A novel architecture for pore network modelling with applications to permeability of porous media

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Abstract

Network models of porous media are beneficial for predicting the evolution of macroscopic mass transport properties. This work proposes a novel bi-regular network model based on truncated octahedral support. With the model, pore systems with different pore coordination spectra for a given average coordination number can be constructed to match experimental data. This feature and the maximum allowed pore coordination of 14 make the proposed model more realistic and flexible than the existing models based on cubic supports. Limestone is used as a study material to illustrate the model performance. Experimental pore space data for this material obtained by X-ray tomography (CT) are used for constructing microstructure-informed model realisations. It is demonstrated that with these realisations the experimentally measured permeability of the material can be predicted. The model is further used to assess the effects of pore connectivity and porosity on the permeability. It is shown that the effect of pore connectivity is substantially stronger than the effect of porosity. A strategy for calculating the evolution of permeability with damage-related pore space changes is also described. The results reveal the effects of the mechanical properties of the medium on the permeability evolution as a function of damage evolution. Developments of this strategy are suggested for deriving mechanism-based constitutive laws for engineering applications.

Keywords: Hydrocarbon reservoirs; X-ray tomography; Pore-space modelling; Bi-regular network; Permeability evolution; Pore-space damage.

1. Introduction

Porous inorganic media, geological or man-made, are typically brittle or quasi-brittle in nature. They contain one or several solid phases with different chemical compositions and mechanical properties along with a system of spatially distributed pores and/or other micro-defects. The rate of mass transport through these media, either via diffusion or via convection/advection, is determined predominantly by the structure of the pore space.

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Important parameters characterising this structure are the porosity, the sizes and shapes of the pores, and the connectivity between the pores. Engineering scale properties, such as diffusivity or permeability, will change if the pore space geometry or connectivity is altered. Alterations may be caused by various physical processes, such as mechanical damage, electrochemical and/or bacterial corrosion. Mechanical damage is defined as the creation and growth of micro-crack population, typical for quasi-brittle media. This is arguably the most effective alteration process as it can cause changes in both the geometry and the connectivity of pore space over short time scales. It can be utilised, for example, during hydraulic fracturing of hydrocarbon reservoirs to increase macroscopic mass transport parameters. In other applications the damage-induced change in the macroscopic parameters is detrimental; for example in the use of low-permeability media for retention of radioactive species in geological repositories for nuclear waste. Either way, the prediction of the evolution of the macroscopic properties with pore space changes is of substantial industrial value. Such predictions can be achieved by coupled models that represent the mechanical behaviour of and mass transport through the medium.

The advances in materials imaging, in particular X-ray Computed Tomography (XCT), and the increase of computational power allowed for mass transport analysis using the reconstructed pore space. This type of image-based modelling has been combined with several analysis techniques, such as Lattice-Boltzmann methods (e.g. Arns et al. 2004; Chen et al. 2009), finite element/difference methods for solving Navier-Stokes flow equations (e.g. Oren et al. 2007; Zhang et al. 2011), and particle-based methods (e.g. Ovaysi and Piri 2010), to study transport through real pore morphologies and to analyse effects of pore space changes due to colloid deposition (Chen et al. 2009). The imaged-based modelling provides invaluable insights into the effects of the local morphologies on the transport parameters (Van Marcke et al. 2010) and can be used to produce macroscopic permeability tensors for engineering scale models (Zhang et al. 2012). However, the analysis is restricted to the imaged volume, which might not be the representative volume for the probed material, i.e. the imaged volume could contain only a limited set of all possible size and connectivity characteristics of the material. As a result it is yet not certain when image-based analyses could provide engineering scale properties.

A historically older approach is the conceptualisation of the pore space with a discrete network of pores appropriately connected by throats, known as pore-network modelling (e.g. Blunt et al. 2002). Pore networks can be considered as meso-scale models, where the physical mechanisms at the pore- or micro-scale level are averaged over and the engineering scale properties emerge from averaged geometrical and topological characteristics of the pore space. Hence, the pore-network models are complementary to the micro-scale imaged-based models in the effort to provide better understanding of the relation between microstructural characteristics and engineering properties. One benefit is that they allow for analysis of larger physical volumes with less computational demand compared to image-based models. Analysis of volumes larger than the currently imaged can capture topological properties of the pore space that may not be observed in the images, e.g. long-range properties of the network. Thus, the pore-network models have the potential to answer the question of the representative volume size. They are also advantageous for studies of mechanical damage effects on transport because they can be linked elegantly to various lattice models for deformation and fracture of quasi-brittle materials (e.g. Chang et al., 2002; Cusatis et al. 2006).

Early 3D pore-network models were based on a regular cubic lattice with a maximum pore coordination of six (Matthews and Spearing 1992; Ioannidis and Chatzis 1993, Reeves and Celia 1996). Later, XCT-obtained experimental data showed that pores with pore coordination numbers larger than six could be substantial fractions of all coordinated pores (Lindquist et al. 2000, Al-Raoush and Wilson 2005; Dong and Blunt 2009). Based on such data irregular pore-network models were also developed as stochastic replicas of the reconstructed pore spaces (Piri and Blunt 2005; Al-Kharusi and Blunt 2007; Van Marcke et al. 2010). The use of regular lattices to modelling pore networks, however, is attractive compared to the irregular image-based lattices, for the same reasons as discussed above. To account for pore coordination larger than six using a regular lattice the network topology needs to be different from the simple cubic lattice. Raoof and Hassanizadeh, 2010, suggested pore coordination increase to 26 based on a cubic support by adding 12 throats along planar diagonals and eight throats along body diagonals to the six throats along the cube principal directions. The large coordination number is one attractive property of this model, but the suggested connectivity is not physically realistic, although topologically admissible, because large numbers of throats intersect at points that are not pores. To the authors' knowledge, the only application of a non-cubic lattice support for pore-network construction uses rhombic dodecahedron as a unit cell (Vogel and Roth 2001). This offers a maximum pore coordination of 12 with throats of equal lengths, i.e. sufficiently large physically admissible coordination. In Section 2.1 we will show that this cell is less representative for the volume around a pore than the cell proposed in this work.

In this paper we present a bi-regular interpretation of the pore space, which conceptualises porous materials at their meso-scale. This is based on truncated octahedral cells providing a maximum pore coordination of 14 with two sets of throats of different lengths. We demonstrate that pore-network models based on the truncated octahedral lattice can be used for describing a rich set of real pore spaces, particularly different pore coordination spectra for one and the same average coordination number. We demonstrate, further, the capabilities of the model to predict experimentally measured permeability of a limestone using pore space data extracted from computed tomography. We analyse the effects of the average pore coordination number and the porosity of a medium on the permeability and show that the former has substantially stronger effect than the latter. We also illustrate how the model can be used to study evolution of permeability with pore space changes with a simple strategy mimicking mechanical damage. The real link to a complementary solid-phase model is under development, but is also discussed briefly. In this work we are mainly concerned with the macroscopic permeability and the relevant engineering applications and do not consider pore level phenomena.

2. Theoretical basis

2.1. Meso-scale and supporting skeleton of pore spaces

In this study, the meso-scale is considered as the length scale dictated by the distances between the pores of a porous medium. Alternatively, it is dictated by the lengths of the throats connecting pores. At the meso-scale, the throats are fluid conduits and the flow is a continuum phenomenon resulting from underlying atomic-scale mechanisms such as convection, advection and diffusion. The pore space is characterised by a set of pores and a set of throats, which are topologically equivalent to a set of sites and a set of bonds, respectively. A 3D domain containing a site (pore) set can be tessellated into cells using a

Voronoi construction. In the resulting cell assembly the sites (pores) reside at the centres of the cells. The members of the bond (throat) set link some of the sites (pores) residing in adjacent cells. This suggests that a good description of the possible pore space configurations can be achieved by analysis of Voronoi tessellations of point sets with random spatial distribution of points. Kumar et al. (1992) have performed a very large series of Voronoi tessellations with point sets distributed spatially by a random Poisson process. The results have produced a statistical picture of the possible cell topologies. The number of cell faces has been found to vary between 4 and 36, with the average number of cell faces $\bar{F} = 15.54$. This suggests that the maximum possible coordination of sites would be 36. The conclusion, of course, is constrained by the limited number of simulations performed, but it provides a good estimate for a maximum possible pore coordination to be experimentally observed in real materials. Indeed, experimental results show the rare appearance of pores of high coordination, e.g. up to 25 in Al-Kharusi and Blunt (2007). Further, the analysis by Kumar et al. (1992) showed that the number of sides per face varies between 3 and 15, with average number of sides per face $\bar{S} = 5.23$. Also, the average number of cell edges is found to be $\bar{E} = 40.63$, and the average number of cell vertices to be $\bar{V} = 27.09$. Hence an average cell in the tessellation of a pore space will have a topology given by the quadruplet $(\bar{F}, \bar{E}, \bar{V}, \bar{S})$. This provides an insight into the selection of a regular cell shape, which can be used to support the construction of pore space topologies.

Four geometric solids can fill the space compactly using a single solid cell. These are: the cube with $F = 6$, $E = 12$, $V = 8$, $S = 4$; the regular hexagonal prism with $F = 8$, $E = 18$, $V = 12$, $S = 4.5$; the rhombic dodecahedron (a solid bounded by 12 equal rhombuses) with $F = 12$, $E = 24$, $V = 14$, $S = 4$; and the truncated octahedron (a solid bounded by six equal squares and eight equal regular hexagons) with $F = 14$, $E = 36$, $V = 24$, $S = 5.14$. A comparison between an average cell from Voronoi tessellations and the space filling solids suggests that the truncated octahedron represents best the space around a pore in an average sense. Fig. 1 shows an illustration of this solid, as well as a 3D assembly of sites and bonds. The single cell (a) is shown with a pore residing in the centre and all possible 14 throats. The assembly (b) shows all possible sites and bonds in the regular supporting skeleton of a pore space.

Fig. 1. Unit cell (truncated octahedron) with all possible bonds (a) and site-bond support for pore space construction (b). Letter S denotes a site or pore; letters B_1 and B_2 denote two types of bonds or prospective throats.

The construction of the site-bond skeleton begins with the seeding of sites. This uses a mapping from integer triplets (i, j, k) into the physical space. Only triplets with three even indices (even triplets) and three odd indices (odd triplets) are mapped into sites. For the mapping, equal spacing between the sites of the assembly in the three principal directions is assumed, i.e. the directions normal to the square faces of the solid cell in Fig. 1(a), denoted by L . This assumption yields a site-bond model corresponding to the cell assembly of Fig. 1(b), with L giving the size of the unit cell in any of the principal directions. With equal spacing in the principal directions, L , the sites of the assembly are seeded at points with coordinates $(i L / 2, j L / 2, k L / 2)$ in the physical space. The sites mapped from even triplets and from odd triplets form two sets of sites in the physical space. The sites from each one set are connected by bonds to the neighbouring six sites of the same set and to the neighbouring eight sites of the other set. The bonds connecting sites belonging to one of the site sets are denoted by B_1 . They have length $L_1 = L$ and are normal to the square boundaries of the unit cell. The bonds connecting sites belonging to two different site sets are denoted by B_2 . They have length $L_2 = \sqrt{3} L / 2$ and are normal to the hexagonal boundaries of the unit cell.

The proposed model is physically admissible, i.e. there will not be throats intersecting outside pores, and offers a sufficiently high maximum coordination, $Z = 14$, to cover the statistically significant coordination numbers observed experimentally (Lindquist et al. 2000, Al-Raoush and Wilson 2005; Dong and Blunt 2009).

2.2. Construction of pore networks from experimental data

We conjecture that the macroscopic property of the porous medium fluid permeability emerges from the underlying atomic-scale processes, predominantly via the meso-scale properties of the pore space. These meso-scale properties are the connectivity of pores and the local conductivity of throats and these are discussed in turn below.

The connectivity of the pore space can be characterised by the fractions of pores coordinated by different numbers of throats. Let n_i be the number of pores with coordination i , where $i = 0, \dots, 14$ with $i = 0$ corresponding to isolated pores and $i = 14$ corresponding to fully connected pores. We denote the sum of n_i for $i = 0, \dots, 14$ (i.e. the total number of pores) with N and the sum of n_i for $i = 1, \dots, 14$ (i.e. the number of connected pores) with $\underline{N} = N - n_0$. The fraction of pores with coordination i are given by: $z_i = n_i / N$, for $i = 0, \dots, 14$ relative to the total number of pores; or $\underline{z}_i = n_i / \underline{N}$, for $i = 1, \dots, 14$ relative to the number of connected pores. The average coordination number of the pore system can thus be calculated as: $z = \text{sum of all products } (i \times z_i)$, for $i = 0, \dots, 14$ if the total number of pores is considered; or $\underline{z} = \text{sum of all products } (i \times \underline{z}_i)$, for $i = 1, \dots, 14$ if the number of connected pores is considered.

The procedure for pore network construction is based on elimination of bonds from the bi-regular support. This uses an elimination number, $0 < \varepsilon < 1$, and a generator for uniformly distributed random numbers $0 < \gamma < 1$. The process is a loop over all bonds in the site-bond assembly, where a bond is accepted as a throat if $\gamma < \varepsilon$, and is eliminated otherwise. The elimination number can be selected to be the same for all bonds in the assembly. In such a case, it will be equal to the fraction of non-eliminated bonds, f , i.e. the bonds accepted as conducting throats. Elimination based on a constant number produces an average pore coordination $z = \varepsilon Z = f Z$ (e.g. Matthews and Spearing 1992; Raoof and Hassanizadeh 2010) but is also very specific to the network distribution of coordination numbers z_i or $\underline{z}_i$. This makes the previously published models rigid with respect to describing possible distributions of pore coordination numbers. In principle, one can select different elimination numbers to reflect various pore-network properties of real materials. In the proposed model for example: the elimination numbers for the seven distinct bond directions can be assigned different values to achieve a required anisotropy; or the elimination numbers for different spatial domains in the assembly can be assigned different values to achieve required inhomogeneity. While these are important possibilities, the proposed site-bond support allows for a special tuning of the network properties without the introduction of anisotropy and inhomogeneity. A selection of different elimination numbers for the two sets of bonds B_1 and B_2 does not yield anisotropy because the two sets are independently isotropic. Blocking the set B_2 leaves an isotropic network with maximum coordination of six; blocking the set B_1 leaves an isotropic network with maximum coordination of eight.

The elimination numbers for the bonds sets B_1 and B_2 are denoted here by ε_1 and ε_2 , respectively. A study of the effects of these elimination numbers on the topological properties of the constructed pore network is straightforward and leads to the following observations. The fraction of throats (retained conducting bonds) follows the expected linear

dependence on the elimination numbers $f = (3\varepsilon_1 + 4\varepsilon_2) / 7$. This is reflected in the expected linear dependence of the average pore coordination on the elimination numbers $z = fZ = 6\varepsilon_1 + 8\varepsilon_2$. Any predefined fraction of throats, f_u , or alternatively average pore coordination number, z_u , can be achieved with any pair $(\varepsilon_1, \varepsilon_2)$ on the line $3\varepsilon_1 + 4\varepsilon_2 = 7f_u$ or on the line $6\varepsilon_1 + 8\varepsilon_2 = z_u$, respectively. The fractions of throats created from bonds B_1 and from bonds B_2 , however, follow non-linear dependences on ε_1 and ε_2 . This is reflected in non-linear dependences of the fractions of pores with various coordination numbers, z_i , on ε_1 and ε_2 . To illustrate this effect here we have selected an average coordination $z_u = 6$ and four points $(\varepsilon_1, \varepsilon_2)$ on the line resulting in this average coordination. Fig. 2 shows the results for the fractions of pores with different coordination numbers in the manner experimentally determined fractions (sometimes called normalised frequency) are reported in the literature (e.g. Dong and Blunt 2009). Fig. 2 demonstrates one of the strengths of the proposed model: a rich class of pore spaces with equal average coordination number can be simulated.

Fig. 2. Fractions of pores with different coordination numbers in a network with average pore coordination $z_u = 6$. These are obtained with different elimination numbers for the two types of bonds -given in the plots.

2.3. Local transport properties

In the proposed model, the throats are represented by pipes of circular cross section with corresponding hydraulic conductivity. The conductivity of a real throat is an emergent property that depends on the viscosity of the fluid being transported and on the morphology of any given throat. In principle, local conductivity values can be determined using fluid mechanics calculations on experimental pore throat geometries (Van Marcke et al. 2010). For a given throat connecting two pores, α and β , with prescribed pressures, $p_\alpha > p_\beta$ (in Pa), the calculations will provide the fluid volume, $Q_{\alpha\beta}$ (in $\text{m}^3 \cdot \text{s}^{-1}$), transported through the throat morphology. The local conductivity of the throat can then be defined with $c_{\alpha\beta} = Q_{\alpha\beta} / (p_\alpha - p_\beta)$, in $\text{m}^3 \cdot \text{Pa}^{-1} \cdot \text{s}^{-1}$. Such calculations can be performed for a selected, sufficiently large, number of throats to obtain a distribution of local conductivity values. These can be used to construct a distribution of bond radii in the site-bond assembly. Assuming laminar flow in the pipes, the total discharge of the pipe between sites α and β is given by:

$$Q_{\alpha\beta} = \frac{\pi R_{\alpha\beta}^4}{8\mu} \cdot \frac{p_\alpha - p_\beta}{L_{\alpha\beta}}, \quad (1)$$

where $R_{\alpha\beta}$ and $L_{\alpha\beta}$ are the radius and the length of the pipe, respectively (in m), and μ is the fluid viscosity (in $\text{Pa} \cdot \text{s}$). From the known local conductivity distribution $c_{\alpha\beta}$, the distribution of bond radii will be given by:

$$R_{\alpha\beta} = \left(c_{\alpha\beta} \cdot \frac{8\mu L_{\alpha\beta}}{\pi} \right)^{1/4}. \quad (2)$$

In the absence of sufficient experimental data to describe throat morphologies, the bond radii can be distributed according to the throat size distribution as a first approximation since such distributions are readily obtainable. Clearly, this approximation does not capture local morphology effects but could provide a sufficiently realistic pore structure at the macroscopic scale. An assessment of how good the approximation is can be made by comparing model predictions with experimental permeability data. The simplest way is to assume that all

throats have morphologies producing conductivity values proportional to the values in pipes of corresponding lengths and cross sections, i.e.

$$c_{\alpha\beta} = m \frac{\pi R_{\alpha\beta}^4}{8 \mu L_{\alpha\beta}}, \quad (3)$$

where m is a morphology coefficient, and $R_{\alpha\beta}$ are now the distributed bond radii. The deviation of m from unity will characterise the effect of local morphology in an average sense.

The process of assigning bond radii requires the cumulative distribution of experimentally measured throat radii, $F(r)$, and a generator of uniformly distributed random numbers. The cumulative distribution is obtained from the set of experimentally measured throat radii using a standard statistical technique. For a set of N throats the measured radii r_i are ordered in ascending order, i.e. $r_i \leq r_{i+1}$ for $1 \leq i < N$, and $F(r_i) = (i - 0.3) / (N + 0.4)$. This ensures that $0 < F(r) < 1$. Then a throat radius is assigned as $R_{\alpha\beta} = F^{-1}(p)$, where p is a uniformly distributed random number. This ensures that the produced distribution of radii is statistically identical to the measured distribution. The process is used to assign radii to the conductive bonds. The non-conducting bonds are left in the model with zero conductivity, see Eq. (1), as they may become conductive when studying the effects of damage evolution on macroscopic permeability with the model described in Section 3.3.

In the proposed model, spherical pores are assumed to reside at the sites of the site-bond assembly. Experimentally determined distributions of pore sizes can be used to assign radiuses, R_α , to these pores. The process is similar to the one for the throats. Such an assignment can be subject to constraints from the preceding assignment of throat sizes. For example, the size of a pore at a given site can be required to be larger than a certain factor times the largest throat coordinating the pore. Irrespective of the assignment process the total volume of the accessible pore space will be:

$$V_p = \frac{4\pi}{3} \sum_{\alpha}^{pores} R_{\alpha}^3 + \pi \sum_{\alpha,\beta}^{throats} L_{\alpha\beta} R_{\alpha\beta}^2, \quad (4)$$

where the sum over the pores includes only the connected pores and the sum over the throats includes only permeable bonds. Note, that $L_{\alpha\beta}$ are proportional to the length scale, L , of the site-bond model, i.e. $L_{\alpha\beta} = \lambda_{\alpha\beta} L$, where $\lambda_{\alpha\beta} = 1$ for bonds of type B₁, and $\lambda_{\alpha\beta} = \sqrt{3} / 2$ for bonds of type B₂. For a given pore size distribution, R_α , and pore throat size distribution, $R_{\alpha\beta}$, Eq. (3) allows for determining L for any given porosity $\phi = V_p / V$, where V is the volume of the domain represented by the site-bond model. For example a model of a domain with N_x , N_y , N_z sites in the three principal directions will represent a volume $V = N_x \cdot N_y \cdot N_z \cdot L^3$. The length scale will then be determined from the cubic equation

$$(\phi N_x N_y N_z) L^3 = V_{pores} + (\pi \sum_{\alpha,\beta}^{throats} \lambda_{\alpha\beta} R_{\alpha\beta}^2) L. \quad (5)$$

Eq. (5) is used to enforce a prescribed porosity via a change of the model length scale after the distribution of pore and throat sizes is made.

2.4. Calculation of macroscopic permeability

The macroscopic permeability of the site-bond model is calculated in a manner similar to the one used by Van Marcke et al. (2010). The model with given boundary conditions formulates a discrete boundary value problem with unknown pressures at the sites. For a bond connecting sites α and β , with pressures p_α and p_β , respectively, the following relation holds: $Q_{\alpha\beta} = c_{\alpha\beta} (p_\alpha - p_\beta)$, where $Q_{\alpha\beta}$ is the fluid volume flowing through the bond per second, and $c_{\alpha\beta}$ is the bond conductivity determined from Eq. (2) for the particular bond length and diameter. The conservation of mass at site α is:

$$\sum_\beta Q_{\alpha\beta} = \sum_\beta c_{\alpha\beta} \cdot (p_\alpha - p_\beta) = 0, \quad (6)$$

where the sums are taken over all bonds coordinating site α . The local conservation equations for the sites of the model form a system of linear equations $\mathbf{C} \cdot \mathbf{p} = \mathbf{f}$, where $\mathbf{C}$ is the matrix of bond conductivity values, $\mathbf{p}$ is the vector of site pressures and $\mathbf{f}$ is the vector of external forces, reflecting the particular boundary conditions. The matrix $\mathbf{C}$ has the following sparse structure: the off-diagonal coefficients $C_{\alpha\beta}$ ($\alpha \neq \beta$) are equal to the conductivity of the bond between the sites α and β , i.e. $C_{\alpha\beta} = c_{\alpha\beta}$, if the sites are connected or zero otherwise; the diagonal coefficients $C_{\alpha\alpha}$ are equal to the sum of the local conductivity values of all bonds coordinating site α , i.e. $C_{\alpha\alpha} = \sum_\beta c_{\alpha\beta}$ for all β .

Natural boundary conditions, i.e. known fluxes at sites, can be prescribed directly as coefficients of the force vector. For example, a known discharge Q_u at site α , is prescribed by setting $f_\alpha = Q_u$ in $\mathbf{f}$. This is typically used to prescribe zero fluxes across impermeable boundaries, i.e. setting $f_\alpha = 0$ for all sites along such a boundary. Essential boundary conditions, i.e. known pressures at sites, are dealt with in a standard manner. This involves changes in the system matrix $\mathbf{C}$ and the force vector $\mathbf{f}$, without altering the system size and the vector $\mathbf{p}$. For example, for a site α with known pressure p_u the following changes are made: $C_{\alpha\alpha} = 1$ and $C_{\alpha\beta} = 0$ in $\mathbf{C}$; $f_\alpha = p_u$ and $f_\beta = (f_\beta - p_u C_{\alpha\beta})$ for all ($\beta \neq \alpha$) in $\mathbf{f}$.

The system of linear equations describes a steady-state fluid flow through the site-bond model and can be solved with any standard matrix solver. The macroscopic permeability of the site-bond model, k , can then be determined from the total fluid discharge across a permeable boundary using Darcy's law:

$$k = \frac{\mu Q_{in} L_m}{(p_{in} - p_{out}) A_m} = \frac{\mu Q_{out} L_m}{(p_{in} - p_{out}) A_m}, \quad (7)$$

where Q_{in} is the total inflow, Q_{out} is the total outflow, p_{in} and p_{out} are the applied pressures, L_m is the model distance between the permeable boundaries, and A_m is the model area through which the flow occurs. These two parameters are different from the cubic based models due to the different topology of the new model. The model distance between two points with physical distance $N \cdot L$, where L is the model length scale, depends on the relative fractions of the two types of bonds and is given by:

$$L_m = N L \left(\frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2} + \sqrt{3} \frac{\varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right). \quad (8)$$

Note, that in the absence of bonds B_2 , i.e. $\varepsilon_2 = 0$, the model length scale coincides with the linear (physical) distance as in the cubic-based models. Also, in the absence of bonds B_1 , i.e. $\varepsilon_1 = 0$, the model length scale represents the zig-zag path between the two points along B_2 bonds. The model area through which the flow occurs equals only the areas of the square

boundaries of the truncated octahedrons, see Fig. 1. For a physical area $(N \cdot L)^2$, the model area is $A_m = (N \cdot L)^2 / 8$, because the area of a square boundary of the unit cell is $L^2 / 8$, where L is the model length scale.

3. Experimental and modelling details

3.1. Experimental methods

By way of an exemplar, this study focuses upon a single sample of a Lower Cretaceous limestone from a producing oil field in the Middle East. A 1.5'' diameter core plug of a skeletal pack-grainstone was sampled, trimmed and a thin section prepared from offcut material (Figure 3). Helium porosity and gas permeability and mercury injection capillary pressure data was provided with the core plug. The sample has a measured total porosity of 24.9% and a gas permeability of 17.2mD. Pore throat size distribution, as determined by mercury intrusion, is shown in Figure 4. Mean pore throat diameter determined by this method is 12 μ m ; varies between 4×10^{-3} μ m and 418 μ m. Image analysis of the thin section using ImageJ software measured a total porosity of 23.5%, with over 50% of the porosity being <100 μ m diameter and an average pore shape of 1.3 (where a pore shape of 1 is spherical (Leben, 2011)). The sample comprises primary interparticle macroporosity, minor mouldic porosity, created by selective dissolution of skeletal debris and rare vugs, following solution enhancement of primary interparticle macropores.

For X-ray CT scanning, samples were prepared as 'match-sticks' up to 4cm in length, and with a diameter of <2mm using rock-cutting equipment. The samples were imaged on the Xradia Micro XCT scanner at the Henry Moseley X-ray Imaging Facility, University of Manchester using x10 and x20 magnification and an exposure time of 20 seconds per projection (Etiese, 2011). The current ranged from 140-200mA, with an energy of 50-70kV. The pixel size was 1.2 μ m for the 10x objective and 0.6 μ m for the 20x objective with exposure times were in the order of 10 hours. An offset correction was applied to centre the rotation axis and ensure it is vertical which improves the sharpness of the reconstructed volume making the segmentation easier but is not expected to greatly affect the inferred pore network. The sample was set to rotate through 180 or 360° during data collection. Reconstruction of the projections to tomograms was by filtered back projection via CT-Pro and XM Reconstructor. Particular emphasis was made on removal of beam hardening effects.

Pore volume, size, shape and connectivity were then quantified. Prior to analysis, the data was filtered to reduce noise using a 3D median filter. Thresholding was then conducted based upon the grey level, in order to segment the porosity from the matrix. To ensure the best threshold level was identified so as to achieve a faithful representation of the pore network, the resulting pore system was calibrated against thin sections and back-scatter electron microscopy images. Regions incorrectly attributed as porosity due to diffuse grey-levels were then removed prior to statistical analysis. A 'skeletal' structure of the pore space was created by progressive thinning of the pores identifying the endpoints (pore centres) and nodes (pore throats). The size, shape and volume, the pore throat diameters, the total number of pore throats, and the co-ordination number for each pore, were then calculated.

The imaged cube is shown in Figure 3(c). The total imaged area of 1.5 x 2.1 x 1.4mm had a resolution of 1.1microns. The extracted pore volume is shown in Figure 3(d), from which a

shape factor of 1.83 was calculated. This is less spherical than the shape factor measured from 2D image analysis and it is unclear if this reflects the 3D geometry, the resolution of the imaging or the smaller size of the sample on which X-ray CT imaging was conducted. The probability density and cumulative distribution function of the pore and pore throat radii are shown in Figures 5 and 6 and the extracted pore and pore throat geometrical data summarised in Table 1. Note that the average pore size is significantly smaller than measured using image analysis of thin sections because a) the sample size was too small to incorporate the larger pores that are seen in thin section and b) the high resolution X-ray CT image is able to resolve a high volume of microporosity that cannot be described from a thin section. Conversely, the average pore throat diameter extracted from the X-ray CT image is higher than measured by mercury intrusion, reflecting the maximum resolution of $1.1\mu\text{m}$ within the image data.

Fig. 3. (a) and (b) representative thin section photomicrographs from thin section of carbonate sample. Thin sections are blue-dye resin impregnated to show porosity. Primary interparticle macropores are arrowed, m=biomoulds, v= vugs. (c) X-ray CT image of sample ($1.5 \times 2.1 \times 1.4\text{mm}$) and (d) separated pore volume (blue). Data derived from Etiese (2010).

Fig. 4. Pore size distribution as determined by image analysis of thin section (a), from Leben (2011) and pore throat diameter as measured by mercury intrusion (b).

Fig. 5. Probability density function (a) and cumulative probability function (b) of pore radii obtained from the experimental data. Probability density function is given by a histogram using a semi-log scale for convenience. Pore sizes are given in semi-log scale on both graphs.

Fig. 6. Probability density function (a) and cumulative probability function (b) of throat radii obtained from the experimental data. Probability density function is given by a histogram using a semi-log scale for convenience. Throat sizes are given in semi-log scale on both graphs.

Table 1. Summary of experimental data extracted from X-ray CT image of limestone sample (Etiese, 2010).

3.2. Models description

Simulations have been performed with models of three different sizes. These are given by the regions ($0 \leq X_1 \leq 20L$, $0 \leq X_2 \leq 20L$, $0 \leq X_3 \leq 40L$), ($0 \leq X_1 \leq 20L$, $0 \leq X_2 \leq 20L$, $0 \leq X_3 \leq 60L$) and ($0 \leq X_1 \leq 40L$, $0 \leq X_2 \leq 40L$, $0 \leq X_3 \leq 40L$) with respect to a coordinate system (X_1 , X_2 , X_3) oriented along the principal directions of the unit cell. The three sizes have been used to check the independence of the results on the length and cross section of the flow. Due to the lack of experimental data for the pore coordination spectrum of the study material, five possible spectra providing the same average coordination number of $z = 2.84$ have been considered. One basic spectrum is such that the two types of bonds are selected as throats with equal probability, which is equivalent to the following relation between elimination numbers $3\varepsilon_1 = 4\varepsilon_2$. The other four spectra are selected so that they have largest differences of all possible spectra. The elimination numbers for producing these spectra are given in Table 2. Comparison between the basic case and these four cases has been used to study the effect of the pore coordination spectrum on the macroscopic permeability.

In addition to the network with $z = 2.84$, we have constructed models with the following average pore coordination numbers: $z = 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6$, obeying the same constraint as the basic case $3\varepsilon_1 = 4\varepsilon_2$. These models have been constructed with the experimentally measured porosity, $\phi = 0.249$. Simulations with these have been used to study the effect of the coordination number on the macroscopic permeability. Further, we have constructed models with $z = 2.84$, obeying the constraint $3\varepsilon_1 = 4\varepsilon_2$, but with the following porosities, $\phi = 0.05, 0.075, 0.1, 0.125, 0.15, 0.175, 0.2, 0.225, 0.275, 0.3, 0.325, 0.35, 0.375, 0.4$. These models have been used to study the effect of pore volume on the macroscopic permeability.

The distribution of pore and throat sizes in all models have been performed using the respective cumulative probability functions shown in Figures 5 and 6. An illustration of a network constructed with the experimental data is given in Fig. 7.

Fig. 7. Network section constructed with experimental data $z = 2.84$ and $\phi = 0.249$. The two types of throats are shown as cylinders with different colours and lengths and radii to scale. Pores are shown with spheres with equal radii for clarity of the illustration, i.e. pore sizes are not to scale.

Thirty different random distributions of connectivity and sizes have been analysed for each of the models described above. The parameters of these models are given in Table 2. The model length scales, L , model flow lengths, L_m , and areas, A_m , are the average values obtained from the thirty distributions. The calculation of the macroscopic permeability for each model instance, however, uses its own length and area parameters. For each of the 30 realisations of each of the models, the experimentally measured pressures, p_{in} and p_{out} ($p_{in} > p_{out}$), have been applied to the sites at planes $X_3 = 0$ and $X_3 = 40L$ ($60L$ for M_1), respectively, and zero fluxes have been prescribed to the sites on the planes $X_1 = 0$, $X_1 = 20L$ ($40L$ for M_2), $X_2 = 0$, and $X_2 = 20L$ ($40L$ for M_2). The macroscopic permeability has been calculated using Eq. (7) in μm^2 . The average CPU time to solve the three model sizes is 26 min for $20 \times 20 \times 40$ models, 45 min for $20 \times 20 \times 60$ models and 150 min for $40 \times 40 \times 40$ models.

Table 2. Parameters of analysed models. The number of throats, lengths and areas shown in columns N_t , L , L_m , and A_m are the average values of thirty different distributions with the parameters in columns Size, z , ϕ , ε_1 and ε_2 .

3.3. Damage simulation

The coupling of the proposed pore space model with a complementary model for the mechanical behaviour of the solid phase is under development. This is discussed further in Section 5. To show how the model will be used to study the effect of mechanical damage on macroscopic permeability a heuristic argument is employed. The evolution of damage is mimicked by local increases in the conductivities of throats in a series of simulations steps and the macroscopic permeability is recalculated after each step.

The model is thought to be subjected to a tensile hydrostatic stress, σ , and the medium to be progressively damaged as this stress increases. Here we refer to damage as a sequence of meso-scale events related to local material failure around pores. This is different from the notion in continuum damage mechanics, where damage describes the change of the macroscopic elastic modulus or equivalently the change of the stress-strain relation at material points. The medium is quasi-brittle, i.e. the material failures are driven by elastic

strains. Consider a pore of radius R_α ($\alpha = 1, \dots, N$, and N is the number of pores) coordinated by C conductive bonds (existing throats) and $(Z-C)$ non-conductive bonds (potential throats), where $Z = 14$ for internal pores and $Z < 14$ for pores on the model surfaces. With respect to these bonds, the pore acts as a stress concentrator. In the worst case scenario it acts as a crack of length $2R_\alpha$ with respect to each pair of collinear bonds. The criterion for material failure around the pore is given by the Griffith criterion $\sigma = \sigma_c = K_{Ic} (2\pi R_\alpha)^{-1/2}$, where K_{Ic} is the fracture toughness of the solid phase and σ_c is the critical stress at failure. The radial displacement of the pore surface prior to failure can be represented as $u_\alpha = M \sigma R_\alpha$, where M is a constant dependent on the elastic modulus and Poisson's ratio of the solid phase (see e.g. Rice et al., 1978). From the failure criterion and the radial displacement, the increase of pore radius at the moment of failure can be written as $dR_\alpha = D R_\alpha^{1/2}$, where D is proportional to the fracture toughness of the material K_{Ic} and the elastic constant M . We refer to D as the material failure coefficient and note that larger failure coefficient corresponds to a material with higher toughness. In the absence of damage, i.e. at sufficiently small σ , pore enlargements are elastic and no change in throat sizes or connectivity, and hence in permeability, is assumed. With increasing σ , the damage starts with a failure around the largest pore in the system and continues via failures around pores of decreasing size. The simplifying assumptions in this work are that the failures are not redistributing stresses in the medium (the model is not yet coupled to mechanical deformation) and that a failure around a pore impacts all adjacent bonds, currently conductive and non-conductive (the load is hydrostatic).

Material failure around a pore of radius R_α is represented by changes in the adjacent bonds. At failure the pore relaxes from its strained configuration ($R_\alpha + dR_\alpha$) to its original size, with associated release of strain energy proportional to the pore volume increase before failure given by $dV_\alpha = (4\pi/3)[(R_\alpha + dR_\alpha)^3 - (R_\alpha)^3]$. The changes in the surrounding bonds are assumed to be such that the increase of their volumes equals the reduction of the pore volume during relaxation. For currently non-conductive bonds the process consists of attaching finite conductivity, which can be viewed as creation of new throats by changing their volumes from zero by the increment :

$$dV_{new} = \frac{Z-C}{(Z-C)^2 + C^2} dV_\alpha. \quad (9)$$

The volumes of the conductive bonds are increased from their current values V_i ($i = 1, \dots, C$) by the increments:

$$dV_i = \frac{V_i}{\sum_{i=0}^C V_i} \frac{C^2}{(Z-C)^2 + C^2} dV_\alpha. \quad (10)$$

These expressions ensure that the consequences of the local damage are represented simultaneously by creation of new flow channels and by local pore space enlargements. Note that the volume of all new conductive bonds, $(Z-C) \cdot dV_{new}$, and the increase of volume of all previously conductive bonds, the sum of dV_i for $i = 1, \dots, C$, equals the replaced increase of pore volume dV_α . For an isolated pore, i.e. $C = 0$, the damage is equally distributed to all previously non-conductive bonds. For a pore fully coordinated by throats, i.e. $(Z-C) = 0$, the damage is distributed to all throats proportionally to their current sizes. For $C = 0$ the increase of the total pore space volume, i.e. pores and throats, is $(V_\alpha + dV_\alpha)$ as the pore is now included in the accessible pore space and contributes to the increase of porosity. For $C > 0$, the increase of the total pore space volume is dV_α . The radii of the newly created throats are

calculated from Eq. (9) and their respective lengths. The new radii of the existing throats are calculated from the enlarged volumes ($V_i + dV_i$) and their respective lengths, where dV_i is given by Eq. (10).

When the above changes are made the system is recalculated to obtain the new macroscopic permeability as well as porosity. The process continues with hypothetically increasing stress σ to the failure of the next pore. At each failure event, the increase of the pore space volume, the average coordination number and the failure stress are recorded. One measure of macroscopic damage used is the relative increase of the system porosity, ϕ / ϕ_0 , where ϕ and ϕ_0 are the current and the initial porosity, respectively. A second measure for macroscopic damage used is the relative increase of the system average pore coordination number, z / z_0 , where z and z_0 are the current and the initial average pore coordination numbers, respectively.

4. Results

4.1. Prediction of permeability

The permeability values calculated by the models based on the experimentally determined pore and throat size distributions and average coordination number, M_0 , M_1 , M_2 , are shown in Fig. 8. The results from the 30 different distributions of throat locations and sizes for each model are shown with stars and the average values with circles.

Fig. 8. Permeability values predicted by the models based on experimental data (M_0 , M_1 , M_2 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the circles show the average values. The sizes of the models, the average values and the local morphology factors defined by Eq. (3) are depicted.

The results demonstrate an excellent agreement between the predicted and the measured permeability. The local morphology factors, m , defined by Eq. (3) and depicted in Fig. 8 are close to one. This suggests that with the proposed model the representation of the throats with pipes of constant cross section and radii from the experimental throat size distribution is sufficiently robust. The scatter in the permeability values decreases with model size, which is to be expected, as the larger size is associated with a more representative extraction of throat sizes from the experimental size distribution. The average predicted permeability seems to increase with the model size for the cases considered. However, the outcomes are not sufficient to judge that the prediction is improved with increasing size as the number of random distributions per model is limited to 30. By and large, the results show independence of the average predicted permeability on the model size. In order to assess the effect of the number of model realisations, we have also performed simulations with 60 realisations of the base model, M_0 . The result of these simulations is an average permeability of 16.9 mD, maximum and minimum values of 12.3 mD and 22.8 mD, respectively. This suggests a moderate change of the spread and improved consistency with the experimental value. It should be noted that while the spread cannot be eliminated so long as the model size is smaller than the representative volume for the material, an increase of model realisations potentially improves the prediction in average because of the wider set of throat sizes involved.

Fig. 9 shows the results obtained with the basic model, M_0 , and the four models, M_3 - M_6 , with different pore coordination spectra. As in Fig. 8, the results from the 30 different

distributions of throat locations and sizes for each model are shown with stars and the average values with circles. The models are ordered with decreasing elimination number for throats along B_1 bonds and increasing elimination number for throats along B_2 bonds, starting with a model nearly depleted of throats along B_2 (M3) and finishing with a model nearly depleted of throats along B_1 (M6).

Fig. 9. Permeability values predicted by the models with variable pore coordination spectrum (M_0 , M_3 - M_6 in Table 2). Each star shows the value obtained with one of 30 different distributions of throat locations and sizes; the circles show the average values. The elimination numbers producing the spectra for these models and the average permeability values are depicted.

The scatters in the predicted permeability values for the five models are similar, suggesting that the scatter is dictated primarily by the model size as shown in Fig. 8. Some increase in the predicted average permeability values is observed as the throats along B_1 decrease and the throats along B_2 increase. This suggests that there might be a dependence of permeability on the pore coordination spectrum. For the considered case of $z = 2.84$ this dependence appears to be marginal, possibly because of the small differences in the spectra that can be produced for this average coordination. However, it is expected that for pore spaces with larger average pore coordination, where large difference in the spectra can be observed such as in Fig. 2, the dependence of permeability on the pore coordination spectrum could be significant.

4.2. Effects of porosity and connectivity

Fig. 10 shows the results obtained with the models with variable porosity, M_7 - M_{20} , together with the results obtained with the model based on the experimental porosity, M_0 . The predicted permeability values are scaled with the average permeability of the model M_0 , $k_0 = 16.0$ mD (see Fig. 8). The curve connecting the average permeability values cannot be approximated by a single power law. It appears that for porosities below 0.25 a power law fit requires a power smaller than one, which is not typical for porous rocks. For porosities above 0.25 a power law fit requires a power larger than one. However, it should be noted that the results are obtained with models with changing porosity but identical pore and throat size distributions. Hence this is not a true porosity-permeability relation. The curve shows that the increase of permeability between a medium with 5% and 40% porosity and constant pore-scale parameters is about 6 times. .

Fig. 10 Normalised permeability values predicted by the models with variable porosity (M_7 - M_{20} in Table 2) and the model based on experimental data (M_0 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the line connects the average values to show the dependence of permeability on porosity.

Fig. 11 shows the results obtained with the models with variable pore coordination number, M_{21} - M_{30} , together with the results obtained with the model based on the experimental porosity, M_0 . As in Fig. 10, the predicted permeability values are scaled with the average permeability of the model M_0 . The line connecting the average values shows the effect of the average coordination number on permeability. The effect is stronger than exponential, since the increase of permeability between a medium with $z = 2.84$ and $z = 6$ is about 15 times, and the increase of permeability between a medium with $z = 2.0$ and $z = 6$ is about 125 times

Fig. 11 Normalised permeability values predicted by the models with variable pore coordination number (M_{21} - M_{30} in Table 2) and the model based on experimental data (M_0 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the line connects the average values to shows the dependence of permeability on average coordination number.

4.3. Evolution of permeability with pore space damage

The process described in Section 3.3 has been applied to one instance of the experimentally-based model M_0 , which produces a permeability nearly equal to the average predicted value $k_0 = 16.0$ mD (see Fig. 8). Simulations for this model have been performed with four failure coefficients, $D = 0.1, 0.2, 0.3, 0.4$, representing media with increasing toughness. The simulations have been terminated after 500 failure events, during which the average pore coordination number increased from $z_0 = 2.84$ to $z = 5.2$. Because the same model has been used, the failures in all simulations are triggered by the same sequence of pores with decreasing sizes. The differences between the four cases are the macroscopic stresses at which these failures occur and the corresponding amount of damage produced.

Fig. 12 shows the calculated evolution of macroscopic permeability, scaled by the initial value, with the relative increase of the average pore coordination number, z / z_0 . If z / z_0 is used as a measure for macroscopic damage, the increase of the toughness of the medium, represented by D , yields an increase of the permeability at one and the same macroscopic damage. Inversely, this means that a larger increase of connectivity is required in a less tough medium to achieve a given increase of permeability. This is due to the smaller amount of local damage inflicted by the failing pores for smaller toughness. The failure events occur at hydrostatic stresses proportional to D . The permeability changes, however, are not proportional to D at any connectivity. The evolution depends in a complex way on the structure of the pore space. Jumps or rapid increases in permeability, i.e. large dk / dz , correspond to damage around well-coordinated pores. This leads mainly to an increase of conductivity of the coordinating throats, some of which are part of the main flow path. Jumps or rapid increases of connectivity, i.e. large dz / dk , correspond to damage around non- or purely-coordinated pores leading mainly to the creation of new flow channels that do not contribute currently to the main flow path.

Fig. 12 Evolution of normalised permeability with pore space connectivity. Relative increase of the average pore coordination number is used as a measure for macroscopic damage. Four media with increasing toughness are shown. Toughness is represented by the failure coefficients D given. Normalised permeability values at four simulation instances are depicted for information.

Fig. 13 shows the evolution of permeability, scaled by the initial value, with the relative increase of porosity, ϕ / ϕ_0 . For a given macroscopic damage, measured by the ratio ϕ / ϕ_0 , the increase of toughness of the medium yields a reduction of the permeability. This also means that a smaller increase of porosity is required in a less tough medium to achieve a given increase of permeability. As before, there is no linear relation between D and the effects of porosity on permeability. In this case, rapid increases in permeability, i.e. large $dk / d\phi$, correspond to damage around smaller, well-coordinated, pores. This leads mainly to an increase in conductivity of the coordinating throats, some of which are part of the main flow path. Rapid increases in porosity, i.e. large $d\phi / dk$, correspond to damage around larger non-

coordinated pores. This leads to a relatively high increase of porosity and the introduction of new flow channels that do not contribute immediately to the main flow path.

Fig. 13 Evolution of normalised permeability with porosity. Relative increase of porosity is used as a measure of macroscopic damage. Four media with increasing toughness are shown. Toughness is represented by the failure coefficients D given. Normalised permeability values at two simulation instances are depicted for information.

5. Discussion

The results presented in Fig. 8 show that the proposed model can deliver very good predictions of macroscopic permeability using a relatively limited set of microstructural data. It is emphasised that the only data used in the model construction are experimentally measured pore and throat sizes, and average pore coordination number. The results suggest that the representation of throats as cylindrical pipes is a reasonable assumption. Evidently, an increase in model size yields a reduction of scatter, which is expected as the throat size population in the model becomes more representative for the experimentally measured distribution. The average permeability prediction does not appear to be affected by the model size.

An additional strength of the model is its ability to represent different pore coordination spectra. This has been demonstrated in Fig. 2 for a relatively large average coordination number. For the rock studied experimentally ($z = 2.84$), the difference in the possible pore coordination spectra is not significant. This translates into a marginal effect of the spectrum on the predicted permeability shown in Fig. 9. However, the trend observed in the figure suggests that the effect of the spectrum might be significant for porous media with larger average pore coordination numbers. Published studies have also emphasised the importance of including full coordination number distributions on reproduction of permeability (eg. Arns et al., 2004b, Raoof and Hassanizadeh, 2012).

The results presented in Figs. 10 and 11 demonstrate very important aspects of the pore space (microstructure)-permeability (macroscopic properties) correlation. The analysed microstructures possess identical pore and throat size distributions. When such microstructures also have the same average pore coordination number but different porosities, an increase of porosity from 5% to 40% is shown to yield a six-fold increase of permeability, Fig. 10. When such microstructures have the same porosity but different average pore coordination numbers, an increase of the average coordination number from 3 to 6 is shown to yield a 15-fold increase of permeability, while an increase from 2 to 6 yields a 125-fold increase of permeability, Fig. 11. This highlights the much stronger effect of the pore space connectivity on the macroscopic flow than the effect of the porosity. This has significant implications to the industry-standard practice of predicting permeability from porosity, which is widely understood to be extremely challenging in carbonate hydrocarbon reservoirs (eg. Lucia, 2007, Hollis et al., 2010) and support observations made using other pore network simulations of single phase permeability and relative permeability of sedimentary rocks (eg. Arns et al., 2004b; Youssef et al., 2007; Raoof and Hassanizadeh, 2012). The mean coordination number $z = 2.84$ used in this study is close to the value of 3 observed by Youssef et al (2007) and is consistent with the authors unpublished data. Knackstedt et al. (2006), Sok et al. (2007) and Al-Kharusi and Blunt (2007) all report an average pore coordination of 3 to 5, with a Z_{max} of more than 24. Overall, however, there is relatively little published

data on the topology of carbonate rocks, and therefore it is difficult at present to draw a relationship between carbonate rock type, pore topology and permeability. What is clear is that without some mechanism by which pore connectivity can be accounted for, permeability prediction will remain an area of considerable uncertainty.

Of key interest to us is the effect of the pore space evolution on the macroscopic permeability, when triggered by different mechanisms, such as corrosion and mechanical damage. The corrosion-induced changes are relatively easy to implement and analyse, as these are associated with local increases of pore and throat sizes. This can be achieved with a complementary model having the same geometry and topology as the pore space model and reflects the understanding that corrosive agents are transported predominantly along the easy pathways of the pore space, rather than through the solid phase. The model can have its own driving forces, such as electrochemical potential gradients or concentration gradients, but can also be informed from the results of the pore space model about local fluid fluxes. Conversely, the results from the complementary model in terms of pore space changes will inform the pore space model.

The pore space changes due to mechanical damage are more difficult to model and analyse, as these are associated with mechanically driven nucleation and growth of micro-cracks. So far mechanical damage has been introduced in a heuristic manner, where the material failure around a pore is represented by the creation of new flow channels to initially unconnected neighbouring pores and by the enlargement of existing flow channels. The process is isotropic, i.e. all coordinating directions of the pore are equally considered, due to the assumed tensile hydrostatic stress field. Even with such a simplification, the simulations revealed interesting properties of the damage-permeability correlation. Figs. 12 and 13 illustrate the complex dependence of the permeability evolution on the structure of the pore space and on the material mechanical properties. They show that the toughness of the medium dictates the manner by which a given change of permeability is achieved. A less tough medium requires a lower increase of porosity and a higher increase of pore space connectivity than a tougher medium, which would require a higher increase of porosity and a lower increase of connectivity. Clearly, a tougher medium requires a higher external load to develop damage, but this load is not linearly related to the material toughness. The evolution of permeability depends on the pore space structure, the material toughness and the applied load in a complex manner. This highlights the importance of coupled models for analysis of the damage-permeability relations.

More realistic studies, in particular to analyse loading cases of practical interest, can be achieved by coupling the proposed pore space model with a complementary model for the deformation of the solid phase of the porous medium. A natural and beneficial approach is to use a discrete representation of the solid phase that has the geometry and the topology of the site-bond support used for the construction of the pore space. In this approach, the sites of the complementary model are again associated with the pores whether they be isolated or connected. The bonds are deformable links between all existing pores, i.e. all bonds of the site-bond support are links in the solid phase model. An important requirement for these bonds is that they must represent all possible relative deformations between the coordinated grains, i.e. three independent relative displacements and three independent relative rotations. This is an emergent requirement at the meso-scale and marks a major difference from e.g. atomic-scale models or discrete element method models, where the bonds between atoms or nodes transfer axial forces only due to the relative displacement of the atoms or nodes along the bonds directions.

Interestingly, the discrete model based on the truncated octahedral lattice has been shown to be the only one that can reproduce the elastic properties of any material of practical interest (Jivkov and Yates 2012). This provides a strong support for the use of such a model for the deformation of the solid phase coupled with the pore space model analysed in this work. To reflect the existence of throats between some pores in the pore space model, the mechanical properties of the corresponding deformable bonds can be altered so that a larger throat yields a weaker deformable bond. A solution of the deformation model subjected to prescribed external loads or internal pore pressures will provide the forces in the bonds. Damage in the deformation model can be assumed to initiate at pores as a result of the forces in its coordinating bonds. Unlike the current work, such damage need not be isotropic in the advanced model. If the failure criterion is met due to the action of a particular pair of forces, only failure perpendicular to this pair can be considered. In the deformation model this can be represented by the removal of the pair of bonds causing the failure. In the pore space model this can be represented by changes in the throats sizes or the creation of new throats in the failure plane, similarly to the approach described in Section 3.3. These ideas are under development and will be reported later. The key benefit with such modelling is that the relation between damage and permeability for a given material could be determined as a function of the amplitudes and the nature of the mechanical loads.

6. Conclusions

In this work we have:

- Conceptualised the meso-scale structure of a porous medium with a simple bi-regular cellular lattice based on truncated octahedral cell;
- Described the construction of pore networks using this regular support and experimental data;
- Demonstrated that the new lattice support can be used for producing a rich set of real pore spaces;
- Described the use of the model for calculations of macroscopic permeability and illustrated this on a set of experimental data;
- Shown that the model can predict experimentally measured macroscopic permeability with very good accuracy;
- Analysed the effects of porosity and network connectivity on permeability, and highlighted the much stronger effect of the latter;
- Proposed a heuristic model for pore space damage that mimics local material failures by connectivity and conductivity changes;
- Demonstrated the importance of the material mechanical behaviour on the evolution of permeability with damage;
- Discussed the potential of the proposed model for developing coupled mechanical-transport models .

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Figures

Fig. 1. Unit cell (truncated octahedron) with all possible bonds (a) and site-bond support for pore space construction (b). Letter S denotes a site or pore; letters B_1 and B_2 denote two types of bonds or prospective throats.

Fig. 2. Fractions of pores with different coordination numbers in a network with average pore coordination $z_u = 6$. These are obtained with different elimination numbers for the two types of bonds -given in the plots.

Fig. 3. (a) and (b) representative thin section photomicrographs from thin section of carbonate sample. Thin sections are blue-dye resin impregnated to show porosity. Primary interparticle macropores are arrowed, m=biomoulds, v= vugs. (c) X-ray CT image of sample (1.5x2.1x1.4mm) and (d) separated pore volume (blue). Data derived from Etiese (2010).

Fig. 4. Pore size distribution as determined by image analysis of thin section (a), from Leben (2011) and pore throat diameter as measured by mercury intrusion (b).

Fig. 5. Probability density function (a) and cumulative probability function (b) of pore radii obtained from the experimental data. Probability density function is given by a histogram using a semi-log scale for convenience. Pore sizes are given in semi-log scale on both graphs.

Fig. 6. Probability density function (a) and cumulative probability function (b) of throat radii obtained from the experimental data. Probability density function is given by a histogram using a semi-log scale for convenience. Throat sizes are given in semi-log scale on both graphs.

Fig. 7. Network section constructed with experimental data $z = 2.84$ and $\phi = 0.249$. The two types of throats are shown as cylinders with different colours and lengths and radii to scale. Pores are shown with spheres with equal radii for clarity of the illustration, i.e. pore sizes are not to scale.

Fig. 8. Permeability values predicted by the models based on experimental data (M_0 , M_1 , M_2 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the circles show the average values. The sizes of the models, the average values and the local morphology factors defined by Eq. (3) are depicted.

Fig. 9. Permeability values predicted by the models with variable pore coordination spectrum (M₀, M₃-M₆ in Table 2). Each star shows the value obtained with one of 30 different distributions of throat locations and sizes; the circles show the average values. The elimination numbers producing the spectra for these models and the average permeability values are depicted.

Fig. 10 Normalised permeability values predicted by the models with variable porosity (M_7 - M_{20} in Table 2) and the model based on experimental data (M_0 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the line connects the average values to show the dependence of permeability on porosity.

Fig. 11 Normalised permeability values predicted by the models with variable pore coordination number (M_{21} - M_{30} in Table 2) and the model based on experimental data (M_0 in Table 2). The stars show values obtained with 30 different distribution of throat locations and sizes; the line connects the average values to shows the dependence of permeability on average coordination number.

Fig. 12 Evolution of normalised permeability with pore space connectivity. Relative increase of the average pore coordination number is used as a measure for macroscopic damage. Four media with increasing toughness are shown. Toughness is represented by the failure coefficients D given. Normalised permeability values at four simulation instances are depicted for information.

Fig. 13 Evolution of normalised permeability with porosity. Relative increase of porosity is used as a measure of macroscopic damage. Four media with increasing toughness are shown. Toughness is represented by the failure coefficients D given. Normalised permeability values at two simulation instances are depicted for information.