing, dispersive solutes in immiscible two-phase flow. Comput Geosci in press. doi:10.1007/s10596-012-9282-6.
[80] Schmid KS, Geiger S, Sorbie KS. A higher order FE-FV method on unstructured grids for transport and two-phase flow with variable viscosity in heterogeneous porous media. J Comput Phys (in review).
[81] Sorbie KS. Polymer-improved oil recovery. Glasgow: Blackie & Sons Ltd.; 1991.
[82] Sorbie KS, Skauge A. Can network modelling predict two-phase flow functions? . Paper SCA2011-29, Society of Core Analysts Symposium; 2011. A thought-provoking paper that discusses the limitations of pore-network simulations to truly predict relative permeability and capillary pressure curves without experimental data.
[83] Tartakovsky AM. Langevin model for reactive transport in porous media. Phys Rev E 2010;82(2):026302. The paper extends a previously developed Langevin model to include chemical reactions and simulate mixing-controlled reactions in heterogeneous porous media. The model is able to predict the mass of the reaction product more accurately compared to conventional modelling approaches.
[84] Tartakovsky AM, Tartakovsky DM, Meakin P. Stochastic Langevin model for flow and transport in porous media. Phys Rev Lett 2008;101(4):044502. The paper describes, for the first time, a stochastic Langeving model, solved via smooth particle hydrodynamics, to accurately model advective and diffusive transport processes in heterogeneous porous media. This allows to account correctly for mixing due to diffusion and dispersion.
[85] Thomas SG, Wheeler MF. Enhanced velocity mixed finite element methods for modeling coupled flow and transport on non-matching multiblock grids analysis and applications to transport of reactive species in multiphase flow through porous media. Comput Geosci 2011;15(4):605–25. The paper discusses a flux-continous discretisation approach that differes from classical finite-volume based models but is readily capable of modelling multi-phase multi-component transport processes on complex geological grids.
[86] Thömmes G, Becker J, Junk M, Vaikuntam A, Kehrwald D, Klar A, et al. A Lattice Boltzmann method for immiscible multiphase flow simulations using the level set method. J Comput Phys 2009;228(4):1139–56. The paper proposes to combine lattice Boltzmann and level-set methods to increase the computational efficiency of two-phase LB calculations and to deal with arbitrary viscosity and density ratios.
[87] Tsakiroglou CD. A multi-scale approach to model two-phase flow in heterogeneous porous media. Transp Porous Media in press. doi:10.1007/s11242-011-9882-y
[88] Tsang Y, Birkholzer JT, Mukhopadhyay S. Modeling of thermally driven hydrological processes in partially saturated fractured rock. Rev Geophys 2009;47:RG3004.
[89] Tyagi M, Jenny P. Probability density function modeling of multi-phase flow in porous media with density-driven gravity currents. Transp Porous Media 2011;87(2):603–23.
[90] Tyagi M, Jenny P, Lunati I, Tchelepi HA. A Lagrangian, stochastic modeling framework for multi-phase flow in porous media. J Comput Phys 2008;227:6696–714. The paper develops a computationally efficient stochastic particle method combined with a classical finite volume approach to model small-scale fluctuations and uncertainties in the residual trapping of CO_2 in heterogeneous geological formations.
[91] Wu K, Jian Z, Ma J, Couples GD, van Dijke MIJ, Sorbie KS. Multiscale pore system reconstruction and integration. Paper SCA2011-36, Society of Core Analysts Symposium; 2011. The paper shows that if two pore-networks, representing micro and macro pores, are combined, the resulting permeability cannot be modelled by averaging the respective permeabilities of the two networks.
[92] Zaretskiy Y, Geiger S, Sorbie KS. Direct numerical simulation of pore-scale reactive transport: applications to wettability alteration during two-phase flow. Int J Oil Gas Coal Technol (in press).
[93] Zaretskiy Y, Geiger S, Sorbie KS, Förster M. Efficient flow and transport simulations in reconstructed 3D pore geometries. Adv Water Resour 2010;33(12): 1508–16. The paper introduces the first computationally efficient finite element – finite volume based simulation algorithm for unstructured grids to model transport processes directly on realistic pore-scale images.
[94] Zeidouni M, Pooladi-Darvish M, Keith D. Analytical solution to evaluate salt precipitation during CO_2 injection in saline aquifers. Int J Greenhouse Gas Control 2009;3(5):600–11.