Porosity and Permeability: Literature Review and Summary

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ABSTRACT: Coupled thermal-hydrologic-mechanical-chemical processes are important for salt radioactive waste repositories and other applications. Because mechanical, chemical, and hydrological processes can all have significant impact on transport properties in salt, these processes should be considered when predicting long-term repository performance. Geomechanical simulations predict porosity changes due to strain accumulation, while multiphase flow models require porosity and permeability to redistribute brine and transport solute. Chemical processes can impact both hydrological and geomechanical properties (i.e., porosity, permeability, and surface area), providing further feedback. While porosity and permeability are clearly related, their functional relationship is not simple. For example, the observed porosity-permeability relationship during granular salt reconsolidation is different from the relationship during damage accumulation in intact salt.

Because the mapping from porosity to permeability is non-unique, it is generally conceded there are important hidden constraints or variables needed to predict permeability, which describe the pore space distribution beyond bulk porosity. Tortuosity, specific surface area, hydraulic radius, and percolation length scale have been proposed as possibly contributing to the response of permeability to mechanical and chemical changes. We summarize theoretical considerations and experimental observations on the relation between porosity and permeability. We consider salt-relevant data and constitutive models, but we draw on the wider literature for our summary.

1   Motivation and Definitions

While our subsurface applications are at the macro-scale, micro-scale features – distribution of pore throats, microfractures, and grain boundaries – critical to comprehensive understanding are often unknown. Pore geometry and pore-scale processes are critical but attaining and integrating this information into macro-scale models is the focus of current research. Large domains (m- to km-scale) are relevant for making long-term repository performance predictions, and repository-scale predictions of coupled thermal-hydrological-mechanical-chemical (THMC) processes need to cover long time scales. The inter-relation between porosity and permeability is one way chemical and mechanical processes feedback to control flow processes. Bulk porosity is created or destroyed mechanically, chemically, or thermally. Mechanical deformation of pores can be elastic (i.e., closing microfractures) or plastic (i.e., grain rearrangement, grain crushing, or creep). Permeability controls porous media flow, which then further affects

the chemical and mechanical evolution of the system. For example, hydrostatic loading will close microfractures, reducing permeability, which may prevent excessive pore pressure from draining, possibly leading to damage and permeability increase.

Several summaries cover the oilfield literature and data regarding relationships between permeability and porosity (Archie 1950, Scheidegger 1972, Thompson et al. 1987, Nelson 1994, David et al. 1994, Bernabé 1995, Bernabé et al. 2003). There is less material in the salt repository literature.

For predictions of salt repository behavior, we are interested in granular (i.e., run of mine), damaged (i.e., disturbed rock zone, DRZ), and intact salt. Geologic salt makes an excellent candidate media for a permanent isolation of radioactive waste from the biosphere because it is self-healing, has low permeability, is relatively dry, has high thermal conductivity, and is biologically simple. In the short-term and at the waste-package scale salt can be complex to predict because: rooms and boreholes deform over months and years, salt essentially dissolves instantly in water (i.e., not kinetically limited), intragranular brine inclusions move and liberate under a thermal gradient, salt's chemical and mechanical properties are highly temperature- and moisture-dependent, and high ionic strength brine chemistry is complex, requiring additional considerations compared to fresh water. Despite these near-field complexities, salt presents a robust alternative for radioactive waste isolation at repository-relevant time and space scales. In this review, we consider the complexities related to the evolving pore space geometry and connectivity in granular and fractured salt. Because of the lack of salt-specific data, our summary assumes salt is similar to more insoluble rocks widely studied in the literature. Clearly, salt-specific data should be used when available. When considering the change of porosity and permeability under load, the creeping behavior of salt may lead to significant deviations from rocks like sandstones.

1.1 *Porous-medium scale characterization*

Naïvely, POROSITY is a scalar measure of void space in porous rocks, but there are many types of porosity. Porosity relates the bulk Darcy flux to the average flux within pores. Porosity and pore compressibility are a medium's primary storage capacity. Porosity typically ranges from 0.1 to 50 percent, and relates mineral properties to bulk properties (e.g., thermal conductivity and density). Variations on porosity in wide use include: effective porosity, dead-end porosity, intergranular, intragranular (i.e., fluid inclusions), matrix porosity, and fracture porosity. Pores and fractures both contribute to porosity, but they contribute to permeability in very different ways. Porosity is straightforward to measure in the laboratory or via borehole geophysics (e.g., neutron porosity, gamma density, sonic, or nuclear magnetic resonance – NMR). It is more difficult to estimate porosity in low-porosity rocks like intact halite (< 1%) than in higher-porosity granular media. The relationships between the different types of porosity are complex in insoluble rocks. Salt contributes an additional complexity, since addition of brine will evolve the distribution of porosity (e.g., dissolution from condensation of vapor), and temperature gradients can lead to significant dissolution and precipitation of salt (Olivella et al. 1996, 2011).

PERMEABILITY is the proportionality constant in Darcy's law, and is generally a second-order tensor relating the fluid driving force and bulk flowrate vectors. Permeability is needed to predict flow and solute transport. Typically, permeability is estimated from a flow test (i.e., perturb pore pressure in a fluid-filled rock, observing the response), which is often more complex than estimating the same rock's porosity. Permeability ranges over more than 10 orders of magnitude and is scale dependent (Clauser 1992), but its definition is essentially universal. The permeability of intact salt is almost unmeasurably low (< 10^{-20} m^2, Beauheim & Roberts 2002). Confined granular salt will eventually reconsolidate and heal to the low permeability and porosity of intact salt. Salt's ultralow permeability arises from its inability to withstand differential stress at the pore scale; open pores cannot resist closing except due to pore pressure.

TORTUOSITY is a bulk estimate of path complexity at the pore scale relevant to the porous medium scale (Clennell 1997), often conceptualized as a ratio of two lengths. A set of straight non-intersecting fractures or tubes have unit tortuosity. Tortuosity also has many possible definitions (e.g., geometrical, flow, diffusion, or electrical). Tortuosity may be a second-order tensor. It can be estimated in the laboratory (e.g., effective diffusion coefficient or electrical formation factor) or with borehole geophysics (e.g., electrical resistivity, NMR).

FORMATION FACTOR is the bulk (brine-saturated rock) electrical resistivity normalized by the pore fluid resistivity (Archie 1950). Formation factor is tortuosity to flow of electric current (Clennell 1997). Electrical resistivity is readily measured in the laboratory or via borehole geophysics. Samples must be permeated with a conducting fluid (e.g., brine or Hg) to estimate their formation factor. Formation factor is also approximated as the ratio of tortuosity to permeability (assuming an equivalence of flow and electrical tortuosities, Paterson 1983) or simply as a monomial expression for porosity (Pape et al. 1999).

1.2 Pore-scale characterization

Modern high-resolution imaging characterizes pore geometry (i.e., shapes and connectivity) directly, rather than inferring it from porous-medium scale measurements. Pore microstructure data can be integrated into geometric models that then represent the macro-scale network, predicting its transport properties (Schwartz et al. 1989, Bernabé 1995, Hilfer 1992, 2002, Fredrich et al. 2006, Keller et al. 2013, and Hilfer & Lemmer 2015). Many geometric models have been developed, including capillary tube models, grain models, network models, percolation models, fractal models, and stochastic reconstruction models (Hilfer 2002). These methods use observable geometric information to infer or differentiate microstructural features that in turn can be discretized and used to predict macroscopic behavior of the porous media. Local porosity theory, local percolation theory, and classical percolation theory have been applied to porous media (Katz & Thompson 1987, Hilfer 1991, 1992, Biswal et al. 1998, Pringle et al. 2009) and granular salt reconsolidation (Keller et al. 2014) with relative success.

2 Permeability Models

We summarize widely used porosity-permeability relationships. These can broadly be grouped into models based on: 1) grain-size distributions, 2) porosity and specific-surface area estimates, and 3) pore-size distributions. Berg (1970) developed a monomial regression model for permeability (k) in terms of porosity (ϕ) for granular materials with $\phi > 30\%$:

$$k_{BERG} = 8.08 \times 10^4 \phi^{5.1} D^2 e^{-1.385p} , \tag{1}$$

where k is in darcys, D [mm] is the median grain diameter, and $p = P_{90} - P_{10}$ is a phi-scale ($P_n = -\log_2 D_n$, with D in mm and n is percent passing a sieve size) sorting term to account for the grain-size distribution. This grain-size based model (or one of the many other models of its type, Nelson 1994) may be useful for characterizing permeability of granular salt used in drift seals or as backfill in a salt repository. They could also be used to estimate the effect different grain size distributions have on permeability (Kröhn et al. 2009, 2017).

Permeability may also be expressed as a monomial of porosity and specific surface area. The most widely used relationship of this type is that of Kozeny and Carman (KC). It is based on an "equivalent channel model", which assumes the porous medium can be represented by a bundle of non-intersecting tortuous tubes of different radii. Tubes are assigned a dimensionless shape factor $1.7 < f < 3$ and a tube length L_a (longer than the sample length L); from this, dimensionless tortuosity is defined as $\tau = (L_a / L)^2$. The KC model is then

$$k_{KC} = \frac{\phi R_h^2}{f\tau} = \frac{\phi}{f\tau \Sigma_p^2} , \tag{2a}$$

Where $R_h = 1 / \Sigma_p$ is hydraulic radius [m] and Σ_p is specific surface area normalized by pore volume [m^{-1}]. If specific surface area is normalized by the rock (Σ_r) or grain (Σ_g) volume ($\Sigma_p = \Sigma_r / \phi = \Sigma_g (1 - \phi) / \phi$), the KC model becomes

$$k_{KC} = \frac{\phi}{f\tau \Sigma_p^2} = \frac{\phi^3}{f\tau \Sigma_r^2} = \frac{\phi^3}{f\tau \Sigma_g^2 (1 - \phi)^2} . \tag{2b}$$

Tortuosity can be replaced with the formation factor $F = \tau / \phi$ (Paterson 1983) to give

$$k_{KC} = \frac{R_h^2}{fF} = \frac{1}{fF\Sigma_p^2} = \frac{\phi^2}{fF\Sigma_r^2} = \frac{\phi^2}{fF\Sigma_g^2 (1 - \phi)^2} . \tag{2c}$$

The typical KC model form assumes k is proportional to ϕ^2 and Σ_r^{-2} . In oil reservoirs, Σ_r is often related to residual water saturation, gas adsorption, or NMR and induced polarization logs, to allow estimation of the parameters in the KC model from geophysics (Nelson 1994, Pape et al. 1999).

The KC model is widely used, but it under-predicts   due to imposed $\Delta\phi$ (David et al. 1994). Many users simply make the porosity exponent an adjustable factor, more typically 3 to 8. There is no physical justification for the high exponents observed or inferred for low-permeability rocks (Thompson et al. 1987, Nelson 1994). Bernabé (1995) used synthetic pore network models to illustrate the effect dead-end pores have on the KC model. The KC model can be derived through upscaling (i.e., homogenization) from Stokes' flow at a length scale longer than average pore sizes (Hilfer 1992).

Pape et al. (1999) used a "pigeon-hole" fractal model for ϕ to arrive at a polynomial expression for k, starting from the KC model. Their piecewise-linear model was regressed to > 600 sandstone and shale data from a German hydrocarbon reservoir:

$$k_{PAPE} = a\phi + b\phi^2 + c(10\phi)^{10},$$ (3)

where a, b and c are empirical basin-specific non-linear regression coefficients estimated from core data. Notably, this model can predict concave-up log-log $k(\phi)$ breaks in slope, sometimes observed in low-porosity data $(\phi < 10\%)$.

The Schwartz, Sen & Johnson (SSJ) model assumes a porous medium comprising insulating solids, conductive pore-filling fluid, and a surface conductivity term arising from the electric double layer (Johnson et al. 1986, Schwartz et al. 1989). They characterize a porous medium by four micro-scale parameters: tortuosities and characteristic lengths of the pore volume (α_3, Λ) and surface area (α_2, λ). They consider Λ an effective hydraulic radius [m]. The distinction between bulk and surface conductance was first proposed in shaly sands (Waxman & Smits 1968) but has seen application to rock types with fractally rough grains. For estimating k, their approach is a modified hydraulic radius model where a weighted averaging procedure is used to reduce the effect of dead-end pores that do not contribute to electrical flow. Bernabé (1995) and Hilfer (1992) present the SSJ model in a simpler form as:

$$k_{SSJ} = \frac{\Lambda^2}{7.3F},$$ (4)

where $\Lambda = 2(\int E^2 d\phi)/(\int E^2 d\Sigma)$, the integral of the pore-scale electric field, E, over the pore volume and grain surface area. Λ represents the size of the connected pore space; in general, $\Lambda \propto \tau^{1/2}\phi/\Sigma_r$ (Hilfer 1992), and as $E \to 0$, $\Lambda = 2/\Sigma_r$. Porosity does not appear in (4), but it factors into the integral in the numerator of Λ. It is a weighted surface-area-to-pore-volume ratio in which only those parts of the pore space that carry current are counted (Schwartz et al. 1989). Bernabé (1995) shows the SSJ model does very well in estimating k when the pore-scale network is sufficiently known (e.g., during an upscaling procedure from pore-scale models or imaging data, Noiriel 2015), but the difficulty in estimating Λ at the field scale is a weakness.

The Katz-Thompson (KT) model is based on fractal percolation theory. This model estimates its characteristic length from mercury-injection data and F to characterize the distribution of pores in the medium (Katz & Thompson 1986, 1987). Nelson (1994) presents the KT model as:

$$k_{KT} = \frac{R_c^2}{56.5F},$$ (5)

where $R_c = l_c / 2$ is a characteristic radius, $l_c = 4\sigma \cos\theta / p_c$ is a characteristic length, σ is a surface tension [Pa·m], θ is a contact angle, and p_c is the Hg-injection entry pressure. The form of (5) is quite similar to (4) and (2c) using a typical Archie's exponent of 2, $F \approx \phi^{-2}$ (Archie 1950, Hilfer 1992). Both SSJ and KT predict variation in characteristic length, rather than ϕ leads to observed variation in k. Their exponents are < 3; much less than typical fits of KC to data, which attribute variations in k to variations in ϕ or specific surface area (Nelson 1994).

3   Evolution of Porosity and Permeability in Coupled Models

Geomechanical models commonly predict volumetric strain (displacement is often their primary variable), which can be translated into $\Delta\phi$, and may further be mapped onto an isotropic Δk. Models in the previous section depended on F or a characteristic length scale related to pore-size distributions (KT) or electric field weighted volume/surface integrals (SSJ). Constitutive models have not yet been developed to relate deformation in a geomechanical model to changes in F or relevant characteristic length scales. Additionally, changes to ϕ, k or τ that occur in the thermal-hydrologic-chemical model must be propagated back into the geomechanical model. These would require still more constitutive models relating changes in porosity back to a volumetric strain or a displacement. In the future, we would also seek to couple the tensorial nature of the mechanical and hydrological problems, rather than just scalar changes.

David et al. (1994) summarize laboratory observations of $\Delta\phi$ and Δk at variable confining pressures in sandstones (14% to 35% initial porosity). They found three primary types of k responses: I) low porosity ($\phi < 5\%$) crystalline rocks, II) porous sedimentary rocks with low pressure-sensitivity of k, and III) porous materials being compacted across their critical stress, associated with the onset of grain crushing. Type I behavior is typical for closure of micro-cracks with moderate hydrostatic loading (typical of intact salt samples from the DRZ):

$$k_{PS} = k_0 e^{-\gamma(p_{eff} - p_0)},$$ (6)

where γ is the pressure sensitivity coefficient [Pa^{-1}], p_{eff} is the difference between confining and pore pressure (i.e., a Terzaghi effective pressure), and subscript zero indicates a reference state. They did not consider the effects of the Biot-Willis coefficient, related to poroelastic coupling (Wang 2000). This type of exponential pressure-sensitivity is also predicted in aquifers; γ is matrix compressibility, which can be related to the specific storage coefficient,

$S_S = \rho_w g(\gamma - c_w \phi)$ [m^{-1}], where ρ_w is the density of water [kg·m^{-3}], g is acceleration due to gravity [m·s^{-2}], and 5.1×10^{10} [Pa^{-1}] is the compressibility of water. Type II and Type III behavior are often characterized by monomial porosity-permeability relationships like

$$k_{\phi S} = k_0 \left(\frac{\phi}{\phi_0}\right)^\alpha, \tag{7}$$

where α is the dimensionless porosity sensitivity coefficient. Type II behavior is associated with lower exponents than Type III behavior. David et al. (1994) showed the pore compressibility $\beta = \gamma / \alpha$ [Pa^{-1}] can characterize a threshold ($\beta \sim 3.3 \times 10^{-3}$ [MPa^{-1}]) between pore squeezing in granular materials and crack closure in fractured materials. The critical stress associated with grain crushing was identified using acoustic emissions. They observed k in tight rocks is more pressure sensitive than granular rocks and β is higher in tight rocks. In rocks with both granular and fracture porosity, they found the monomial form of $k(\phi)$ is not well-defined; this result is similar to observations of Pape et al. (1999). Reconsolidating granular salt to low porosity or salt in the DRZ may possess both types of porosity and may similarly foil prediction with simpler monomial models.

Bernabé et al. (2003) present a discussion of trends in the permeability and porosity of porous rocks during deformation and chemical processes. Their primary point is that a local monomial relation ($k \propto \phi^\alpha$) holds during deformation, but $\alpha \propto \phi_e / \phi_{ne}$, the ratio of effective and non-effective porosity. Bernabé et al. (2003) defines ϕ_{ne} as porosity where fluid velocity is less than a small fraction (e.g., 1%) of the mean velocity. Their heuristic argument is analogous to the more rigorously derived SSJ model (see Equation 4), where is defined by contribution to the bulk electrical conduction response, but Bernabé et al. (2003) do not present a quantitative relationship for ϕ and ϕ_e, based on their contribution to pore-scale flow. They illustrate how data with a concave-downward break in slope in their log-log $k(\phi)$ plot can be converted to simpler linear trends using ϕ_e instead of ϕ. Data distinguishing ϕ_e and ϕ_{ne} would require a pore-scale characterization effort.

Verma & Pruess (1988) present models to predict Δk given $\Delta \phi$ from silica redistribution in basalt. Using geometrical arguments, they develop predictions of ϕ and k for collections of tubes or planar fractures of constant diameter and aperture along their length (i.e., the KC model), and for collection of tubes that vary diameter stepwise along their length. They found different distributions (linear, triangular, and semi-Gaussian) of uniform tube diameters or fracture apertures do not have a large impact on the overall macroscopic relation between porosity and permeability, but the "series" model with tubes of variable radii had a large impact on the relationship (Scheidegger 1972). Having multiple tube radii effectively introduces an irreducible porosity $\phi > 0$ when $k \to 0$. Reis & Acock (1994) present laboratory data showing the effects of uniform salt precipitation on permeability in Berea Sandstone. They also found the KC uniform tube model did not capture the observed Δk, given the observed $\Delta \phi$. As an improvement to the stepwise-change "series" tubes of Verma & Pruess (1988), they present a non-uniform pore model with a sinusoidal pore cross-sectional shape, which gives a more

realistic flow distribution along the pores. They concluded that exponential and power-law models for permeability reduction are accurate for modest porosity reduction (≤ 80%), but their sinusoidal model is required for better estimates of Δk when ϕ reduction is significant (KC under-predicts Δk for a given $\Delta \phi$). During salt reconsolidation to very low porosities, this known deficiency should be considered.

4   Low-Porosity Characterization Methods

A multitude of techniques exist to characterize porosity (Lowell & Shields 2013) and permeability, but here we mention methods focused on low-porosity, microporous samples, where traditional porosimetry methods become less accurate and useful. Computed methods offer a possible solution to probe the micropore range – synchrotron micro-tomography can resolve on the order of 100 microns (Bernard 2005), X-ray micro computed tomography (micro-CT) can resolve at the sub-micron scale (Noiriel 2015), and focused ion beam nano-tomography (FIB-nT) can resolve in the 2 to 20 nm range (Keller et al. 2014). Understanding the data from computed tomography, especially dealing with numerical noise and reconstruction discretization artifacts, remains a critical challenge (Fredrich et al. 2006, Noiriel 2015). Keller et al. (2014) contends micro-CT and Fib-nT should be combined to measure both the macro-scale and micro-scale pore distributions.

Pore-scale characterization presents a potential route at low-porosities when traditional macro-scale porosity-permeability relationships break down. Once the pore-structure is reconstructed, percolation methods can be used to quantify pore-connectivity, which can then be combined with Lattice-Boltzmann (Fredrich et al. 2006) or other pore-scale flow solvers to predict permeability (Manwart et al. 2002, Biswal et al. 2009). Pore-scale characterization of entire large (> cm-scale) samples is still not possible, requiring sub-sampling.

5   Recommendations Relevant to Salt

There are three primary regions to characterize in a salt repository: 1) granular salt in backfill and drift or shaft seals, 2) DRZ surrounding excavated drifts, and 3) intact salt in the far-field. Granular salt ($20\% \lesssim \phi \lesssim 45\%$) will eventually reconsolidate to the low porosity of intact salt ($\phi \lesssim 1\%$). Similarly, k may decrease by 10 orders of magnitude. These enormous changes in flow properties may include a structural change in the pore network, not just a simple scaling of the initial structure. Different laboratory methods are used to estimate ϕ and k at either end of the ϕ spectrum. Kröhn et al. (2017) discussed some multi-year duration oedometer reconsolidation tests, where initial results show negative porosity at final compaction. Measuring small porosities during long tests is difficult, especially when adding brine to salt (leading to mass gain or loss through dissolution and precipitation). Run-of-mine salt obtained directly from mining operations is compositionally and chemically heterogeneous. Bedded salt may include ~5% non-halite components (e.g., clays, polyhalite, and anhydrite), and therefore

may exhibit non-uniform chemical, mechanical, and hydrological responses at the pore-scale, contributing to inter-test variability at the meter-scale.

Kröhn et al. (2009) showed $k(\phi)$ data for reconsolidating granular salt, where some samples exhibited concave-up or concave-down breaks in slope. A monomial with a single constant exponent cannot describe this non-linear log-log $k(\phi)$ relationship. Concave-up variation can be modeled with a polynomial $k(\phi)$ and can be explained by a material having multiple characteristic length scales (Pape et al. 1999) or a combination of both granular and fracture porosity (David et al. 1994). Bernabé et al. (2003) illustrated qualitatively how concave-down log-log $k(\phi)$ distributions might be "rectified" to linear ones by plotting k against effective porosity (i.e., excluding dead-end or low-flow porosity), rather than total porosity.

In the DRZ, salt porosity includes microfractures; pore compressibility will be quite different from the same porosity in a granular medium (David et al. 1994). A slight $\Delta(\phi)$ (~1%) may lead to a Δk of several orders of magnitude. Often this is treated with a large exponent in a monomial law, i.e., the ϕ^{10} term in Equation 3. Because fracture porosity is quite pressure-sensitive, DRZ salt may be better represented by a $k(p)$ model such as Equation 6 or Bandis et al. (1983), rather than a monomial $k(\phi)$. If the salt is brine-saturated, resistivity geophysics may be useful for estimating the connected porosity (Jockwer & Wieczorek 2008).

Intact salt has very low porosity and permeability. We typically do not attempt to estimate a $k(\phi)$ relationship under intact conditions, but constitutive models derived for higher ϕ and k under other conditions should be consistent with this endpoint (i.e., during reconsolidation and healing of granular or DRZ salt) or starting point (i.e., during the damage accumulation process from drift excavation or hydrofracture).

Different methods should be used to estimate permeability depending on the data available. If porosity is high (>20%) and only grain-size distribution data are available, Berg (1970) works well. If estimates of the formation factor or tortuosity are available, the KC or SSJ methods could be used. If the air-entry pressure is known, or other characteristic pressure from the moisture-retention curve (e.g., Cinar et al. (2006) or Hg injection data), the KT model does well. There are several proposed models for estimating changes in permeability for granular pores and fractures, but accurately understanding the dynamics of pore/fracture consolidation, requires considering the poroelastic behavior of the salt-fluid system (Wang 2000, Ghabezloo et al. 2009). In the low porosity range (<5%), tomographic pore-scale characterization methods combined with SSJ, local porosity, or percolation theory, offer promising approaches. Upscaling methods are an area of active research and will improve as imaging technologies continue to advance.

Acknowledgements

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