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Grain-mixing modelling of the porosity and permeability of binary mixtures

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Summary

The porosity and permeability of binary mixtures of spherical grains were modelled theoretically and studied empirically against such variables as grain-size, grain-size ratio, grain volume fraction and grain packing. The results confirmed that binary mixing of different-sized grains always results in a porosity loss. The degree of porosity loss was found to be a function of the grain-size ratio. Consequently, the mixture with the highest grain-size ratio of 3 dropped to the lowest minimum porosity of 0.3116 while the mixture with the minimum grain-size ratio of 1.5 experienced the highest minimum porosity of 0.3716. The observed porosities could not be described by some of the existing porosity models including the ideal and fractional packing models due to the assumptions of ideal packing and no-mixing respectively underlying these models. Thus, a corrected fine packing (or replacement) model was developed during this research to incorporate the grain-size ratio effect on porosity. Together with the interstitiation model, the corrected replacement model gave the best fit to the observed porosities. The mixtures' permeabilities could not be modelled by the grain-size/porosity-dependent permeability models because these models tend to mimic the trend of the representative porosity used. The weighted geometric/harmonic mean permeability models (weighted by volume fraction) described the observed permeabilities best.

Introduction

The understanding of how grain mixing and packing control the porosity (Dias et al., 2004; Kamann et al., 2007), permeability (Bernabe and Maineult, 2015), acoustic transmission (Leurer and Brown, 2008), heat flow (Wallen et al., 2016) and electric current in rocks (Glover, 2015) is very useful in various fields of science. Among these fields are Soil Science (Zhang et al., 2011), Petrophysics (Sakaki and Smits, 2015) and Hydrology (Zhang et al., 2009). However, our focus is on porosity and permeability studies.

Various models have been developed to predict the porosity (i.e. a measure of storage capacity) and permeability (i.e. a measure of fluid-flow permission) of a single-sized grain pack and ideally packed binary mixtures (Kozeny, 1927; Carman, 1937; Kamann et al., 2007; Glover, 2006). However, real rocks are made of the mixture of grains of various sizes with non-ideal packing. These scenarios need to be considered when analysing three-dimensional packing in rocks. Thus, we have undertaken this research to model the effects of grain size, relative grain size, grain fraction and grain packing on the porosity and permeability of granular mixtures (as typified by clastic rocks). However, given the extreme complexity in the modelling of packing in rocks with very poor grain sorting, we have focused on binary mixtures which consists of only two sizes of grains. These mixtures can considerably represent certain real facies like shaley sands (Marion, 1990) and pebbly sands.

Theoretical Background

Various binary-mixing porosity and permeability models have been developed. These include the ideal-packing porosity models (Kamann et al., 2007; equations 1a-b), the fractional-packing porosity model (Koltermann and Gorelick, 1995; equation 2), the fine packing porosity model (Dias et al., 2004; equation 3), the interstitiation/non-cutting replacement porosity models (P. Glover, personal communication, 2017; equations 4a-b), the Kozeny-Carman permeability model (Kozeny, 1927; Carman, 1937; equation 5), the RGPZ permeability model (Glover et al., 2006; equation 6) and the weighted mean permeability model (Glover et al., 2006).

We have endeavoured to implement/validate these equations via experimentation with binary mixtures of spherical grains. For each mixture, the porosity and hydraulic permeability were measured by specially designed apparatuses. The result of this research is applicable not only to geosciences, but also to all fields that require the knowledge of porosities and permeabilities, including material science, process engineering and soil science.

The ideal coarse packing model,

$$\Phi_n = \Phi_c - r_f(1 - \Phi_f) \qquad r_f < \Phi_c;\ V_m = V_c \qquad (1a)$$

The ideal fine packing model,

$$\Phi_N = r_f \Phi_f \qquad r_f > \Phi_c;\ V_m = V_f + V_{SC} \qquad (1b)$$

where Φ_c is the porosity of the premixed coarse components, Φ_f is the porosity of the premixed fine components, r_f is the ratio of the premixed volume of the fines to the volume of the mixture, V_m is the volume of the mixture, V_c is the volume of the coarse component, V_f is the volume of the fine component and V_{SC} is the volume of the solid coarse component (kamann et al., 2007).

The fractional packing model (equation 2) considers that both fine and coarse packing may occur together. It categorizes a mixture into region A (with coarse packing) and region B (with fine packing).

$$\Phi_{fractional} = \frac{VVCA - VSFA}{VA}\frac{VA}{VM} + \frac{VVFB}{VFB + VSCB}\frac{VB}{VM} \quad (2)$$

where VA is the volume of region A, VB is the volume of region B, VM is the volume of the mixture, VVCA is the volume of void in the coarse grained component of region A, VSFA is the volume of solid fine grains in region A, VFB is the volume of fine component in region B, VVFB is the volume of voids in the fine component within region B, VSCB is the volume of solid coarser grains in region B (Kamann et al., 2007; Koltermann and Gorelick, 1995).

Dias et al. (2004) acknowledged the effect of grain size ratio on binary mixtures' porosity and incorporated a correction function $\{\exp(1.2264 X_D\sqrt{D/d})\}$ to give a fine packing model defined as $\mathcal{E} = \frac{\mathcal{E}_d^0(1 - x_D)exp\left(1.2264 x_D^{\sqrt{D/d}}\right)}{1 - \mathcal{E}_d^0 x_D}$ $X_D \leq X_{D,min}$ and $D/d \geq 10$ (3)

where $\mathcal{E}_d^0$ is the porosity of a uniform bed of small particles, D/d is the ratio of coarse grain size to fine grain size, x_D is the coarse particle volume fraction (Dias et al., 2004). Since the above corrected model is limited to grain size ratios greater or equal to 10, it could not be used in this work.

The interstitiation model,

$$\Phi_n = \frac{\Phi_c - X_{vf}}{1 - \Phi_c} \qquad X_{vf} < X_{crit} \quad (4a)$$

The non-cutting replacement model,

$$\Phi_N = \Phi_f\left[\frac{X_{vf}(1 - 2\Phi_f)}{1 - \Phi_f - \Phi_f X_{vf}}\right] \qquad X_{vf} > X_{crit} \quad (4b)$$

where Φ_c is the porosity of the premixed coarse components, Φ_f is the porosity of the premixed fine components, X_{vf} is the fines' volume fraction, X_{crit} is the critical fines' volume fraction at the minimum porosity (P. Glover, personal communication, 2017).

The Kozeny-Carman permeability model,

$$k = \frac{d_m^2 \Phi^3}{180(1 - \Phi)^2} \quad (5)$$

where d_m is the median grain diameter and Φ is the representative porosity (Kozeny, 1927 & Carman, 1937).

The RGPZ permeability model,

$$K = \frac{d_{grain}^2}{4am^2\,\Phi^{-m}(\Phi^{-m} - 1)^2} \quad (6)$$

where k is the permeability (m^2), d_{grain} is the effective grain diameter in (m), Φ is the porosity, a is a constant which is equal to 8/3, m is the cementation exponent which is equal to 1.5 for spherical grains (Glover, 2006; Glover, 2015).

The weighted mean permeability models (Glover et al., 2006).

$$K_{arithmetic} = K_f V_f + K_c V_c \quad (7a)$$

$$K_{harmonic} = \frac{1}{\frac{V_f}{K_f} + \frac{V_c}{K_c}} \quad (7b)$$

$$K_{geometric} = {K_f}^{V_f} {K_c}^{V_c} \quad (7c)$$

where V_f and V_c are the grains' volume fractions of the fine and coarse constituents respectively, and k_f and k_c are the permeabilities of the fine and coarse constituents respectively.

Results and Discussions

Figure 1 reveals that the ideal packing model has a similar trend (but not values) to the observed porosities due to the impracticability of ideal packing. Conversely, the fractional packing model is dissimilar (both in trend and values) to the observed porosities. For $X_{vf} > X_{crit}$, the fractional-packing porosity progressively increased from the fines end-member's porosity (at 100% fines) towards the coarse end-member's porosity as the coarse grains fraction increased due to the assumption of no mixing. For $X_{vf} < X_{crit}$, the fractional packing porosity reduces to an ideal situation.

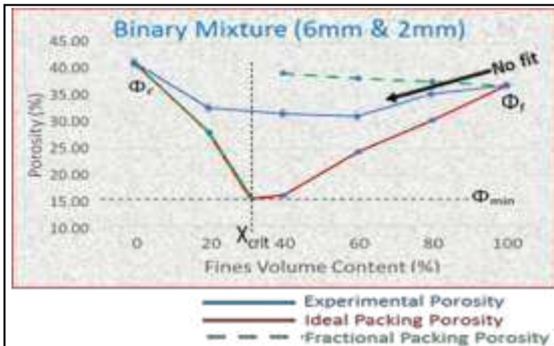

Figure 1: The observed porosities in comparison with the ideal and the fractional packing models for the grain-size ratio of 3.

Figure 3 shows that the interstitiation model gave a good prediction for the experimental porosity in the range of coarse packing. However, the non-cutting replacement model (equation 4b) was tested mathematically and found to vary with the form of cell used. Also, it has not accounted for the grain size-ratio effect on the packing porosity. Consequently, we developed a corrected fine packing (replacement) model (equation 10) that accounted for the grain size ratio effect and that correctly describes the fine packing porosity following this mathematical routine:

Consider a cylindrical cell, fine spherical grains of radius ŕ and coarse spherical grains of radius, Ŕ. Let the height of the cell be h and the cross-sectional radius be h/2. We define a scaling relationship between the grain sizes and the cell height, ŕ = hr and Ŕ = hR, where r and R are dimensionless reperesentation of the fine and coarse grain sizes respectively. We start by filling the cell with n fine grains (figure 2). The porosity of the resultant structure is given by

$$\Phi_f = \frac{\frac{\pi h^3}{4} - \frac{4}{3}n\pi(hr)^3}{\frac{\pi h^3}{4}}$$

Grain-mixing modelling

Now, let us replace some of the fine grains by coarse grains. This fine packing or replacement process results in a net porosity reduction since some of the fine grains and their associated porosity are replaced by solid coarse grains.

Figure 2: Porosity-measuring cylindrial cell.

The porosity of the resultant structure is given by

$$\Phi_N = \frac{\frac{\pi h^3}{4} - \frac{4}{3}n\pi(hr)^3 - \frac{4}{3}N\pi(hR)^3 + \frac{4}{3}N\pi(hR)^3(1-\Phi_f)}{\frac{\pi h^3}{4}}$$

$$\therefore \Phi_N = \Phi_f\left(1 - \frac{16}{3}NR^3\right) \qquad (8)$$

where $+\frac{4}{3}N\pi(hR)^3(1-\Phi_f)$ is a replacement term which represents the volume of solid fine grains replaced by $\frac{4}{3}N\pi(hR)^3$ volume of solid coarse grains. The remaining volume of solid fine grains in the binary mixture is given by $V_f = \frac{\pi h^3}{4}(1-\Phi_f)\Phi_c$. The fines volume fraction can therefore be defined as

$$X_{vf} = 1 - \frac{\frac{4}{3}N\pi R^3}{\frac{\pi}{4}(1-\Phi_f)\Phi_c + \frac{4}{3}N\pi R^3}$$

This implies that $N = \frac{\frac{\pi}{4}(1-\Phi_f)\Phi_c(1-X_{vf})}{\frac{4}{3}\pi R^3 X_{vf}}$ (9)

Expressing this model in terms of the fines volume fraction (X_{vf}) by substituting equation 9 into equation 8 =>

$$\Phi_N = \Phi_f\left(1 - \frac{16}{3}\left(\frac{\frac{\pi}{4}(1-\Phi_f)\Phi_c(1-X_{vf})}{\frac{4}{3}\pi R^3 X_{vf}}\right) * R^3\right)$$

$$\therefore \Phi_N = \Phi_f - \frac{(1-\Phi_f)(1-X_{vf})\Phi_{min}}{X_{vf}} \qquad X_{vf} > X_{crit} \quad (10)$$

where Φ_f is the porosity of the premixed fine components, X_{vf} is the fines' volume fraction and Φ_{min} is the minimum porosity. Φ_{min} represents the grain size ratio effect.

Although we initially assumed a cylindrical cell in the process of formulating equation 10, the equation is independent of the form of cell used. Additionally, since Φ_f and X_{vf} cannot be greater that unity, it follows that the term $\frac{(1-\Phi_f)(1-X_{vf})\Phi_{min}}{X_{vf}}$ in equation 8 cannot be negative. This confirms that the fine packing or replacement process always results in porosity loss. Another interesting fact about this corrected replacement model is that it can be negative at very low value of X_{vf}. If this happens we know that we have moved into the range of coarse packing and should use the coarse packing (or interstitiation) model instead.

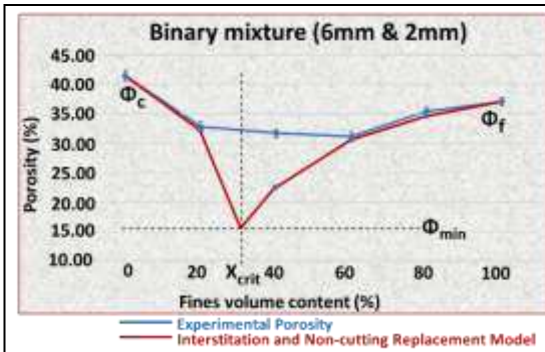

Figure 3: Observed porosities in comparison with the interstitiation/corrected replacement models for the grain-size ratios of 3.

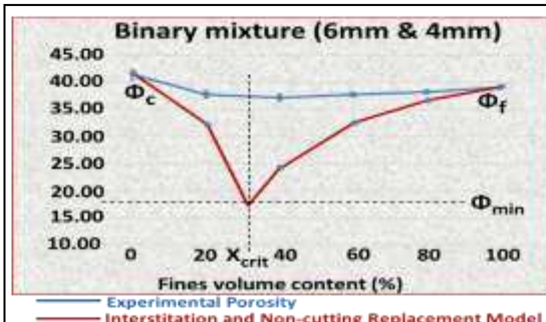

Figure 4: Observed porosities in comparison with the interstitiation/non-cutting replacement models for the grain-size ratios of 1.5.

Together with the interstitiation model, the corrected replacement model gave a good fit to the experimental porosities except at the minimum porosity figure 3. The reason for this discrepancy at the region of minimum porosity ($0.25<X_{vf}<0.35$) is due to the wedging of the fine particles between the coarse particles (Dias et al., 2004). This wedging effect produces a higher minimum porosity than theoretical expectations.

However, even though the interstitiation/non-cutting replacement model gave the best prediction of the experimental porosities, its degree of fitness decreases with a decrease in grain-size ratio (figure 4). This is because the grain-size ratio is a determinant of the effectiveness of binary mixing. Also, for the mixtures with small grain size ratio, wall effect tend to be more pronounced and this increases the overall mixtures porosity (Scott, 1960; Le Goff et al., 1985; Zou et al., 1995). Thus the least grain-size ratio of 1.5 gave the worst fitness between the observed data and the interstitiation/corrected replacement model (figure 4).

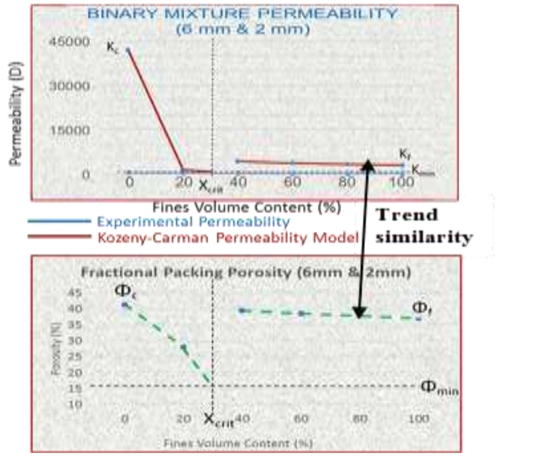

Figure 5: The Kozeny-Carman permeability model in comparison with the fractional packing model.

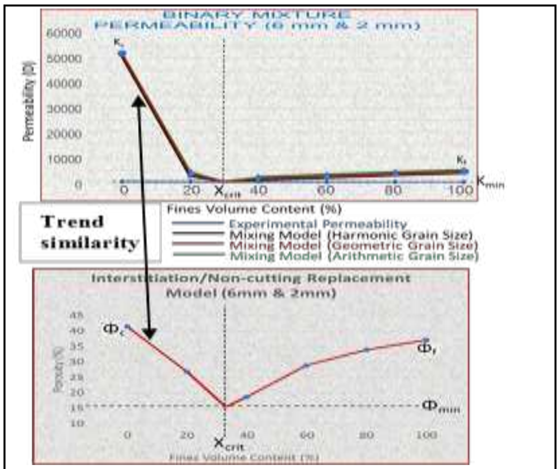

Figure 6: The RGPZ permeability model in comparison with the interstitiation/Corrected replacement models.

Figure 5 shows that the trend of the Kozeny-Carman model tends to mimic that of the fractional packing porosity which was used as its representative porosity. Conversely, figure 6 shows that the trend of the RGPZ model tends to mimic the trend of the interstitiation/Corrected replacement porosity which was used as its representative porosity. This is because the grain-size/porosity-dependent permeability models (including the Kozeny-Carman and the RGPZ models) are unduly controlled by their representative porosities. Thus, these permeability models are insufficient in predicting the observed permeabilities.

The observed permeabilities of the binary mixture were best fitted by the weighted averages of the end members permeabilities (weighted by volume fraction; figure 7). This validates that the permeability of a binary mixture is controlled by the end members' permeabilities (rather than the representative porosity as proposed by the grain-size/porosity-dependent permeability models).

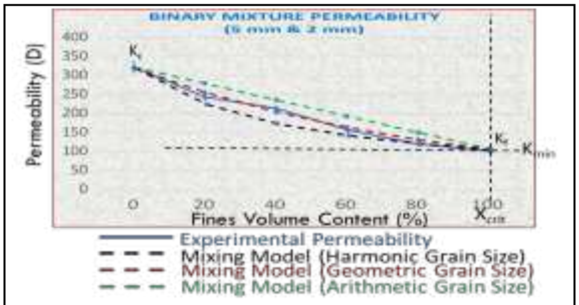

Figure 7: Observed permeability in comparison with the weighted mean permeailities for grain size ratio of 2.5.

Conclusions

Grain-size ratio is an important determinant of binary mixtures porosity. Thus, a good model should incorporate not only the effects of grain sizes and constituent volume fractions, but also the grain size ratio effect. Regarding permeability, grain size/porosity-dependent models are not sufficient because it is possible for a rock to be highly porous like pumice and yet impermeable. Thus, the weighted mean permeability models performed best in modelling the observed permeabilities. Since these models depend on end members permeabilities (and not directly on grain size), we have used the volume fraction of each end member (rather than the number of grains) as the best choice of weight.

Additionally, it should be noted that the experiments conducted in this research represent real cases of binary mixtures. Geological processes could present different scenarios. These may include cases of more than two grain sizes or cases where diagenesis has taken its toll on the rock. In all these cases, the porosity and permeability will be different from the models describing pure binary mixtures. The magnitude of the disparity could then be used to measure the extent of these processes.

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