Particulate structure and microstructure evolution of concrete investigated by DEM

Part 2: Porosimetry in hydrating binders

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Durability of concrete in engineering structures is becoming more and more of a major problem. Research into such problems is complicated and expensive, however. Developments in computer technology make it possible nowadays realistically simulating cementitious materials and studying its pore network structure. In this paper use is made of the dynamic DEM (Discrete Element Method) denoted HADES (Habanera's Discrete Element Simulator), introduced earlier, and a new vector-based hydration simulation system, XIPKM (Extended Integrated Particle Kinetics Model) . Inspired by developments in robotics, a pore exploration system is developed in DraMuTS (Double Random Multiple-Tree Structuring). The tree structure inside pores governs pore topology, including pore continuity. For determination of pore geometry such as pore size, a second uniform random point system is used. In each of these points, star volume measurements govern local pore size, while the collected data allow constructing a volume-based pore size distribution. The method is illustrated by means of data pertaining to Portland cement (PC) paste and rice husk ash-blended PC. This approach is demonstrated providing all necessary pore network information relevant for durability estimation.

Keywords: Concrete, cement, DEM, hydration simulation, pore connectivity, pore size distribution, blended cement

1 Introduction

Durability is becoming an issue of major concern. Hence, it would be attractive exploiting the modern computer facilities for this purpose, favourably competing with experimental research that is mostly more time-consuming and laborious. Since many of the properties of interest will be structure-sensitive, a realistic dispersion of the binder particles would be a prerequisite for getting reliable data on the pore network structure that is at the basis of transport-based durability problems. This can be accomplished by DEM. In this paper use is therefore made of the dynamic DEM, HADES described in Part 1. We have argued that the popular random sequential modelling systems (RSA) do not provide proper dispersion characteristics: particles will be too evenly distributed in container space (Stroeven, 1999; Williams and Philipse, 2003; Stroeven *et al.,* 2010). Moreover, the effect of improper cement particle dispersion in the fresh state exerts significant influences on the pore de-percolation process during hardening, as shown in Part 1. The influences of dispersion on porosity and pore size distribution are moreover demonstrated by a simple example in Stroeven *et al.* (2009). The example was based on comparing DEM- (by SPACE: Software Package for the Assessment of Compositional Evolution) and RSA-generated cement particle dispersions (1-10 μm particles with volume fraction of 0.4 in 50 μm container). Fig. 1 gives two sections of the respective cubes. Also a comparison between the sections of SPACE-generated particle dispersions presented in Fig. 2 of Part 1 and HYMOSTRUC3D-generated ones, such as Fig. 9 in Ye and van Breugel (2009), clearly reveals the characteristic dispersion differences. This leads among other things to the obvious improvements in the pore de-percolation process predicted by DEM simulation, as dramatically demonstrated in Fig. 1 of Part 1.

Particle packing in the fresh state is discussed in Part 1 of this issue (He *et al.*, 2013). Next stage in producing a realistic hardening cementitious binder involves hydration simulation. An improved version of the well-known vector approach is used. This is denoted Extended Integrated Particle Kinetics Model (XIPKM). It is an extension of the Integrated Particle Kinetics Method (IPKM) that was first used by Jennings and Johnson (1986). Navi and Pignat (1996), van Breugel (1991) in HYMOSTRUC3D and Stroeven (1999) in SPACE have used IPKM. Once the material is available in virtual reality, the pore network characteristics have to be assessed. A robotics-inspired new exploration method is developed and will be introduced herein. It is denoted "Double Random Multiple-Tree Structuring" (DRaMuTS). When completed, the pore network structure is represented by trees existing of dispersed points connected by lines *inside* the pore system. Next, a uniform random point system is generated for performing local measurements in such points on the pore system. The fraction of points inside the pore system directly yields porosity. Basically, pore topology, including pore connectivity can be directly derived from the tree structure. For assessment of pore size distribution the so called star volume method is applied (Gundersen *et al.*, 1988). This is a very significant advancement in terms of economy and reliability over the serial sectioning and 3D reconstruction technique that is commonly used in life sciences in experimental designs and was developed for application to virtual concrete by Ye (2003).

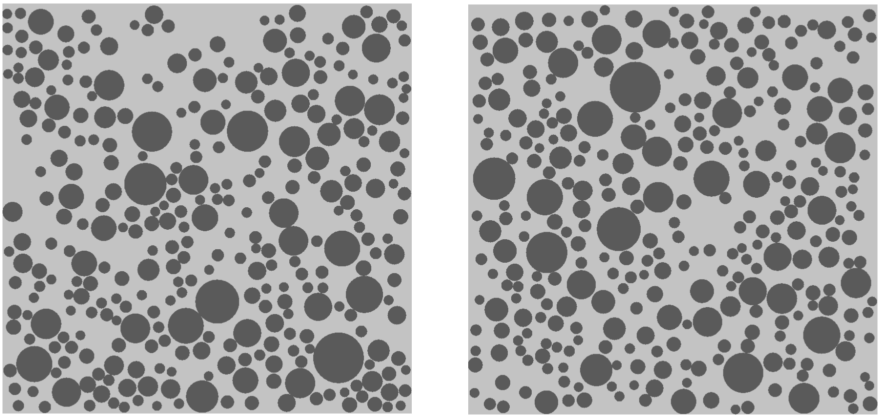


Figure 1. Range of particle sizes packed in container with rigid boundaries at 0.4 volume fraction. At the left is a section of a DEM (SPACE)-produced cube (by dynamic mixing), at the right is a section from a cube with the same ensemble of particles obtained by RSA procedure.

2 Hydration simulation of (blended) Portland cement paste

In this research, a new numerical multi-phase model for simulating hydration of (pozzolanic blended) cement is utilized. Herein, the hydrating grains are simulated by spherical integrated particles based on the so called 'integrated particle kinetics model' (IKPM), coupling a fresh core of material and its hydration product (CSH) (Stroeven and Stroeven, 1997; Le and Stroeven, 2012). Nonetheless, different from IKPM model that is used for only single phase material (C_3S), each fresh spherical core also incorporates information of its components, i.e. percentages of phases in this model. So, the model is referred to as 'extended integrated particle kinetics model' (XIPKM).

The present model takes into account the two major phases of PC, i.e., tri-calcium silicate (C_3S) and di-calcium silicate (C_2S). Yet, it could be expanded to cover more phase components. Fig 2 is an illustration of the hydration model with three types of particles.

Besides the two composite/integrated PC particles (left and middle ones in Fig. 2), another hydration product (CH) is modelled as single spherical particles (right one in Fig. 2). Researches have demonstrated that the CH product diffuses and nucleates randomly either in the pore space or precipitates on the surface of the existing CH grains. The quality of the new hydration concept is verified on the basis of experimental data in Fig. 2. Much better

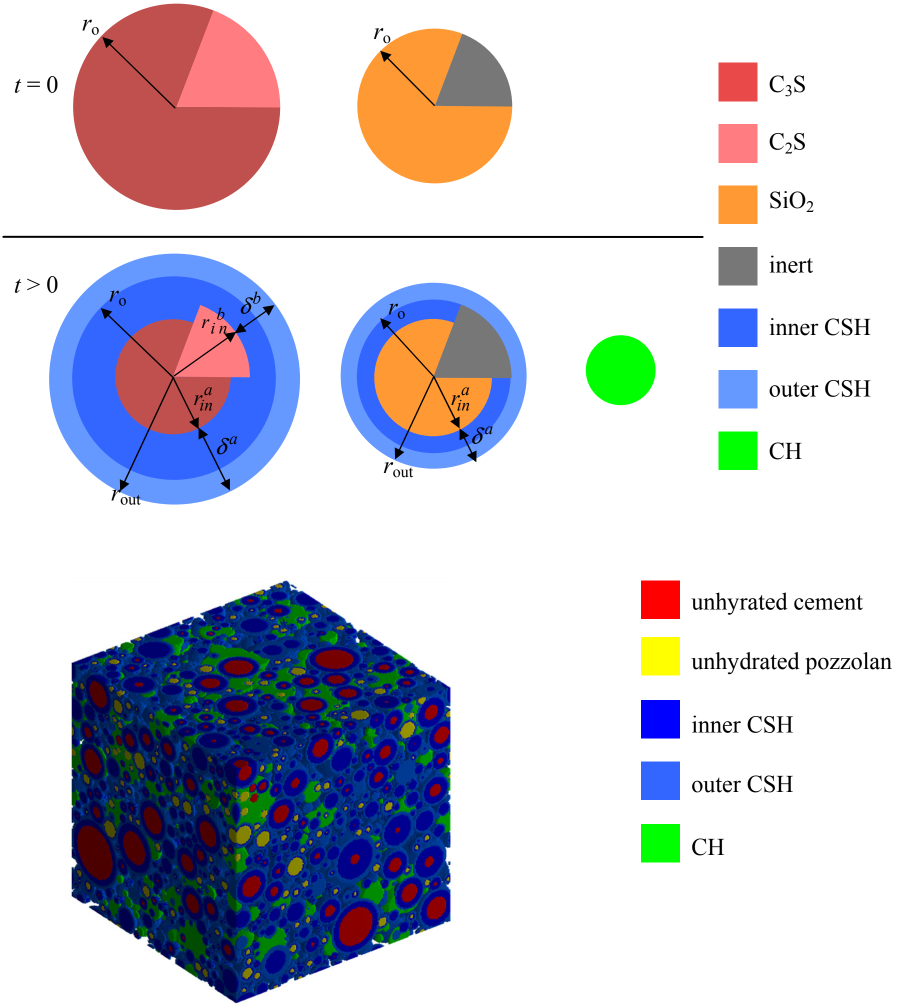


Figure 2. Particle models of cement, pozzolanic admixture and hydration product (at the left). Microstructure visualized with the phase voxel system (at the bottom), whereby each unhydrated multi-phase core is represented by a sphere whose volume equals the total volume of the phases. (This figure is in colour at www.heronjournal.nl)

correspondence is found than can be expected from popular random sequential systems, as argued by Williams and Philipse (2003).

Hydration of a hydraulic material involves its chemical reactions with water. The volume change of each phase (cement components, pozzolan, free water and hydration product) can be computed via the chemical equilibrium equations. In the present model, the cement is assumed to be composed of its two major compounds C_3S and C_2S. So, the hydration products are only calcium silicate hydrate (CSH) and calcium hydroxide (CH). The chemical equilibrium equations can be expressed in relative volume ratios of water and hydration products to C_3S and C_2S according to Bentz *et al.* (1994)

$$1.0V_{C_3S} + 1.34V_H \rightarrow 1.521V_{CSH} + 0.610V_{CH} \qquad (1)$$

$$1.0V_{C_2S} + 1.49V_H \rightarrow 2.077V_{CSH} + 0.191V_{CH} \, . \qquad (2)$$

Similarly, for the silica (SiO_2) in the pozzolanic admixture, Bentz *et al.* (2000) gives

$$1.0V_S + 1.35V_{CH} + 1.87V_H \rightarrow 3.77V_{CSH} \qquad (3)$$

Notice that in these equations the standard cement chemistry abbreviations are used:

C = CaO, S = SiO_2 and H = H_2O.

Complicated interactions resulting from hydrating neighbour particles are modelled in XIPKM. For details see Le *et al.* (2013). The microstructure simulated by the hydration model is visualized by the 'digital-image-based' technique. The simulated space is subdivided by a 3D lattice system into small cubes, called 'voxels' (similar to image pixels), each of which is used to represent a certain phase. Herein, the microstructure of the hydrating paste is composed of C_3S and C_2S of the unhydrated cement cores, of SiO_2 and the inert phase of the unhydrated pozzolanic cores, of CSH-in and CSH-out, of CH and of the pore space (free water). However, for simplification in visualization, the phases constituting the unhydrated core of each particle are merged into a representative phase, 'fresh cement' or 'fresh pozzolan', represented by a spherical core whose volume equals the total volume of the phases. Fig. 2 at the bottom is an example of the microstructure visualization by the voxel system, whereby the red and yellow indicate the fresh cement and fresh pozzolanic cores, respectively. Some voxels are able changing their phases during the cement hydration process; fresh cement or fresh pozzolanic voxels can change into CSH-in ones, pore voxels can change into CSH-out or CH ones and CH voxels can change into pore ones (pozzolanic hydration). Notice that this voxel system is only for representing the microstructure of the hydrating paste and thus does not affect the hydration simulation process.

3 Hardened state of the binder - DRaMuTS design

Presently, a modern and sophisticated methodology is in development. Successively, assessment of pore characteristics in 3D virtual hydrated paste are investigated by DRaMuTS approach in which randomized data structures are built incrementally in two stages. Firstly, the porous medium is rapidly explored. Secondly, pore features such as porosity, gradient structures and connected fraction are evaluated. This allows distinguishing not only between de-percolated pores and pores that are mutually connected between opposite sides of the cube specimen, but also between continuous pore channels and dead-end branches of the above-mentioned percolated pores. Finally, also pore size distribution can be assessed by star volume measurements on the basis of the randomized point system. See Stroeven *et al.* (2012b;c).

Inspiration for the present approach is derived from the so called ‘Rapidly exploring Random Tree’ (RRT) algorithm developed in LaValle and Kuffner (2001). This efficient path planning algorithm pursues finding a way from point A to B, avoiding any collision with dispersed obstacles. Path planning is implemented by generating a ‘virtual tree’ system that includes sets of nodes (‘vertices’) and lines (‘edges’) that connect pairs of nodes (like branches of real trees). This tree grows incrementally and randomly in 3D. The procedure starts by generating a random point that is moved towards the nearest vertex, thereby defining a maximum incremental distance. Next, a check for collision with an obstacle is executed. No collision leads to addition of a new point and segment to the tree. At collision, a new random point is generated and the procedure is repeated until the goal is achieved. The expansion of the tree is illustrated in Fig. 3 (top).

This method needed upgrading for porosimetry applications. At a certain point of the simulation procedure a random point is generated and connected to the closest point of the tree. This may involve intersection with obstacles (solid phase in hydrated cement paste. In the present approach, instead of boosting the no-collision trials by regenerating a new random point as in RRT approach, intersections of the tested segment and obstacles are detected. Next, a point is trimmed between the nearest intersection and the considered vertex as in Fig. 3 (bottom). This excludes making iterations, because there is always one new vertex in the generation process. This speeds up the generation of the whole tree system and constitutes therefore a significant improvement of the RRT algorithm. Moreover, it allows investigating also dead-end branches of continuous pore channels.

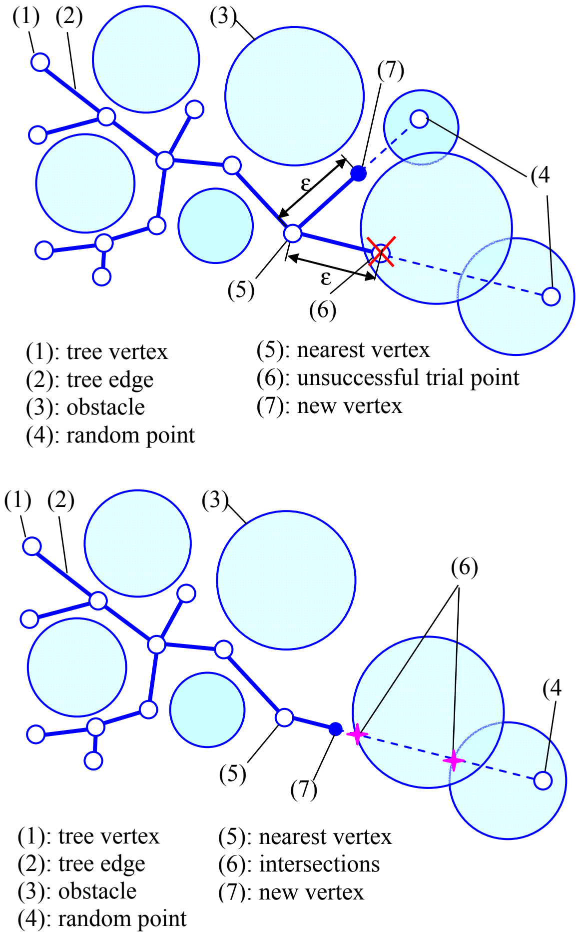


Figure 3. (top) Expansion of the tree systems by RRT and (bottom) by DRaMuTS approaches

Exploration by a single tree system seems not appropriate in porosimetry. Parallel development at the same time leads to the so called ‘multiple-tree’ network. Herein, tree systems grow incrementally from a set of different points referred to as ‘seeds’, which are presently placed on both sides of the specimen on pore sections. Upon completion of the generation process, the connectivity between the tree systems is checked. If so, they will merge into a single system.

The tree morphology governs the topology of the pore network structure. So, a distinction can be made between continuous pores (trunks, or channels), connecting external surfaces of the cube specimen, dead-end pores branching off these trunks, and fully isolated pores. A visualized pore network structure delineated by the tree edges is shown in Fig. 4 for a cement paste. Note that the obtained pore network trees are sensitive to the number of tree edges in the tree system. Basically, an increase in the number of tree edges of the system raises the chances of detecting the smaller pores. This will be more explicitly demonstrated in the example on Rice Husk Ash-blended PC.

4 Assessment of pore characteristics

Advanced methods for porosimetry based on sections are discussed in Hu (2004) and Hu and Stroeven (2005; 2006). This involves among other things the opening distribution technique that could also be applied to sections of the simulated cube specimen. However, the spatial character of the virtual specimens can be employed more effectively. For that purpose, a second uniform random point system is thereupon generated (note “Double Random” in the name of the method). This is shown in Fig. 5. The node fraction inside the

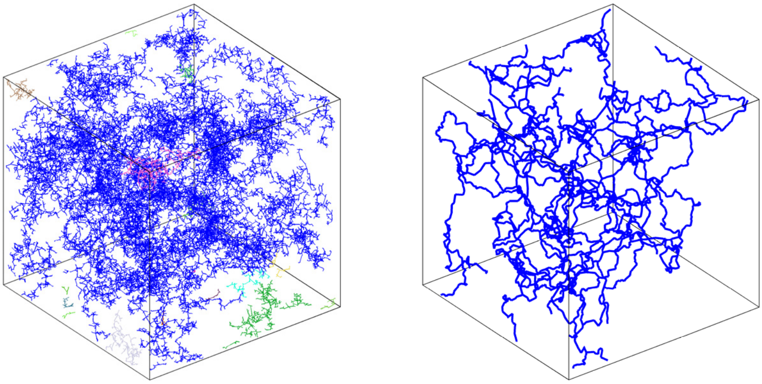


Figure 4. Pore exploration by virtual tree system of an 100µm cube for a cement paste. All trees are shown at the left (blue colour is for trees connected to outside specimen surfaces) and the main trunks in continuous pore channels (not including dead-end pores) are shown at the right. (This figure is in colour at www.heronjournal.nl)

pores directly governs porosity because point fraction is an unbiased estimator of volume fraction.

All points inside the pores are thereupon provided with pikes in systematically arranged orientations. The pikes connect the relevant node with the pore surface in the given direction (length l_i). By averaging all cubed values of pike length in a point and thereupon taking the cubic root, a measure is obtained for local pore radius. Hence, the local pore size associated with the node is estimated as $d_j = 2\left(\overline{l_i^3}\right)^{1/3}$. This is the so called star volume method that can also be instrumental for obtaining this 3D information from 2D sections (Stroeven *et al.*, 2012a; b). This basically experimental setting is illustrated in Fig. 6. The ensemble of such local spheres can be used for the construction of a volume-based pore size distribution function (PoSD), which renders possible studying the effects of technological measures on the PoSD. With the eye on use of pore size characteristics in a transport-based model, it seems more logic determining the local pore throat. This is defined as the smallest pore area of random plain sections through the random point. A 2D

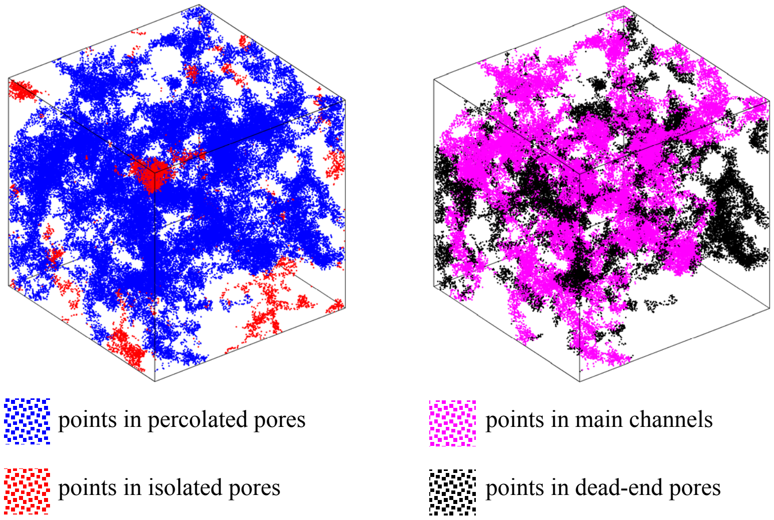


Figure 5. Second uniformly random point system in a hydrated cement paste. At the left, only points inside pores are displayed with a distinction between points in percolated pores and those in isolated pores. The distinction between points in main pore channels and those in dead-end pore branches is shown at the right. (This figure is in colour at www.heronjournal.nl)

star is defined in such a section by a random or systematic set of pikes in the section plane. Pike lengths l_i are determined per point, squared and averaged; cross section area is $\pi\overline{l_i^2}$. The area-based pore throat size distribution function is obtained by collecting all local pore throat area measurements. The curves are not fundamentally different from earlier mentioned PoSD.

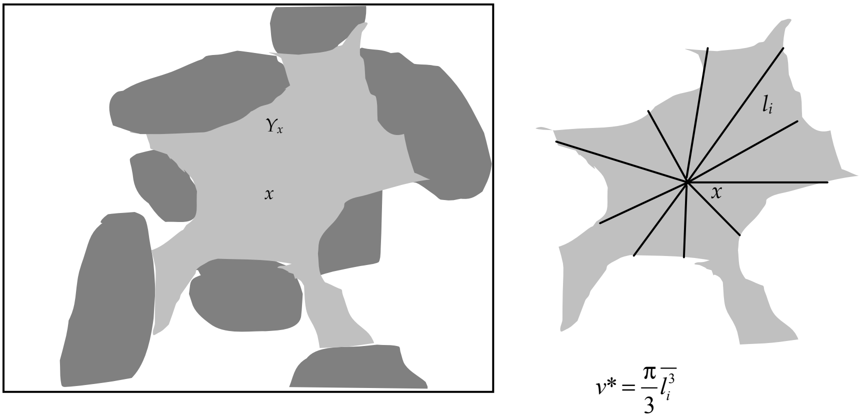


Figure 6. Part of schematised field image in which the connected pore area (Y_x) that can be observed from random point x is indicated in light grey (left). The star in x measures in random directions in the plane the intercept lengths, l_i.. Their average value is used to define the star volume v as indicated at the right.*

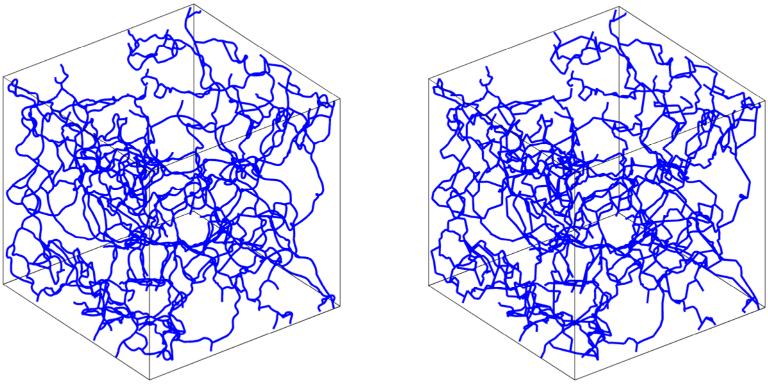


Figure 7. Mid-point smoothening (left) and end-point smoothening (right) of tree channels.

A final operation could be smoothening of the zigzag lines in the pore channels to get a more appropriate measure for their tortuosity. Relevance is derived from the expectation that pore size (throat distribution) and pore tortuosity would be major parameters in a transport model. An example for a test case simulation is presented in Fig. 7. Mid-point smoothening and end-point smoothening are presented. They can be combined for optimum solutions.

5 Cement blending by rice husk ash (RHA)

Portland cement (PC) production contributes by about 6% to global emissions of CO_2. One of the obvious contributions to reducing detrimental effects of Portland cement production on global warming as a result of CO_2 emissions is to reduce PC content significantly (Stroeven *et al.*, 2002). Use of an admixture of vegetable origin such as RHA will additionally contribute to waste management and energy conservation (Stroeven *et al.*, 1995). Experimental research with Vietnamese participation performed at Delft University of Technology (DUT) during the last decades of the previous century also exploited the gap-grading particle packing principle successfully in designing aggregate (very fine sand and coarse aggregate) as well as binders (Portland cement (PC) blended by rice husk ash, diatomite earth or metakaolin) (Bui, 2001; Vu, 2002). Detwiler and Mehta (1989) and Goldman and Bentur (1993) showed PC binders blended with an inert admixture also to lead to proper strength levels provided the blend was gap-graded, revealing the crucial importance of particle packing. The profitable packing effect of gap-graded blending by mineral admixture was already earlier successfully confirmed on SPACE-simulated RHA-blended PC (Bui *et al.*, 2005). The more complicated impact on the pore network system underlying transport-based durability issues is approached in this example. Earlier publications were focusing on aspects of this matter (Stroeven and Le, 2011; Le and Stroeven, 2012; Stroeven *et al.*, 2012a; b; c)

As an illustrative example, the plain PC and RHA-blended PC samples specified in Table 1 were simulated. Figs. 8-10 present some of the results obtained by way of the described modern methodology. Note that the prime interest is highlighting the effects of blending. The estimated pore sizes of the simulated samples (Fig. 9 at the right) are slightly larger than those of experimental ones. For examples, Lange *et al.* (1994) showed that pore sizes of a cement paste of w/c of 0.4 obtained by image analysis techniques range from 0.2 μm to

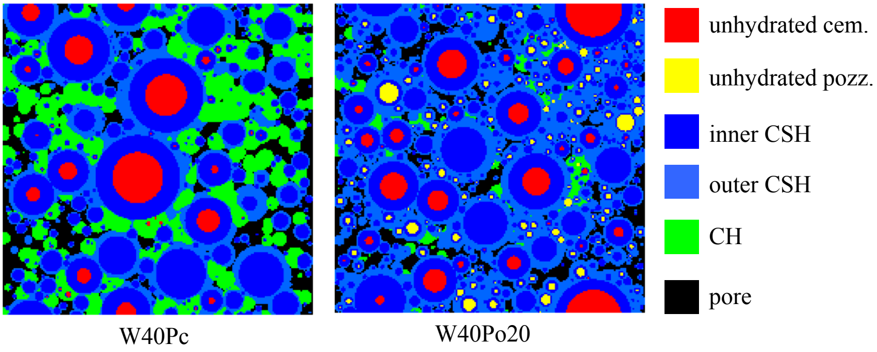
Table 1: Hydration simulation input

Sample	W40Pc	W40Po20
w/b	0.40	0.40
% Replacement	0	20
Number of cement particles	16562	12689
Number of model RHA particles	-	13480

PC:	CEM I (PC32.5) (van Eijk, 2001); Blaine: 286 m²/kg
Composition PC:	66% C_3S, 16% C_2S, 7% C_3A and 11% C_4AF
RHA:	$RHA_{(18+)}$ (Bui, 2001); BET: 58 m²/g
Model PC:	Rosin Rammler PSD with n=1.107, b=0.023 and size range of 1~30 μm
Model RHA:	PSD function of $RHA_{(18+)}$ (Bui, 2001) and size range of 1~13 μm

5.5 μm and have largest density at around 1.7 - 3.2 μm. The relatively coarse materials in the virtual set up inevitably lead to this small overestimation of pore size.

Fig. 9 at the right demonstrates that the pores in the plain PC are apparently larger in the Interfacial Transition Zone (ITZ), whereas this tendency is significantly reduced for the blended PC! This may have favourable impact on transport-based durability issues. Further, blending leads to a reduced extension of the ITZ, as revealed by Fig. 9 at the left, in which the pore volume density is displayed as a function of distance to the rigid wall (by summing up the pore densities at equal distances to both walls). The reader is referred to Stroeven *et al.* (2012a) for another example on cement blending revealing similar effects on porosity.



W40Pc W40Po20

Figure 8. 2D sections of the hydrated PC and blended PC samples specified in Table I. (This figure is in colour at www.heronjournal.nl)

Finite values of connected porosity are found in the middle zone between the ITZs (Fig. 9 at the left). This deviates from earlier observations by Chen *et al.* (2004) and Chen *et al.* (2006) based on SPACE-generated fresh PC specimens that were upon hydration subjected to serial sectioning and 3D reconstruction (Ye, 2003). By gradually removing surface layers (like with an onion) a cube specimen finally resulted without channels connecting top and bottom surfaces. So, connected porosity seemed zero in this middle zone. However, the present investigations demonstrate that branches of the tree channels in the ITZ connect in the middle zone, providing it with transport capability to the outside of the specimen. Total transport capacity will as a consequence not be dominantly governed by ITZ percolation as also found in experiments (Maghsoodi and Ramezanianpour, 2012a; b).

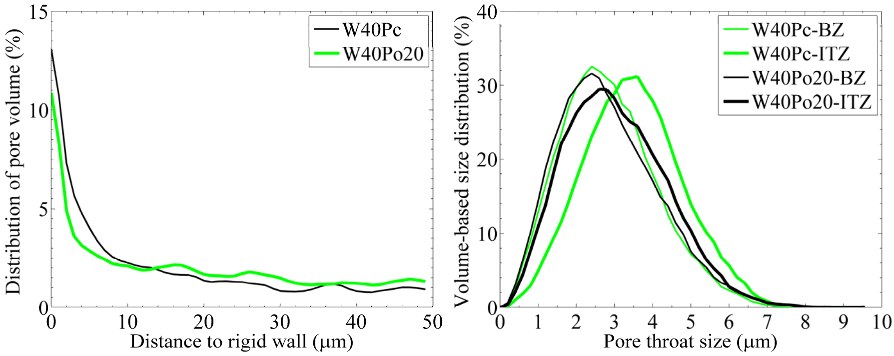


Figure 9. Effect of blending on ITZ extension (left) and on volume-based size distribution of pores in ITZ and bulk zone (BZ) of plain and blended cement.

Fig. 10 reveals for another case of plain PC and blended PC an important feature of the DraMuTS approach. Obtained data depend on the sensitivity selected by the researcher. The chances of finding smaller and smaller capillary pores will increase by taking still larger numbers of connected edges in the tree structures (so, by enhancing the number of generated points). Finally plateau values are reached at a high degree of pore connectivity as reflected by Fig. 10. Such tiny pore connections can be expected not providing major contributions to transport capacity, however. A lower and practical value for the sensitivity should therefore be used in practical approaches. This will reduce the pore connectivity of the network system in which most pores will contribute to the transport capacity, however.

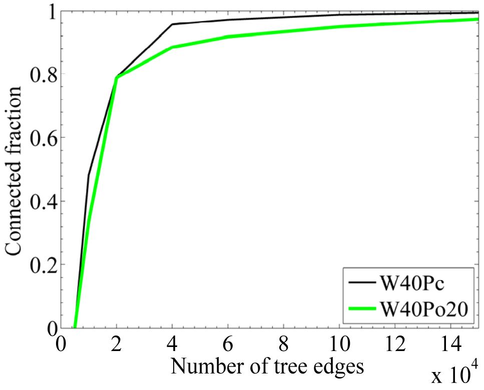


Figure 10. Sensitivity analysis of the fraction of connected edge lengths

Fig. 11 shows this decline in connected fraction of the pore systems when gradually eliminating pores from the system proceeding from small to larger sizes. The 'cutting pore size' is defined as a threshold value below which pores are neglected for the assessment of the connected pore fraction. To do so, the points in the second uniformly random point system that can be associated with a local pore throat size smaller than the cutting value will be eliminated in the further analysis. The connected fraction is then estimated by an independent method, RaNoS (Random Node Structuring) (Stroeven *et al.*, 2012c), in which the connectivity among the random points is detected by a clustering process. The cutting pore size at zero value of the connected fraction can be referred to as the 'depercolation threshold' in conformity with the general definition. This implies according to Fig. 11 that pores having sizes smaller than around 4.6 μm in the plain PC (W40Pc) and 3.8 μm in the RHA-blended PC (W40Po20) are essential in the transport system of these *model* materials.

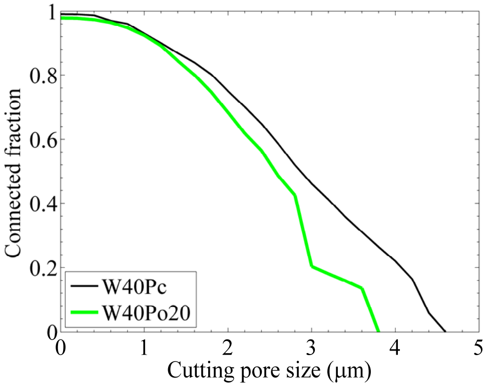


Figure 11. Connected fractions at different values of the cutting pore size

Again, this capability of estimating durability risks related to transport through the capillary pores is not the major issue of this paper. However, this discussion may present the contours for such future applications.

6 Conclusions

A modern versatile and economic methodology for simulating particulate materials like cementitious ones, and for quantitatively investigating the topology (e.g. continuity) and geometry (tortuosity, size distribution) of the pore network structure is presented.
This methodology starts by DEM simulation of the particle packing structure. This would be dense random packing for aggregate and at low water to cement ratios the loose random state for binder particles. In the latter case, next will be hydration simulation by the newly-developed XIPKM, based on the so called vector approach.

The pore structure in the hardened material is explored by the robotics-inspired double random multiple-tree structuring approach (DRaMuTS). It provides quantitative information on pore topology, among other things involving pore continuity. Finally, geometry of the pore network structure as delineated by the DRaMuTS trees is quantitatively assessed by star volume measurements in 3D. This is a straight forward approach that can yield volume based pore size distributions or pore throat size distributions. In 2D this is a method applied to experimental settings in life sciences.

Usage is illustrated on the basis of rice husk ash blended cement. The effect of blending the PC with fine-grained rice husk ash is demonstrated. In the first place, the extent of the ITZ is reduced and secondly, its internal pore structure is refined. These effects promote better durability resistance.

Transport-based durability issues will not be significantly dominated by ITZ percolation, because transport capacity in the middle zone is provided by connected tree branches of the channels in the ITZ.

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