On the use of Darcy's law and invasion-percolation approaches for modeling large-scale geologic carbon sequestration

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Abstract

Most large-scale flow and transport simulations for geologic carbon sequestration (GCS) applications are carried out using simulators that solve flow equations arising from Darcy's law. Recently, the computational advantages of invasion-percolation (IP) modeling approaches have been presented. We show that both the Darcy's-law- and the gravity-capillary balance solved by IP approaches can be derived from the same multiphase continuum momentum equation. More specifically, Darcy's law arises from assuming creeping flow with no viscous momentum transfer to stationary solid grains, while it is assumed in the IP approach that gravity and capillarity are the dominant driving forces in a quasi-static two-phase (or more) system. There is a long history of use of Darcy's law for large-scale GCS simulation. However, simulations based on Darcy's law commonly include significant numerical dispersion as users employ large grid blocks to keep run times practical. In contrast, the computational simplicity of IP approaches allows large-scale models to honor fine-scale hydrostratigraphic details of the storage formation which makes these IP models suitable for analyzing the impact of small-scale heterogeneities on flow. However, the lack of time-dependence in the IP models is a significant disadvantage, while the ability of Darcy's law to simulate a range of flows from single-phase- and pressure-gradient-driven flows to buoyant multiphase gravity-capillary flow is a significant advantage. We believe on balance that Darcy's law simulations should be the preferred approach to large-scale GCS simulations.

Introduction

Modeling and simulation are essential tools for the design and performance prediction of geologic carbon sequestration (GCS) sites. GCS relies heavily on modeling and simulation because each site has its own unique and site-specific characteristics that need to be evaluated, thereby diminishing the value of prior performance data from other sites. In addition, there simply are not yet very many CO_2 injection sites around the world from which observations of GCS processes can be gathered.

As tools for design and performance, it is essential that large-scale GCS simulations be accurate and defensible. First, policymakers need to objectively evaluate whether GCS is an affordable, technically feasible, and safe way to mitigate growing greenhouse gas (GHG) emissions. Second, industry needs to be able to economically design and operate GCS sites. At the same time, regulatory bodies need to ensure safety and evaluate performance to analyze environmental hazards and risks of GCS. Challenges in modeling large-scale GCS include inherent uncertainty about the deep subsurface, the critical importance to failure likelihood that can arise from a few small-scale features (e.g. fractures in cap rock) over large spatial scales, and the importance of modeling performance over very long time scales, on the order of thousands of years or more.

State-of-the-art simulation work in GCS site design and performance prediction makes use of reservoir simulation approaches that have been developed and applied over the last 50 years in the oil and gas industry[1] and for water resources studies.[2] The approaches for simulating the flow of two or more phases (e.g., supercritical CO_2, brine, and/or hydrocarbon fluids) are based on well-established multi-phase versions of Darcy's law. In GCS, active modeling and simulation groups from around the world have compared simulation results for test problems using different, and sometimes the same, numerical simulation codes.[3-7] Results of these studies have increased confidence in the ability of suitably trained and qualified users to produce defensible modeling results of large-scale GCS processes.

Recently, the advantages of invasion-percolation (IP) modeling have been presented in the literature.[8-12] The advantages of IP modeling come from the simplifications in the CO_2-brine flow equations arising from neglect of pressure-gradient-driven flow. IP instead considers only the balance between capillary forces and buoyancy. This simplification is defensible for CO_2-brine flow at distances far away from the injection well where pressure gradients no longer drive the flow, or at long times following the cessation of injection. The value of the simplification is that it vastly lowers computational demand and thereby allows much higher spatial resolution in numerical grids relative to grids that are practical for solving flow and transport problems using approaches based on Darcy's law. As such, IP modeling allows the use of large-scale flow domains that resolve relatively small-scale features like fracture zones and faults. But the simplification comes with certain costs, most significant among which are the loss of formal dynamics, i.e., a way of measuring how long the migration process takes.

In this paper, we review both Darcy's law and IP approaches with an emphasis on clarifying their advantages and disadvantages for simulating large-scale GCS. We start with a derivation of both Darcy's law and the IP approach from the continuum momentum equation for two fluid phases mixed with a solid phase. This presentation makes it clear which terms are accounted for and

which are neglected in the two approaches. Following the mathematical equation development, we present two sections focused on the use, advantages, and disadvantages of the two approaches for modeling CO_2 flow and transport in GCS applications. Along the way, we review both Darcy's law and IP approaches but the emphasis of the paper is on clarifying the advantages and disadvantages of the two approaches for modeling large-scale GCS rather than comprehensive review of the literature on Darcy's law and IP approaches.

Momentum equation

The starting point for the comparison of Darcy's law to IP approaches for modeling CO_2migration in deep geologic formations is the time-dependent continuum momentum equation in Cartesian coordinates applicable to a mixture containing two fluid phases and one solid phase,

(i) (ii) (iii) (iv) (v) (vi) (vii) (viii)

$$\rho_\beta \frac{Du_\beta}{Dt} = -\nabla P_\beta + \mu_\beta \nabla^2 u_\beta - \rho_\beta g\mathbf{k} - \mu_\beta \phi S_\beta \left[\frac{1}{k_{s\beta}} \left(\frac{u_\beta}{\phi S_\beta} - u_s \right) + \frac{1}{k_{nw}} \left(\frac{u_\beta}{\phi S_\beta} - \frac{u_{\alpha,\alpha\neq\beta}}{\phi(1-S_\beta)} \right) \right]$$

Inertia | Pressure gradient | Viscous dissipation | Gravity body force | Fluid-solid stress | Fluid-fluid stress

(1)

where $\beta = w, n$ are the wetting (w, aqueous or water) and non-wetting (n, CO_2) phases, and s is the solid phase (matrix grains in the porous medium). The left-hand side (i) and first three terms (ii – iv) on the right-hand side are the standard total derivative, which includes the inertial terms, the pressure gradient, viscous stress, and gravitational body force terms.[13] The fluid-solid interphase stress term is after Bennon and Incropera,[14] and the fluid-fluid interphase stress is after Brutsaert and El-Kadi.[15] The applicable coordinate system **i**, **j**, **k**, with g positive downward, and **k** pointing upward is shown in Fig. 1, along with a sketch of the multiphase system consisting of solid grains (gray), aqueous wetting phase (light blue), and CO_2 non-wetting phase (white).

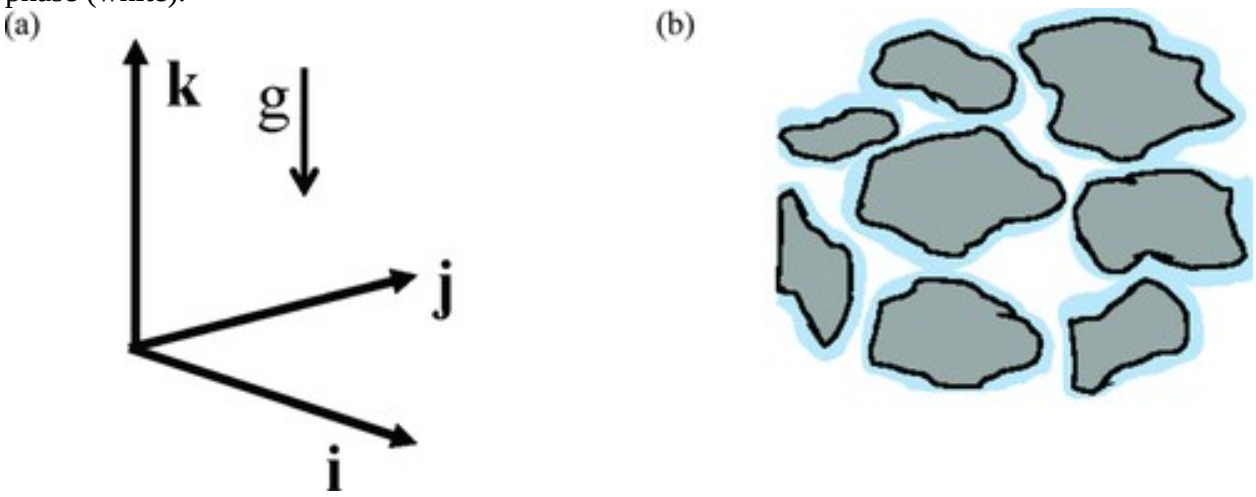

Figure 1
Open in figure viewerPowerPoint

(a) Coordinate system for the multiphase flow system, and (b) sketch of the phases where light blue is the wetting phase (w) and white is the non-wetting phase (n), and dark gray is the solid phase (s).
Caption

For the wetting phase, capillary pressure acts to reduce effective driving force by the effects of interfacial tension (γ) relative to the non-wetting phase. The effects of capillary pressure in porous media can be represented by the equation

$$P_w = P' - P_{cap} \quad (2)$$

where in two-phase conditions, the reference pressure (P') is the non-wetting-phase pressure, i.e.,

$$P_n = P' \quad (3)$$

Considering only the wetting phase, $\beta = w$, we have

$$\rho_w \frac{Du_w}{Dt} = -\nabla P' + \nabla P_{cap} + \mu_w \nabla^2 u_w - \rho_w g\mathbf{k}$$
$$-\mu_w \phi S_w \left[\frac{1}{k_w}\left(\frac{u_w}{\phi S_w} - u_s \right) + \frac{1}{k_{wn}}\left(\frac{u_w}{\phi S_w} - \frac{u_n}{\phi(1-S_w)} \right) \right] \quad (4)$$

We note as an aside that Eqn 4 was used by Oldenburg and Spera16 for a single-fluid phase (silicate melt) and its solidifying/melting crystals by omitting the capillary pressure and fluid-fluid stress term, while including the entrainment or crystal-locking behavior of solidified melt through the application of an *arctan* function to turn on/off the fluid-solid stress (Darcy flow) term depending on the fraction of solid, *fs* (*fs* = 1-φ).

Introducing the following scaling factors for converting the parameters into dimensionless forms,

$$\hat{\nabla} = L\nabla, \quad \hat{\nabla}^2 = L^2\nabla, \quad \hat{u}_w = \frac{u_w}{V_w}, \quad \hat{t} = t\frac{V}{L},$$
$$\hat{P} = \frac{P'L}{\mu_w V_w}, \quad \hat{P}_{cap} = \frac{P_{cap}L}{\gamma_0} \quad (5)$$

where L is a characteristic length scale that may vary for different processes, V is a characteristic velocity, and γ_0 is the surface tension of water in contact with CO_2, and omitting the analogous dimensionless form of the non-wetting phase for brevity, we can write Eqn 4 as

$$\frac{\rho_\beta V^2}{L}\frac{D\hat{u}_w}{D\hat{t}} = -\frac{\mu_w V}{L^2}\hat{\nabla}\hat{P}' + \frac{\gamma_0}{L^2}\hat{\nabla}\hat{P}_{cap} + \frac{\mu_w V}{L^2}\hat{\nabla}^2\hat{u}_w - \rho_w g\mathbf{k}$$
$$-\mu_w\phi S_w V\left[\frac{1}{k_w}\left(\frac{\hat{u}_w}{\phi S_w} - \hat{u}_s\right) + \frac{1}{k_{wn}}\left(\frac{\hat{u}_w}{\phi S_w} - \frac{\hat{u}_n}{\phi(1-S_w)}\right)\right] \quad (6)$$

Multiplying through by $L^2/(\mu_w V)$, we obtain

$$\frac{\rho_w L V}{\mu_w}\frac{D\hat{u}_w}{D\hat{t}} = -\hat{\nabla}\hat{P}' + \frac{\gamma_0}{\mu_w V}\hat{\nabla}\hat{P}_{cap} + \hat{\nabla}^2\hat{u}_w - \frac{\rho_w L^2}{\mu_w V}g\mathbf{k}$$
$$-\phi S_w L^2\left[\frac{1}{k_w}\left(\frac{\hat{u}_w}{\phi S_w} - \hat{u}_s\right) + \frac{1}{k_{wn}}\left(\frac{\hat{u}_w}{\phi S_w} - \frac{\hat{u}_n}{\phi(1-S_w)}\right)\right] \quad (7)$$

Defining the Reynolds, Richardson, Capillary, and Darcy numbers, respectively, as follows,

$$\mathrm{Re} = \frac{\rho_w L V}{\mu_w}, \quad \mathrm{Ri} = \frac{gL}{V^2}, \quad \mathrm{Ca} = \frac{\mu_w V}{\gamma_0}, \quad \mathrm{Da} = \frac{k_0}{L^2} \quad (8)$$

we have for the wetting phase, $\beta = w$, the final general dimensionless equation:

$$\mathrm{Re}\frac{D\hat{u}_w}{D\hat{t}} = -\hat{\nabla}\hat{P}' + \frac{1}{\mathrm{Ca}}\hat{\nabla}\hat{P}_{cap} + \hat{\nabla}^2\hat{u}_w - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k}$$
$$-\frac{1}{\mathrm{Da}}\left[\frac{k_0}{k_w}\left(\hat{u}_w - \hat{u}_s\phi S_w\right) + \frac{k_0}{k_{wn}}\left(\hat{u}_w - \frac{\hat{u}_n\phi S_w}{\phi(1-S_w)}\right)\right] \quad (9)$$

Equation 9 is the full continuum dimensionless momentum equation for the wetting phase of an incompressible two-phase fluid-solid mixture in which the solid may have motion relative to the fluids, move identically with the fluid (fully suspended), or be stationary (rigid solid matrix). Different flow scenarios can be described by Eqn 9 by the values of the four dimensionless numbers, Re, Ri, Ca, and Da.

By comparing various end-member flow scenarios, familiar limiting forms of the full momentum equation can be derived. For example, assuming a single-phase ($\beta = w$) high-velocity and constant-viscosity flow of suspended solid grains with no interphase mass transport, we obtain the dimensionless Navier-Stokes (NS) equation for the mixture

$$\mathrm{Re}\frac{D\hat{u}_\beta}{D\hat{t}} = -\hat{\nabla}\hat{P}_\beta + \hat{\nabla}^2\hat{u}_\beta - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} \quad (10)$$

which upon re-dimensionalization becomes

$$\rho_\beta \frac{Du_\beta}{Dt} = -\nabla P_\beta + \mu_\beta \nabla^2 u_\beta - \rho_\beta g\mathbf{k} \quad (11)$$

Derivations of Darcy's law and the gravity-capillary balance equation

Darcy's law

Assuming steady-state flow and a single-phase ($P = P'$, $\beta = w$) where the flow is creeping (no inertial effects), low permeability, and a stationary solid matrix, Eqn 9 becomes

$$0 = -\hat{\nabla}\hat{P} - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} - \frac{1}{\mathrm{Da}}\hat{u}_\beta \quad (12)$$

which upon rearrangement and re-dimensionalization becomes the familiar form of Darcy's law for a single-phase fluid, $\beta = w$,

$$\frac{1}{\mathrm{Da}}\hat{u}_\beta = -\hat{\nabla}\hat{P}_\beta - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} \quad (13)$$

$$u_\beta = -\frac{k_0}{\mu_\beta}\left(\nabla P_\beta + \rho_\beta g\mathbf{k}\right) \quad (14)$$

Assuming creeping two-phase flow in low-permeability media in which friction forces from the rigid solid grains of the matrix dominate over interphase friction, we have for the wetting phase

$$0 = -\hat{\nabla}\hat{P}' + \frac{1}{\mathrm{Ca}}\hat{\nabla}\hat{P}_{cap} - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} - \frac{1}{\mathrm{Da}}\frac{k_0}{k_w}\hat{u}_w \quad (15)$$

Pressure gradient | P_{cap} gradient | gravity body force | Darcy flow

Re-dimensionalizing Eqn 15, we obtain Darcy's law for two-phase flow:

$$u_\beta = -\frac{k_\beta}{\mu_\beta}\left[\nabla\left(P_\beta + P_{cap,\,\beta\neq n}\right) + \rho_\beta g\mathbf{k}\right] \quad (16)$$

Where k_β is the effective permeability of phase β in the formation which equals the product of the absolute permeability and the relative permeability.

Gravity-capillary balance

Considering creeping two-phase flow in low-permeability media where the capillary forces completely dominate over dynamic pressure, i.e., very low Ca, Eqn 9 can be written

$$0 = -\hat{\nabla}\hat{P}' + \frac{1}{\mathrm{Ca}}\hat{\nabla}\hat{P}_{cap} - \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} - \frac{1}{\mathrm{Da}}\frac{k_0}{k_w}\hat{u}_w \quad (17)$$

Now if we also assume that migration is very slow (i.e., $u \sim 0$), we obtain

$$-\hat{\nabla}\hat{P}' + \frac{1}{\mathrm{Ca}}\hat{\nabla}\hat{P}_{cap} = \mathrm{Re}\,\mathrm{Ri}\,\mathbf{k} \quad (18)$$

Upon re-dimensionalization, the equations for wetting and non-wetting fluid phases become, respectively

$$\begin{aligned} -\nabla P' + \nabla P_{cap} &= \rho_w g\,\mathbf{k} \\ -\nabla P' &= \rho_n g\,\mathbf{k} \end{aligned} \quad (19)$$

Subtracting the non-wetting phase flow equation from the wetting one, we obtain

$$\nabla P_{cap} = (\rho_w - \rho_n) g\mathbf{k} \quad (20)$$

IP modeling of Eqn 20 assumes a steady-state equilibrium between capillary pressure gradient and buoyancy driving force as can be inferred from the lack of any time-dependent term. The key control in Eqn 20 is the saturation-dependent capillary exclusion process that prevents non-wetting phase from entering pores of a certain size below which the capillary entry pressure is not exceeded for the given buoyancy driving force. In IP modeling, the spatial discretization sets a length scale over which sequential steps of CO_2-water redistribution under gravity-capillary equilibration are carried out, the result of which is an apparent migration of fluid phases, if conditions of capillary entry are satisfied. A review and discussion of IP modeling in GCS will be presented below following discussion of the use of Darcy's law in GCS.

Darcy's law in GCS

Introduction

The large number of successful GCS numerical reservoir simulation applications using equations similar to Eqn 6 precludes even a cursory review here, but we note the review paper by Schnaar and DiGiulio[17] which documented existing simulation studies up to 2008, and Birkholzer *et al*.[18] who provided a review of the ten years between 2005 and 2015. A recent benchmark of the state-of-the-art is the work by Senel *et al*.[19] who modeled the Midwest Geologic Sequestration

Consortium (MGSC) injection in Illinois.[20] As the cited review articles confirm, the multiphase version of Darcy's law (Eqn 16) is the flow equation most often solved by large-scale reservoir simulators such as TOUGH2.[21, 22] To simulate heat and mass transfer, the flow equation needs to be coupled to a thermal energy equation for heat transfer, and to various advective-diffusive transport equations (ADTE) for chemical component mass transfer. Between the time-dependence of the ADTE and the fluid velocity which couples Darcy's law with the ADTE, the partial differential equations (PDEs) that are solved numerically in reservoir simulators are transient and faithfully model the time-dependence of flow and transport processes. Numerical solution of the transient coupled PDEs for Darcy flow and coupled heat and/or mass transport is computationally demanding relative to IP approaches which are based on simple saturation-capillary pressure comparisons on a lattice at a series of time-free steps.

Darcy's law is also the basis for numerous analytical and semi-analytical solutions of CO_2migration that take advantage of various simplifications to permit analytical solutions. Reviews of these analytical and semi-analytical solutions can be found in Celia and Nordbotten,[23]Birkholzer *et al.*,[18] and Mukhopadhyay.[24] These analytical and semi-analytical approaches permit practical estimation of CO_2 plume migration without the need for supercomputers or large-scale simulation software.

Limitations of Darcy's law

The form of Darcy's law given by Eqn 16 is applicable to a wide range of porous media flow scenarios, but not to all porous media flow scenarios. For example, in the above derivation of Eqn 16 we specified creeping flow to justify exclusion of inertial terms, and we assumed the largest resistance to flow was from the fluid-solid friction. To handle porous media flow scenarios in which these conditions are not strictly met, ad hoc additions to Darcy's law have been developed. For example, in some flow problems, such as near an injecting or producing well, the fluid velocity can be much larger than appropriate for creeping flow. This has led to additions to Eqn 16 referred to as Forchheimer terms[25] that add back in inertial effects. Another addition to Eqn 16 is the Brinkman term[26] which involves essentially adding back in the viscous term of Eqn 9 that was excluded in the derivation of Eqn 16 by the assumption that the averaging volume is larger than the pore size so that resistance to flow can be parameterized by permeability. The Brinkman term allows momentum transfer (e.g., viscous drag) from the fluid to the solid grains of the matrix, such as might be relevant in the gap between the sandpack in a laboratory flow column and the column wall. It is important to note that retaining the appropriate terms already present in Eqn 9 is preferred if one needs to solve problems outside of the range of assumptions of Eqn 16 rather than adding terms to the reduced Eqn 16. But the ad hoc approach

has been a natural historical development given that Darcy's law was developed empirically from flow experiments under creeping flow conditions rather than mathematically from the continuum momentum equation.

In theory, Darcy's law can describe the physics of pressure-gradient and capillary-pressure-driven flow for single-phase and multiphase flows. In practice, however, the computational demands of Darcy's law coupled with ADTE lead many modelers to use large cell sizes relative to the length scales of the processes being modeled, i.e., to under-resolve their flow domains. This often leads to excessive numerical dispersion, resulting in erroneous estimates of the plume shape and its extent. In addition, modelers often apply relationships (such as capillary-pressure and relative permeability functions) calibrated at the laboratory scale to the much larger grid-block scale of their discretized domain. By doing so, they are often inadvertently applying inaccurate and overly dispersive model equations to their flow and transport problems.

Strengths of Darcy's law

Darcy's law for single-phase flow is a simple flow equation in which the flow rate is linear with the pressure gradient and body force terms, as opposed to the non-linear flow described by the full momentum equation (Eqn 9). This is a huge advantage from an algorithmic and computational point of view. In contrast, single-phase flow of air in a building or water in a stream requires solving the highly non-linear NS equation (Eqn 11). The difficult non-linearity in porous media flow arises when two (or more) phases are present and the permeability of each phase is a function of the saturation of the other phase. Nevertheless, generally speaking, even the multiphase version of Darcy's law is not particularly computationally demanding (e.g., relative to turbulent flow) and numerical reservoir simulators based on Darcy's law have been used extensively in the oil industry since the mid-1960s and throughout subsurface applications in hydrology, nuclear waste disposal, and geothermal energy ever since. Darcy's law models gravitational instability and resulting buoyant plumes and “thermals”[27] as widely demonstrated in GCS applications.[28-30] Significant research has been carried out for GCS using Darcy's law flow models coupled with other process models for geochemical transport and reactions, e.g., TOUGHREACT,[31] and coupled hydro-geomechanical processes, e.g., TOUGH-FLAC.[32]

In Darcy's law, time-dependent fluid velocity is the unknown being solved for as a function of the gradients in the pressure field and buoyancy forces. In addition, time-dependence enters through the control of ADTE that are coupled to Darcy's law through the fluid velocity term. In implicit time-stepping schemes in numerical reservoir simulators such as TOUGH2, which have adaptive time step adjustment capabilities, if temporal changes in the flow velocity become very

small, the time-step size can grow to become very large, making long-time simulations very efficient while the equations remain formally transient.

Invasion-percolation in GCS

Introduction

Knackstedt and Paterson[33] provide an extensive list of applications which involve slow displacement of one fluid by another such as non-aqueous phase liquids into soil and penetration of air into porous materials during drying. GCS in deep saline aquifers also represents an instance of slow displacement of one fluid phase (e.g., the resident brine) by another (the injected CO_2 phase), particularly far away from the injection source. To understand and simulate these slow displacement processes, the concepts of invasion percolation (IP), a term which was first used by Wilkinson and Willemsen,[34] has been often invoked. Extensive literature exists on invasion percolation with applications in porous media.[35-37] Before discussing the strengths and limitations of IP, particularly in the context of GCS modeling, we first provide a brief review of the evolution of the IP algorithm.

The IP algorithm history

As discussed previously, the basic equation that is solved in IP-based flow modeling is Eqn 19. For modeling slow displacement of one fluid by another in a porous medium, which is often conceptualized as a network of sites and bonds,[38-40] IP implementation begins by assuming that all the sites and bonds of the network are filled with a defending fluid. When a second fluid (i.e., the invading fluid) is subsequently injected slowly into the porous medium such that the capillary forces dominate the viscous forces, invasion is controlled by the size of the local pore or throat via the equation

$$P_{cap} = c\frac{\gamma}{r_i} \quad (21)$$

where P_{cap} is the capillary pressure, γ is the interfacial tension, r_i is the size (e.g., radius) of an individual bond (or pore throat) i, and c is a constant. In drainage, where the wetting fluid (WF) is the defending phase and the non-wetting fluid (NWF) is the invading one, it is obvious from Eqn 21 that the capillary forces are maximal at the narrowest of the pore throats. IP in drainage, which is the original version of IP studied by Chandler *et al.*[41] without using the name IP, thus involves a series of discrete jumps across throats in which the NWF displaces the WF via the largest throat, which offers the least resistance to displacement.[33] IP in imbibition, which was first studied by Wilkinson and Willemsen[34] and which involves displacing the NWF slowly with the WF, can be described by a series of discrete jumps in which at each time step the WF advances through the smallest available pore. Algorithms to compute these discrete jumps are

fundamentally different from continuum PDEs such as those for Darcy's law flow and transport that solve for flow variables continuously in space and time. Instead, IP algorithms are based on a time-free series of steps at which comparison is made of adjacent pore sizes to specify where fluid flows during the step, making these algorithms computationally highly efficient.

It will be worthwhile noting a few characteristics of the original IP at this point. For example, IP always starts with a well-defined interface (inlet) and displaces the defending phase in a systematic way until spanning the system. To put it another way, all invaded sites are ultimately connected to each other through the injection source, typically a side (of a two-dimensional lattice) or face (of a three-dimensional lattice) from which the “invasion” spreads. Each individual invasion changes the interface; after each invasion, the new interface is scanned for the site or bond with the least resistance which will be invaded next. There must be a continuous pathway of invaded pores or bonds from the invasion source to the pore or bond under consideration.[42] Another important characteristic of IP is the concept of trapping. Once a cluster of unoccupied pores or bonds is surrounded by occupied pores or bonds, it is “trapped” and the pores or bonds in that cluster cannot be invaded. Thus, once a cluster of pores filled with the WF (for example) is surrounded by the NWF during drainage, the WF cannot escape and the NWF cannot displace it.

IP was originally developed to model two-phase displacements in porous media; however, to be of practical significance and have utility, additional physics needed to be included in the original version. Using a mean field description of fluid flow, Wilkinson[43] extended the original IP to include viscous forces, which was further extended for large and small viscosity ratios by Xu *et al*.[44] For small viscosity ratios, they determined that displacement could be modeled by a form of gradient percolation in a stabilizing gradient, involving a particular percolation probability profile.[33] Displacement with large viscosity ratios, on the other hand, could be described by gradient percolation in a destabilizing gradient; this led to capillary viscous fingering.[33] The original IP model was also subsequently modified to address additional experimental observations, including capillary snap-off, film flow, and mixed wettability issues.[45-47] However, these studies still remain as basic developments and there is no clear path to incorporate coupled effects of capillary, buoyancy, and viscous forces without actually solving for the pressure field.

The most significant change in the original IP model, however, was needed to address the effects of gravity. Gravity was first introduced into the IP algorithm by Wilkinson[36, 43] through the application of a simple linear weighting on the invasion thresholds in the direction of buoyancy. Afterwards, Meakin *et al*.[48] performed a series of computer simulations to investigate IP with a gravity-destabilized gradient. In their conceptualization, they assign each bond a random

threshold of the form $y_i = x_i + gh_i$, where x_i is a random number in the range [0,1], g is a term representing gravitational effects on the fluids, e.g., buoyancy, and h_i is the height of bond i. They concluded that as the gravity term (g) was increased, the displacement pattern became more focused. In other words, fewer bonds needed to be invaded before a spanning cluster was formed. This finding, which is also consistent with the findings of Catalan *et al.*,[49] made IP with gravity (or buoyancy) an attractive algorithm for modeling secondary petroleum migration.

A variation of the IP approach was used by several researchers[50-55] in large domains where each lattice site represents a macroscopic domain defined by local effective properties (i.e., equivalent pore size or equivalent entry pressure, or local capillary pressure-saturation and relative permeability functions). This approach, referred to as the Macroscopic IP (MIP) by some researchers and reviewed by Bandilla *et al.*,[56] has also been used to develop upscaled relationships for the two-phase flow parameters in large computational grid domains with sub-grid scale heterogeneities.[57]

Application of IP to secondary petroleum migration

Secondary petroleum migration is the slow process occurring over geologic timescales where petroleum migrates from the source rocks where it is formed into structural or stratigraphic traps. Summarizing from Carruthers,[58] in secondary petroleum migration, the driving buoyancy force originates from the density contrast between the petroleum phase and the formation waters. Where the buoyancy force exceeds the capillary force, the system is said to be out of capillary equilibrium, or gravity destabilized, and migration of petroleum occurs. According to Berg,[59] for this migration to occur, a critical column height z_c is required, which can be defined as

$$z_c = \frac{2\gamma\left(\frac{1}{r_t} - \frac{1}{r_p}\right)}{g\left(\rho_w - \rho_0\right)} \quad (22)$$

where r_t and r_p are the pore throat radius of the caprock and reservoir rock, respectively, and ρ_w and ρ_o are the densities of the water and petroleum phases, respectively. As long as the buoyancy force is lower than the capillary force, petroleum remains trapped at a pore throat. However, as additional petroleum becomes available, the length of the ganglia increases through coalescence to the point where the critical height is reached, and migration occurs.[58-60] Berg[59] therefore concluded that petroleum would migrate as a discrete separate phase (as “stringers”), whose trajectory could be predicted, provided that sufficient information was available regarding the capillary entry pressure distribution of the host reservoir. Note that several experimental investigations have supported this capillary-dominated stringer-like migration of petroleum (see Carruthers[58] and references therein).

Because of the discrete characteristics of the migration process, Carruthers[58] showed that it is possible to model secondary petroleum migration using the modified IP algorithms discussed earlier. The immediate advantage of adopting the IP approach is that one does not have to perform a full two-phase flow simulation based on Darcy's law, which makes it an attractive choice computationally. Note that, while accepting IP as a reasonable choice for modeling secondary petroleum migration, Carruthers[58, 61] also pointed out two significant limitations of the traditional IP scheme. First, traditional IP models, which assume that the invading phase is in constant pressure communication, are only applicable to small systems, and are not really applicable in cases where there exist vertical or lateral dimensions of a few kilometers. Second, IP models assume that the invading phase originates from a single source. For a “real” petroleum system, where petroleum is being sourced from many concurrent source points and areas, this is a severe limitation. The first limitation was alleviated by including the mechanism of capillary snap-off in the IP algorithm, which was based on the assumption that pressure communication existed within the petroleum phase only when the saturations were greater than the critical saturation. The second limitation was eliminated by allowing concurrent development and coalescing of invasion clusters.[61] These modifications of the IP algorithm allowed researchers[43, 46, 47, 58, 61, 62] to simulate one-phase constant composition petroleum flow in models containing tens of millions of grid cells in a matter of minutes, while honoring dominant mechanics of secondary migration.

Note that Pegaz-Fiornet *et al*.[63] did a comparison of different approaches available for basin-scale secondary and tertiary hydrocarbon migration. They observed that simulations based on Darcy's law, even though they were numerically difficult and therefore time consuming, were indeed appropriate for slow hydrocarbon movement and were able to provide a good description of cap-rock leakage. The IP-based simulations, while quick and especially useful in modeling secondary migration, did not have the capability for predicting the timing of trap-filling. Pegez-Fiornet *et al*.[63] finally concluded that IP-based approaches, which are built around capillary-gravity equilibrium and completely ignore the viscous terms in the momentum equation, may not be fully adequate for basin-scale hydrocarbon migration.

Application of Invasion Percolation in GCS migration modeling

The partial success of IP in enabling high-resolution basin-scale secondary petroleum migration modeling has prompted some researchers to use it in the context of GCS modeling, more specifically for modeling the slow flow of a buoyant CO_2 phase under the cap rock in a saline aquifer over many years. Most of these research efforts[8, 64, 10, 12] have been directed towards understanding and replicating the rapid ascension of the buoyant CO_2 plume through eight thin

shale barriers within the Utsira Formation, offshore Norway, in the Sleipner CO_2capture and storage project, in which more than 14 Mt of supercritical CO_2 has been injected between 1996 and 2013.[12, 65] Based on repeat seismic surveys at the Sleipner site, it has been estimated that the injected CO_2 plume has ascended more than 200 m from the injection point (1012 m below sea level, mbsl) within the Utsira Formation to the sealing cap rock (at 800 mbsl) in the three-year period 1996–1999. It has also been suggested that the plume has encountered and breached eight shale baffles within the storage site. Because of these shale barriers, the plume exists in nine vertically stacked layers, with each layer being approximately 10–20 m thick, and extends laterally for hundreds of meters (see Cavanagh and Haszeldine[12]and references therein).

One reason for the rapid ascension of the CO_2 plume at Sleipner can be the storage formation's relatively shallow depth, which results in a stronger than expected density differential between the brine and CO_2 phases. However, as has been suggested by the above-cited researchers, strong density differential alone cannot explain the plume behavior at the Sleipner site, and there are other finer aspects of the plume that remain unexplained.[12] Singh *et al*.,[8] Cavanagh,[64] and Cavanagh and Haszeldine[12] hypothesize that the vertical stacking of the CO_2 plume at the Sleipner site is the result of “buoyant gas percolating through the vertical heterogeneity of sandstones and shales found in the Utsira Formation, in a manner similar to hydrocarbon migration.” Based on the estimated speeds of 2 and 10 μm/s vertically and horizontally, respectively, which result in $Ca < 10^{-7}$ for the CO_2 plume at Sleipner, these researchers argue that CO_2 flow is completely dominated by buoyancy and capillary forces, and it can be captured by IP algorithms with unprecedented spatial resolution.

As mentioned in Cavanagh and Haszeldine,[12] previous attempts[66-68] at replicating the vertical stacking of the CO_2 plume using Darcy's-law-based simulators have not been successful, even after these Darcy's law models have “imposed discrete vertical pathways to bypass the thin shale layers or assumed a convenient juxtaposition of pre-existing holes for the eight intra-formational shale barriers.”[12] Additionally, Cavanagh[64] and Cavanagh *et al*.[65]performed a benchmark study of the Sleipner CO_2 plume behavior using both an IP-based migration model and a Darcy's-law-based flow model. The IP model, according to Cavanagh,[64]while not yielding a perfect match to observed plume behavior, gave a better approximation of the CO_2 distribution beneath the cap rock and replicated the unusual morphology of the uppermost shale layer, which was strongly influenced by the cap-rock topography. The Darcy's-law-based simulations, on the other hand, again according to Cavanagh,[64] was insensitive to cap-rock topography and developed a cone-shaped radial/sub-elliptical CO_2distribution, in contrast to the vertically stacked plume profile observed in the seismic surveys. Cavanagh[64] and Cavanagh *et al*.[65] opined that this was

“primarily a result of a strong pressure artifact associated with injection” which happens because of the Darcy's-law dependence on a pressure gradient to model flow in permeable media. Note that, while the IP-based models gave a reasonable approximation to CO_2 migration patterns at Sleipner in the early years (1999–2002), subsequent (2004–2008) comparisons were less satisfactory, mostly because of insufficient data for accurate representation of spatial heterogeneities.[64] Cavanagh *et al.*[65]concluded that Darcy's law reservoir simulations gave a better match to observations than IP when the decay of injection pressure was included, indicating the plume migration was dynamic and therefore slightly different from the quasi-static IP result.

Limitations of Invasion Percolation in GCS modeling

While it is encouraging to note that suitably modified IP algorithms can reasonably replicate the CO_2 plume behavior beneath the cap rock at Sleipner, we believe some caution needs to be exercised before making conclusions regarding IP’s applicability for CO_2 flow and transport modeling in saline aquifers or inadequacies of Darcy's-law-based flow simulators for the same purpose. It is apparent that, even after noting its limitations in predicting the timing of trap-filling effects,[63] IP or revised IP models may be useful for basin-scale secondary petroleum migration modeling in cases in which the flow regime is governed by buoyancy and capillary forces (i.e., viscous forces are not dominant effects) from the source to the trapping locations. At the same time, we note that CO_2 flow and transport modeling in the context of GCS involves active injection and therefore is a mixed flow regime problem with the viscous forces controlling the flow behavior near the injection well locations and during active injection periods. On the other hand, the capillary forces control the flow behavior at locations farther away from the injection locations and during the post-injection time frames, under which circumstances the viscous forces play a diminishing role. It is difficult to know in the formation where or when the flow crosses over from the viscous regime to the capillary regime. While Darcy's-law-based modeling can still be used in both flow regimes (though improvements may be warranted), IP-based migration modeling cannot be applied in the viscous flow regime at all, i.e., such an approach addresses only a subset of the entire modeling challenge associated with GCS.

As for the ubiquitous gravitationally unstable configuration of GCS, e.g., where less-dense CO_2underlies denser brine, IP models this by honoring the gravity-capillary balance. However, the flows produced are not classic natural convective flows as governed by the porous medium Rayleigh number[69] which includes viscous effects. Similarly in the shallow subsurface above the water table where CO_2 is gravitationally stable, IP can model CO_2 migration but only in the

limiting case of no viscous or pressure-gradient driving forces, whereas Darcy's law has been shown to match field experiments involving such flows very well.[70]

Discussion

As discussed above, Darcy's law and IP formulations each have their ranges of applicability and advantages and disadvantages in modeling large-scale GCS. Figure 2 shows a sketch of a hypothetical GCS reservoir during injection, with a dry-out zone, which is a single-phase CO_2region extending a short distance from the well, followed by an extensive two-phase region and a fully aqueous-phase brine region. As shown, the IP approach is most applicable to the far-field where gravity and capillarity dominate the flow. On the other hand, Darcy's law is applicable over nearly the entire domain, save perhaps for the region of vigorous flow right up against the well where inertia effects may be most significant (i.e., the creeping flow assumption is not valid). Some authors have stated that the Darcy flow approximation breaks down at low fluid flow rates when the viscous resistance is negligible.[8] These same authors stated that grid resolution limitations when solving Darcy's law have led some researchers to neglect capillary pressure. We are not aware of any evidence supporting these statements. The fact is that Darcy's law is the de facto standard for solving classical creeping flow through porous media, including capillary pressure and gravity effects.

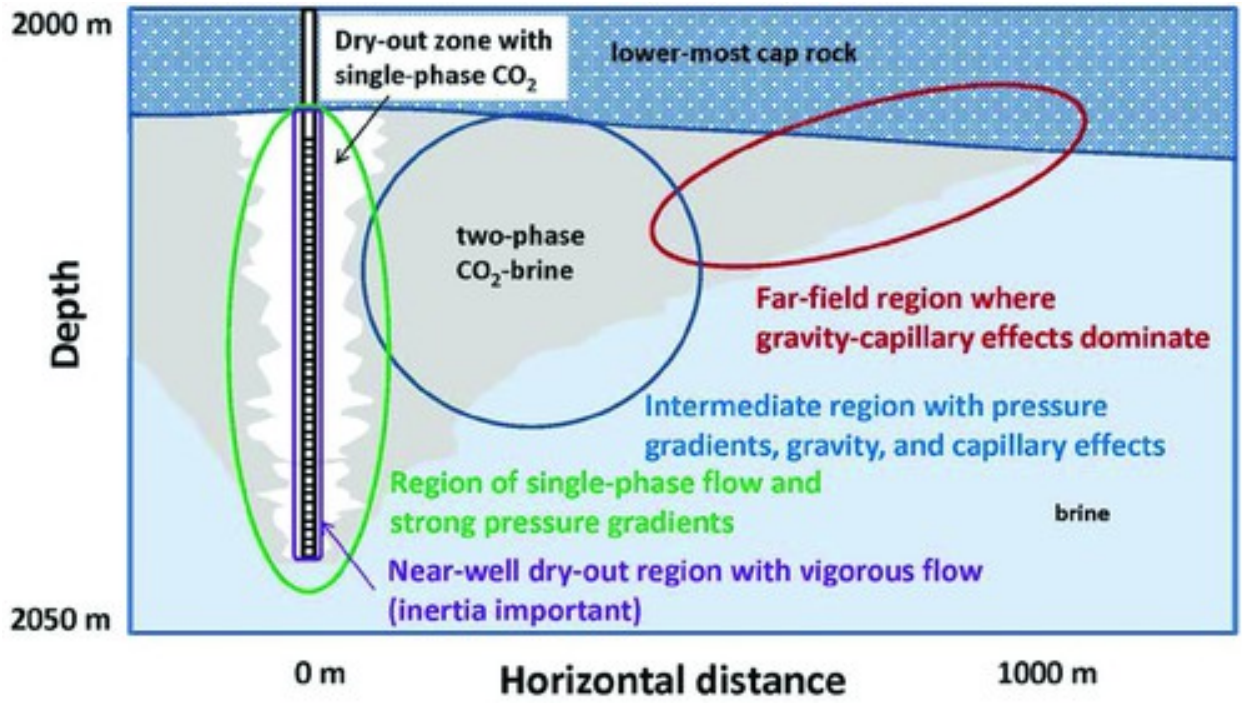

Figure 2
Open in figure viewerPowerPoint

Sketch of CO_2 injection into a hypothetical GCS reservoir with near-well dry-out zone, single-phase region, large two-phase region, and single-phase brine region. While Darcy's law is applicable throughout most of the domain except in the region nearest to the well-bore, IP is applicable only in the far-field region and even there lacks time-dependence.
Caption

The primary challenges associated with using Darcy's-law-based simulations for GCS modeling are practical challenges related to computational demand. Theoretically, if one could use a numerical mesh with infinitely small grid-block sizes, and one could populate these grid-blocks with rock and rock-fluid interaction properties at that scale, there is nothing in Darcy's law itself that would make it inappropriate for GCS modeling, except in the immediate vicinity of the injection wells. And this approach would be valid even in the post-injection capillarity-controlled quasi-static regime, granted that it would require a long time to complete the simulations, especially when hysteresis in constitutive models is included. The combined result of the lack of spatial resolution and improper upscaling of rock properties has been that Darcy's-law-based simulations often generate unsatisfactory results, even though the law itself is rooted in well-understood physics (see derivation of Eqn 16).

The challenge with IP-based migration models, on the other hand, is that of over-simplification of the underlying physics of flow to gain a computational advantage. Broadly speaking, within the domain of fluid displacement in porous media, the IP-based models belong to the “quasi-static” model group, where the pores and throats change their configurations one at a time, the ordering of which is controlled by capillary forces and the flow rate is infinitesimally low. There are several circumstances where the approximation of quasi-static displacement and its implementation through IP or similar algorithms is not valid. Al-Gharbi71 provides several such application areas, including fracture flow where flow rates might be as large as hundreds of meters a day; displacements with very low interfacial tension that substantially reduce capillary forces such as near-miscible gas injection, gas condensate reservoirs, surfactant flooding; near well-bore flow; flow involving polymers, gels and foams where very large pressure gradients are found; and some cases where wetting-layer flow is significant, such as spontaneous wetting into a dry soil.

Even if we restrict ourselves to GCS modeling, there are several limitations to adopting IP-based algorithms. Many GCS sites are highly heterogeneous and likely to include many small- and large-scale fractures plus numerous faults. It is unclear how IP-based models can be used to simulate CO_2 plume migration in such storage formations, where the flow rates in the fractures are likely to be large. Apart from that, IP assumes an immiscible migration of the fluid phases, which is not completely true for supercritical CO_2-brine systems, where the dissolution of the

CO_2 in the brine phase is one of the main mechanisms of storage (i.e., solubility trapping). Note also that the present capability of IP-based models is limited to a situation in which one fluid displaces another under constant pressure-temperature-volume conditions. These assumptions are mostly violated during actual CO_2 injection into a saline aquifer. In addition, it is not clear how IP-based algorithms can be used for reactive transport modeling, which is a critical component of GCS modeling given the importance of mineral trapping as a storage mechanism. While it has been suggested[43] that IP algorithms can be extended to perform compositional modeling because the fluid migration paths are exactly tracked in IP, we are not aware of any research work focused towards IP-based reactive transport modeling for GCS. IP does not include the needed time element for designing GCS projects based on injection duration and rate, or for post-injection site care (PISC), which has strict regulation-based time periods. In addition, insofar as pressure is a primary control parameter for fracturing and induced seismicity, the IP approach cannot be used because it ignores the effects of pressure.

Conclusions

Darcy's law and the IP equation can be derived from the continuum momentum equations considering flow of fluid and solid phases. Both Darcy's law and IP are applicable for certain ranges of properties and processes, while not applicable to others. Briefly, Darcy's law is applicable to creeping flow through porous media. With additional terms such as the Forchheimer or Brinkman terms, or if using the full continuum momentum equation (Eqn 9), it is possible to simulate flows across the continuum from creeping flows through stationary solid grains to vigorous viscous flows of suspended solids. As a significant simplification of the continuum Eqn 9, the IP equation is far more limited. Specifically, IP is applicable to quasi-static flows where gravity and capillary forces dominate. There is no time-dependence or dynamics in the IP equation. There is no pressure-gradient term, viscosity, or entrainment of solids or gases (bubbles). In short, the IP approach has a very narrow region of applicability for situations of very slow migration dominated by buoyancy and capillary forces. The IP approach has proven useful for oil migration problems where the details of timing of processes are not important. In GCS modeling, which often focuses on permanence and leakage processes, the timing and dynamics of the flow process are critical parts of the simulation objective. We present in Table 1 a summary of the strengths and weaknesses of Darcy's law and IP approaches.

Table 1. Summary of degree of capability of Darcy's law and invasion percolation approaches for various large-scale GCS driving forces and processes

Capability Low ○ ● High ●	Darcy's law	Invasion percolation	Comment
Time-dependence, dynamics	●	○	Darcy's law is time-dependent via fluid velocity terms; IP is quasi-static.
Single-phase flow	●	○	IP models capillarity which is not present in single-phase flow
Two- (or more) phase displacement under quasi-steady conditions	●	●	Darcy's law extension to two or more phases is standard simulation practice
Flow near active injection or production well	●	○	IP does not model pressure-gradient driving forces
Flow far from injection well and/or at long times post-injection	●	●	In the limit of gravity-capillary dominance, IP is applicable
Ability to model flow in open fractures	●	○	Limited in Darcy's law but can be addressed with Forchheimer term and/or full continuum momentum equations
Buoyancy-driven flow	●	●	IP models buoyancy-driven flow under capillary-dominated conditions
Viscous resistance to flow	●	○	Attempts have been made to extend IP to include viscous effects[36]
Capillarity	●	●	Capillary pressure gradients are added to fluid pressure gradients in Darcy's law
Inertia	●	○	Forchheimer term adds inertia to Darcy's law
Viscous momentum transfer (e.g., entrainment stress)	●	○	Brinkman term adds viscous momentum transfer to Darcy's law
Mixed wettability	●	●	IP has been extended to include mixed wettability[40]

Because of its greater complexity, Darcy's law requires more computational resources than IP, which leads to coarse grids for Darcy's law simulations and finer grids for IP modeling. Large-scale GCS simulations of CO_2 migration during post-injection periods can be modeled using IP at high spatial resolution. This advantage of IP is tempered by the lack of true time-dependence for the modeled migration process. On balance, we believe Darcy's-law-based simulations are needed for large-scale GCS applications that involve large-scale pressurization (and related induced seismicity hazard), regions of single-phase flow, pressure gradients near wells, and critical interest in time-dependence. Current and future efforts should be dedicated to improving the performance of Darcy's-law-based simulators so that high-resolution large-scale simulations can be carried out over practical time periods using commonly available computer resources.

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Biographies

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