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## **UPSCALING OF PERMEABILITY OF POROUS** MATERIALS: FIRST INSIGHT INTO THE EFFECT OF PORE-SPACE CHARACTERISTICS

Xian Liu, 1,2 Matthias Zeiml, 1 Roman Lackner, 3\* & Herbert A. Mang 1

<sup>1</sup>Institute for Mechanics of Materials and Structures, Vienna University of Technology, Vienna,

<sup>2</sup>Department of Geotechnical Engineering, Tongji University, Shanghai, China

<sup>3</sup>Material Technology Innsbruck, University of Innsbruck, Innsbruck, Austria

\*Address all corespondence to R. Lackner E-mail: Roman.Lackner@uibk.ac.at

The material phase "air" (pore space) in porous materials determines the amount of fluid flow into and through the material and, hence, the time scale of physical/chemical degradation processes in durability aspects of materials and structures. Hereby, the pore-space characteristics, such as pore-size distribution and pore arrangement, both being accessible via respective experimental techniques, influence the transport properties of the material. In this paper, this influence is investigated within the multiscale framework, employing a so-called random pore-network model. Hereby, random arrangements of prescribed pore-size distributions are modeled, giving – under the assumption of steady-state flow conditions - access to the macroscopic permeability of the material. More specifically, three idealized pore-size distributions, i.e., (i) two different radii and (ii) constant and (iii) normal pore-size distribution, are investigated by means of several sets of network configurations. From the obtained results, both mean value and standard deviation of the macroscopic permeability corresponding to a certain pore-size distribution are determined, giving new insight into the impact of pore-space characteristics on the permeability and its variation in porous materials.

**KEY WORDS:** pore-size distribution, permeability, network model, upscaling

## 1. INTRODUCTION

It is well known that the pressure-driven transport of fluids in porous materials is governed by the permeability of these materials. For example, in the case of high- lating macroscopic permeability properties to the matetemperature loading of concrete structures, vaporization rial microstructure are based on digital images (Garboczi of physically and chemically-bound water results in an increase of pore pressure, which in case of low transport ability causes spalling of near-surface concrete lay- Carmeliet et al, 1999). The accuracy of these models, ers. This pressure-driven transport of water vapor is commonly described by Darcy's law with the permeability as about the microstructure, accessible via proper experithe governing parameter (Zeiml, 2008).

material is treated as a continuum, and is related - if at all - to pore-space properties (e.g., porosity) by means of empirical relations (Mehta and Manmohan, 1980; Marchand and Gerard, 1997). More advanced models of reand Bentz, 1996; Sandouki and van Mier, 1997; Ye et al., 2006) and pore networks (Galle and Daian, 2000; mental techniques such as mercury-intrusion porosime-In general, the permeability of porous materials is de- try (MIP) and image analysis. These techniques give acfined at the so-called macroscale, i.e., the scale where the cess to the pore-size distribution and the total pore vol-

ume, which may, however, build up different pore arrangements with different permeability properties.

In this paper, the impact of the pore-size distribution and pore arrangement on the macroscopic permeability of porous materials is investigated. Taking the random nature of the pore arrangement into account, a random porenetwork model is developed in order to relate the macroscopic permeability to characteristics of the pore space. The macroscopic permeability is regarded as a stochasties obtained from random pore networks.

The paper is organized as follows: In Section 2, the framework of the random network model, including basic model assumptions, pore-space generation, and the solution procedure of the random network, is presented. Based on results obtained from the random network model, the impact of the pore-size distribution and the pore arrangement on the macroscopic permeability is investigated in Section 3, taking three types of pore-size distributions into account.

### 2. MODEL DESCRIPTION

In order to build up the pore space of a porous material, the following assumptions are taken into account:

- 1. Each single pore of the network is treated as a tube with circular cross section. In the case of steadystate flow, the Hagen-Poiseuille law (Wikipedia; Sutera and Skalak, 1993) is used to describe fluid flow in this pore tube.
- 2. All pores in the network have the same length.
- 3. Finally, for the design of the pore network, a 2D arrangement - already capturing most features of a 3D pore structure (Carmeliet et al, 1999) – is considered in order to study the main effects of the pore-space characteristics on the macroscopic permeability. The methods developed herein, however, can also be applied to 3D network models.

Following the above assumptions, the fluid flux Q (in cubic meters per second) through a single pore of length l(in meters) and radius r (in meters) is given by the Hagen-Poiseuille law as (Wikipedia; Sutera and Skalak, 1993)

$$Q = -\frac{\pi r^4}{8 \,\mu} \frac{\Delta p}{l},\tag{1}$$

pore and  $\mu$  (in Pascal times second) is the viscosity of of the 2D network model)

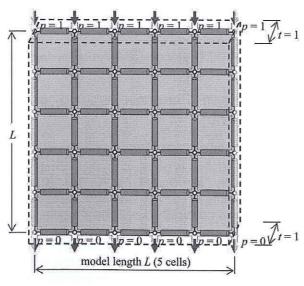
the fluid. Based on the fluid flow in a single pore, a 2D network is used to model the pore space. Hereby, a 2D cross-squared network composed of cylindrical pores is constructed using a regular lattice (see Fig. 1, illustrating an  $N \times N$  pore network, with N = 5).

Based on the underlying pore-size distribution, pores with different radii are placed in the network in a random manner. In the case of a continuous pore-size distribution. the finite number of available pores within the network, tic material property, determined from transport proper-  $n_p$ , represents the pore-size distribution in a discretized manner. Figure 2 illustrates this approximation for a constant pore-size distribution and the respective linear cumulative pore volume represented by a finite number of pores within the network model.

> For a given pore network, the macroscopic permeability can be calculated by imposing a unit pressure gradient at two opposite sides (top and bottom side, see Fig. 1) of the employed 2D network. For determination of the flux through the network, the pressures in the connection points of the single pipes (nodes) are used as state variables. Thus, the flux through the ith pore of the network system is given by the Hagen-Poiseuille law (1) as

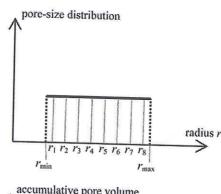
$$q_i = -\frac{\pi \, r_i^4}{8\mu} \frac{\Delta p_i}{l_i},\tag{2}$$

where  $\Delta p_i$  (in Pascal) is the pressure difference between the end and beginning node of the considered pore, re-



**FIG. 1:** Two-dimensional idealized  $N \times N$  pore network where  $\Delta p$  (in Pascal) is the pressure difference within the for N=5, consisting of  $n_p=2N(N+1)$  pores (L: size

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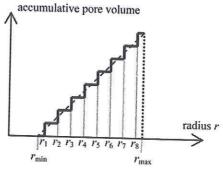


FIG. 2: Approximation of given linear accumulative pore volume (constant pore-size distribution) by eight

spectively. At each node, mass conservation must hold, yielding

$$\sum_{i \in J_{\text{conn}}} q_i = 0, \tag{3}$$

where  $J_{\mathrm{conn}}$  represents the set of pores connected to the considered node.

As boundary conditions, the left and right side of the network model are considered as sealed (no-flow condition), giving equal flux for the top and bottom sides of the model. Considering the initial condition of an imposed unit pressure gradient, inserting Eq. (2) into Eq. (3) gives one equation per node for determination of the unknown pressure at each node of the network model. Based on the computed pressures and, thus, fluxes through the individual pores, the overall flux through the network model,  ${\cal Q}$ (in cubic meters per second), is computed as

$$Q = \sum_{i \in J_{\text{bottom}}} q_i, \tag{4}$$

where  $J_{\mathrm{bottom}}$  represents the pores connected to the bottom side of the network model (see Fig. 1).

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Finally, the effective (macroscopic) permeability K (in meters squared) of the network model is determined by Darcy's law, setting the out-of-plane dimension of the model t (in meters) to 1 m, giving

$$Q = \frac{KA}{\mu} \frac{\Delta P}{L} = \frac{K(t \times L)}{\mu} \frac{\Delta P}{L} = \frac{K}{\mu} \to K = Q\mu, (5)$$

where t=1 m and  $\Delta P=1$  Pa were considered, with  $A = t \times L$  (in meters squared) as the cross-sectional area of the top and bottom sides, and  $\Delta P/L = 1/L$ (in Pascal per meter) as the imposed unit pressure gradient. Accounting for the random arrangement of pores, the described procedure is carried out for various porespace configurations. Let  $n_a$  be the number of considered pore arrangements; then the mean value and standard deviation can be computed for the  $n_a$  – in general differing - macroscopic permeabilities as follows:

$$\overline{K} = \frac{1}{n_a} \sum_{i=1}^{n_a} K_i \tag{6}$$

$$D = \sqrt{\frac{\sum_{i=1}^{n_a} (K_i - \overline{K})^2}{n_a}},\tag{7}$$

where  $K_i$  refers to the permeability of the *i*th pore arrangement.

## 3. APPLICATION

In order to investigate the influence of the pore-size distribution on the macroscopic permeability, the following three different pore-size distributions are considered (see Fig. 3):

(a) Two-radii pore-size distribution,

$$f_V(r) = \begin{cases} f_1, r = r_1 \\ f_2, r = r_2 \end{cases}$$
 with  $f_1 + f_2 = 1$  and  $r_1 < r_2$ , (8)

where  $f_i$  is the volume fraction when radius r takes the value of  $r_i$  (i = 1, 2).

(b) Constant pore-size distribution.

$$f_V(r) = \frac{1}{r_{
m max} - r_{
m min}}$$
 with  $r_{
m min} \le r \le r_{
m max}$  and  $\overline{r} = \frac{r_{
m min} + r_{
m max}}{2}$ ,

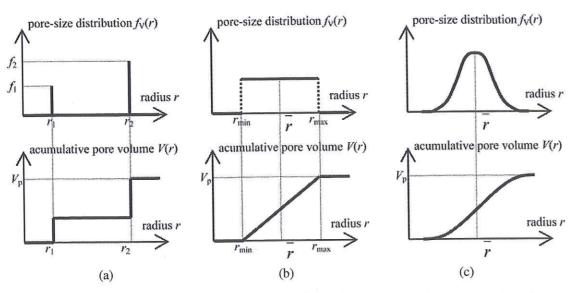


FIG. 3: Investigated pore-space configurations: pore-size distribution and accumulative pore volume for (a) tworadii, (b) constant and (c) normal pore-size distribution

where  $\overline{r}$  is the mean radius of the pore-size distribution.

(c) Normal pore-size distribution,

$$f_V(r) = \frac{1}{\sqrt{2\pi}D_r}e^{-[(r-\overline{r})^2/(2D_r^2)]},$$
 (10)

of the pore-size distribution, respectively.

Within the numerical studies, the length of each pipe was set to 50 m, giving a model length for, e.g., a network model with N=20, of L=1000 m. In order to focus exclusively on the effect of pore-space characteristics given by the pore-size distribution and the pore arrangement, the overall pore volume  $V_p$  (in cubic meters) is directly related to the number of pores  $n_p$  [i.e., the model size N, with  $n_p = 2N(N+1)$ ]. This yields, e.g.,  $V_p = 1,495,000 \text{ m}^3 \text{ for } N = 20 \text{ (giving } n_p = 840 \text{ and }$ L = 1000 m).

## 3.1 Two-Radii Pore-Size Distribution

Within the analysis of the two-radii distribution (see Fig. 3(a)), the input parameters of the model  $(r_1, r_2, f_1, f_2)$  are varied. By setting  $V_p = 1,495,000 \text{ m}^3$ constant, two of the four parameters can be chosen. Throughout the analyses,  $r_1$  and  $f_1$  were chosen as input parameters, yielding the remaining parameters as

 $f_2 = 1 - f_1$ (11)

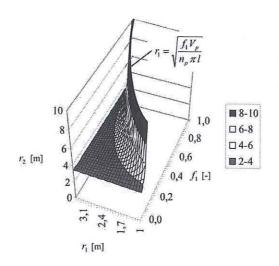
$$r_2 = \sqrt{\frac{V_p(1 - f_1)}{[n_p - (f_1 V_p / (r_1^2 \pi l))] \pi l}},$$
 (12)

with  $\overline{r}$  and  $D_r$  as mean radius and standard deviation with  $n_p = 2N(N+1)$  as the number of pores and  $l=50~\mathrm{m}$  as the pore length. Starting with the case of a uniform pore-size distribution (i.e.,  $r_1 = r_2 = r$ ), the resulting pore radius is given as  $r = \sqrt{V_p/(n_p\pi l)}$  $\sqrt{1.495,000/(840 \cdot \pi \cdot 50)} = 3.36$  m. Figure 4 shows radius  $r_2$  as a function of the input parameters  $r_1$  and  $f_1$ . For the general case of two different radii  $r_1$  and  $r_2$ ,  $[n_p - (f_1 V_p/r_1^2 \pi l)] > 0$  in Eq. (12) yields a condition for the choice of input parameters as (see Fig. 4)

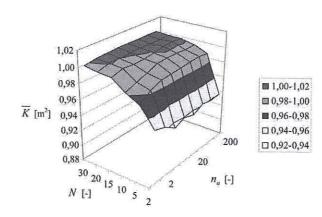
$$r_1 > \sqrt{\frac{f_1 V_p}{n_p \pi l}}. (13)$$

In order to study the convergence behavior of the employed analysis scheme for determination of the macroscopic permeability, both network size N and the number of analyzed pore arrangements  $n_a$  are varied (see Fig. 5). For small N, the convergence behavior is not satisfactory since boundary effects (no-flow condition at left and right boundary of the network) apparently influence the results. For larger networks, the convergence behavior is

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**FIG. 4:**  $r_2$  as a function of input parameters  $r_1$  and  $f_1$ for the two-radii pore-size distribution



the employed analysis scheme: mean value for the permeability,  $\overline{K}$ , as a function of network size N and number of analyzed pore arrangements  $n_a$  (input parameters:  $r_1 = 3 \text{ m}, f_1 = 0.1; r_2 = 3.42 \text{ m}, f_2 = 0.9 \text{ according to}$ Eqs. (11) and (12))

improved, even allowing the use of fewer pore arrangements  $n_a$ . For the subsequent analyses, N=20 and  $\log V_p=1,495,000~\mathrm{m}^3=\mathrm{constant}$  for N=20) different  $n_a = 200$  are chosen.

Based on these satisfactory observations regarding the convergence behavior of the employed analysis scheme, with  $r_{\min} = r_{\max} = \overline{r} = r = 3.36$  m is obtained. parameter studies are performed. Figure 6 shows representative random pore arrangements with different results ments considered within the analyses. Figure 10 contains for the macroscopic permeability K. The respective results for the mean value of the macroscopic permeability,  $\overline{K}$ , are shown in Fig. 7(a). Hereby, pore-size distributions radius  $\overline{r} = (r_{\min} + r_{\max})/2$  (i.e., for increasing slope), the

with either  $f_1 = 0$  or  $r_1 = 3.36$  m refer to the special case of a uniform pore system (with r = 3.36 m), giving the analytically-obtained value for the permeability according to Eqs. (2) and (5) as

$$K = Q\mu = N q \mu = N \frac{\pi \cdot r^4}{8 \cdot \mu} \frac{\Delta p_i}{l_i} \mu$$
$$= 20 \cdot \frac{\pi \cdot 3.36^4}{8} \frac{1}{1000} = 1.0 \text{ m}^2,$$
 (14)

with  $\Delta p_i/l_i = \Delta p/L = 1/L$ . For other  $r_1$ ,  $f_1$  combinations (i.e., nonuniform pore systems), the obtained macroscopic permeability is apparently smaller, with a steep decrease of  $\overline{K}$ , illustrating the effect of small-size pores on the macroscopic permeability. For a given value of  $f_1$ , a decrease of  $r_1$  results in more pores with this respective radius and therefore an increased number of so-called bottle necks within the pore system. For a given  $r_1$ , an increase in  $f_1$  has the same effect, also reducing the macroscopic permeability. The region with  $\overline{K} = 0$  refers to the above-mentioned case where condition (13) is not satisfied, i.e., no pore system can be generated. When investigating the standard deviation for the macroscopic permeability (Fig. 7(b)), a peak can be observed for certain  $r_1$ ,  $f_1$  combinations. These combinations are in the region where the diversity of the pore system is the highest. (As mentioned before,  $f_1 = 0$  and  $r_1 = 3.36$  m refer to the special case of a uniform pore system, leading to D = 0.  $r_1$ ,  $f_1$  combinations close to the region where condition (13) is not satisfied, i.e., D = 0 in Fig. 7(b). also lead to almost uniform pore systems.) When scaling the standard deviation by the respective mean value for FIG. 5: Investigation of the convergence behavior of the macroscopic permeability, again a peak for certain  $r_1$ ,  $f_1$  combinations is observed (see Fig. 7(c)).

## 3.2 Constant Pore-Size Distribution

Based on the above observations, the constant pore-size distribution (see Fig. 3(b)) is investigated in the following. Hereby, the slope of the so-obtained linear cumulative pore volume is varied (see Fig. 8), yielding (consider $r_{\min}, r_{\max}$  pairs and, hence, different mean radii  $\bar{r}$ . For the special case of infinite slope, a uniform pore system

Figure 9 shows representative random pore arrangethe analysis results with the respective permeability distributions displayed in Fig. 10(a). For decreasing mean pore

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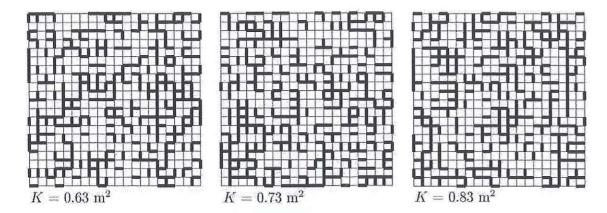


FIG. 6: Representative random pore arrangements for two-radii pore-size distribution with different results for the macroscopic permeability K (input parameters:  $r_1 = 1.75$  m,  $f_1 = 0.1$ ,  $r_2 = 4.02$  m,  $f_2 = 0.9$ )

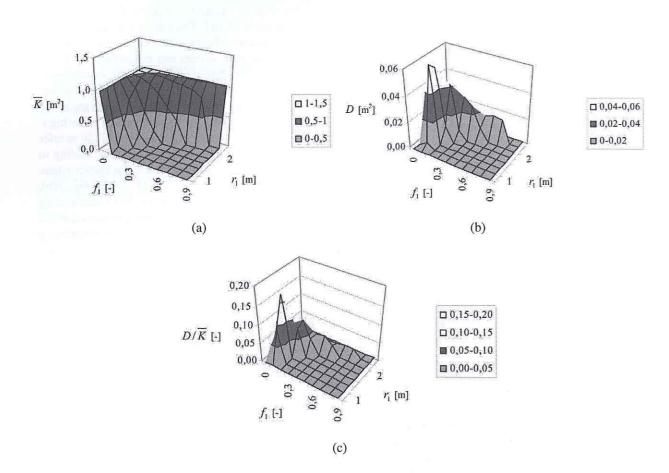


FIG. 7: Investigation of pore networks characterized by a two-radii pore-size distribution: (a) mean value  $\overline{K}$ , (b) standard deviation D, and (c)  $D/\overline{K}$  as a function of  $r_1$  and  $f_1$ 

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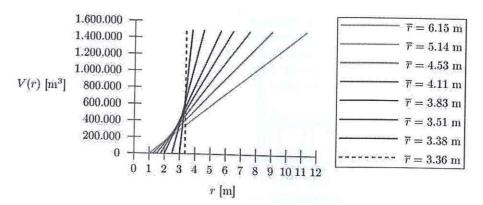


FIG. 8: Investigated constant pore-size distributions with different mean radii  $\overline{r}$  (and, hence, different  $r_{\min}$ ,  $r_{\max}$ pairs), leading to a linear cumulative pore volume

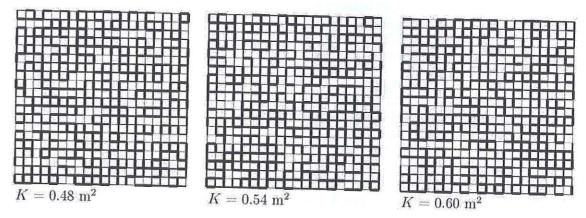


FIG. 9: Representative random pore arrangements for constant pore-size distribution with different results for the macroscopic permeability K (input parameter: mean radius  $\overline{r}=4.11~\mathrm{m}$ )

mean value for the permeability,  $\overline{K}$ , increases (also refer of the macroscopic permeability  $(D/\overline{K})$ , see Fig. 10(b)) to Fig. 10(b)). This can be explained by the increasing shows that the deviation increases monotonously with inregularity of the pore system for decreasing values of  $\overline{r}$ , creasing irregularity of the pore system (i.e., with increaswith  $\overline{K}$  approaching the respective value for a uniform  $\overline{r}$  or decreasing slope). Moreover,  $D/\overline{K}$  approaches pore-size distribution ( $K = 1.0 \text{ m}^2$ , see dashed line in zero for the case of a uniform pore-size distribution (at Fig. 10(a) as well as circle in Fig. 10(b)). In the case of  $\overline{r} = r = 3.36$  m), since  $D \to 0$  (see circle in Fig. 10(b)). increasing  $\overline{r}$  and, hence, decreasing slope of the cumulative pore volume,  $r_{\rm max}$  increases. However, only a small number of larger pores ( $\overline{r} < r < r_{\rm max}$ ) are present in the network, whereas – at the same time –  $r_{\min}$  decreases and hence the number of small-size pores  $(r_{\min} < r < \overline{r})$ increases rapidly, reducing the macroscopic permeability. As shown in Fig. 10(a), the width of the permeability distribution (i.e., the standard deviation D) seems to have a maximum for a specific value of  $\overline{r}$  (i.e., a specific slope of the cumulative pore volume). However, scaling the standard deviation by the respective mean value

## 3.3 Normal Pore-Size Distribution

Within further analyses, normal pore-size distributions (see Fig. 3(c)) are investigated considering different combinations of mean pore radius  $\overline{r}$  (in meters) and standard deviation  $D_r$  (in meters) (see Fig. 11), taking into account the condition of constant cumulative pore volume for a given network size, with  $V_p = 1,495,000 \text{ m}^3$  for N = 20.

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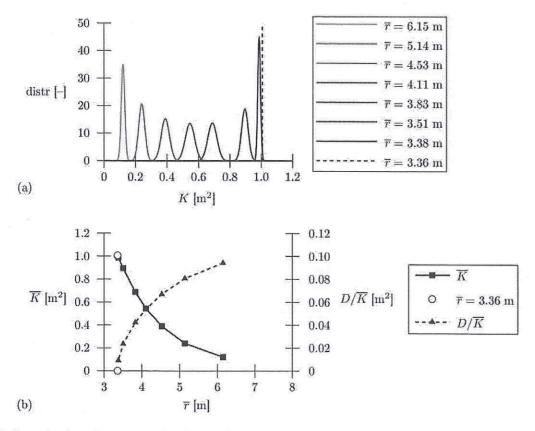
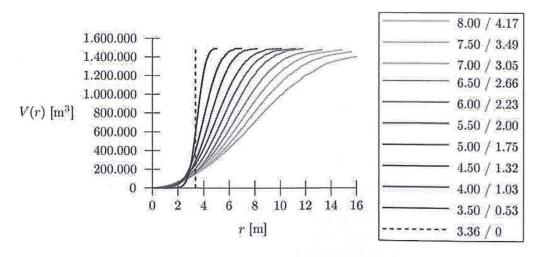


FIG. 10: Investigation of pore networks characterized by a constant pore-size distribution: (a) obtained permeability distributions; (b) mean value for the permeability,  $\overline{K}$ , and standard deviation D scaled by  $\overline{K}$  as a function of mean pore radius  $\overline{r}$ 



**FIG. 11:** Investigated normal pore-size distributions with different  $\bar{r}$  and  $D_r$  (notation:  $\bar{r}/D_r$ )

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Figure 12 shows the obtained numerical results. As observed before for the constant pore-size distribution, the mean value of the macroscopic permeability,  $\overline{K}$ , increases with increasing regularity of the pore system (i.e., with decreasing mean value for the radius of the normal poresize distribution, see Figs. 12(a) and 12(b)). Additionally, the results approach the case of a uniform pore system, characterized by  $\overline{r}=r=3.36~\mathrm{m}$  and  $K=1.0~\mathrm{m}^2$ (see Fig. 12(b)). The variation of the macroscopic perme- The transport properties of porous materials are a key ability again seems to have a maximum for a certain normal pore-size distribution (for the performed analyses, the maximum in D refers to a mean pore radius of  $\overline{r} = 4.5 \text{ m}$ , see Fig. 12(a)); however, when scaling the deviation of

tion error (with the cumulative pore volume - given by the discrete number of pores - starting to significantly deviate from the target value of  $V_p = 1,495,000 \text{ m}^3$ ), on the other hand. The latter also explains the observed oscillations in the scaled standard deviation shown in Fig. 12(b).

## 4. SUMMARY AND OUTLOOK

parameter concerning durability aspects of materials and structures. Hence, prediction of the permeability based on information about the pore space, where the latter can be influenced during the construction process, is of high imthe permeability results (giving  $D/\overline{K}$ , see Fig. 12(b)), a portance. In this work, a so-called random pore-network monotonously increasing trend is observed up to a mean model is developed in order to determine the mean value pore radius of  $\overline{r} = 6$  m. For higher mean pore radii, this and standard deviation for the macroscopic permeability trend is reversed and  $D/\overline{K}$  decreases again. This obser- of porous materials for different pore-size distributions. vation is explained by the rather small magnitude of both In this way, in addition to the influence of the shape of the D and  $\overline{K}$ , on the one hand, and an increasing discretizapore-size distribution, the influence of the arrangement of

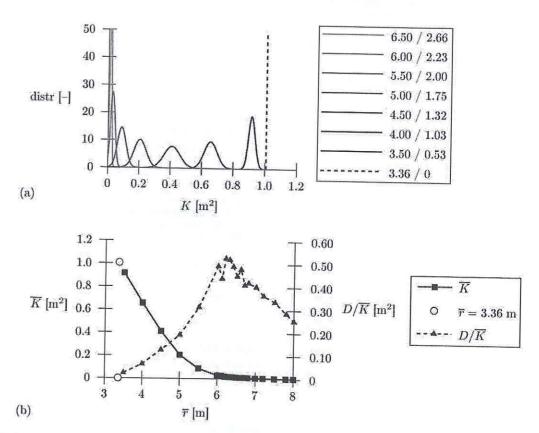


FIG. 12: Investigation of pore networks characterized by a normal pore-size distribution: (a) obtained permeability distributions (notation:  $\overline{r}/D_r$ ); (b) mean value for the permeability,  $\overline{K}$ , and standard deviation D scaled by  $\overline{K}$  as a function of mean pore radius  $\overline{r}$ 

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the respective pores on the macroscopic permeability is tions and will finally be employed to predict the macroinvestigated.

In a first step, the developed model was applied to three idealized pore-size distributions, namely, (i) two-radii, (ii) constant and (iii) normal pore-size distribution. Investigation of the two-radii pore-size distribution showed that the size and volume fraction of small-size pores are the governing factors with respect to the macroscopic permeability of the pore system. Moreover, the diversity of the pore system had an effect on the stochastic nature of the permeability (i.e., the respective standard deviation). In the case of the constant pore-size distribution, the mean value for the macroscopic permeability decreased with decreasing slope of the cumulative pore volume, whereas the standard deviation of the permeability increased with respect to the mean value for the permeability at the same time. This was explained by the increasing irregularity of the pore system. Even though large-size pores become larger for decreasing slope, only a small number of these pores exist in the network and their effect is apparently overshadowed by an increasing number of small-size pores with decreasing radius. In the case of the normal pore-size distribution, again the mean value for the permeability decreased for increasing irregularity of the pore system, whereas the standard deviation increased with respect to the mean value for the permeability up to a certain poresize distribution (i.e., a certain value for the mean pore radius). This again demonstrated the influence and the dominating effect of small-size pores on the macroscopic permeability. With continuing increase in irregularity of the pore system, discretization of the pore-size distribution and respective errors introduced into the analysis caused slight fluctuation of the numerical results.

Within future applications, the developed model shall be applied to other types of idealized pore-size distribu-

scopic permeability of building materials based on poresize information obtained from respective experiments.

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## EFFECTS OF HIGH TEMPERATURE ON MESOSCALE PROPERTIES OF CONCRETE

# Petr Kabele,\* Jaroslav Pekař, & Jiří Surovec

Czech Technical University in Prague, Faculty of Civil Engineering, Thákurova 7, 166 29 Praha 6, Czech Republic

\*Address all corespondence to P. Kabele E-mail: petr.kabele@fsv.cvut.cz

This paper presents a complete experimental methodology for identification of parameters that are necessary for mesoscale numerical modeling and analysis of damage and degradation of concrete at high temperatures. For this purpose, a series of specialized mesoscale experiments are devised and carried out. The experiments target mechanical and fracture properties as well as characteristics of heat transfer of the main mesoscopic phases of concrete, namely, cement mortar, limestone aggregate, and their interface. The tests are conduced on samples that were exposed both to room environment and high temperatures. Results are presented in terms of temperature-dependent material characteristics.

KEY WORDS: elastic modulus, tensile strength, compressive strength, fracture energy, coefficient of thermal conductivity, specific heat, coefficient of thermal expansion, temperature dependence

### 1. INTRODUCTION

Damage of concrete exposed to high temperatures, such as those arising from fire, is associated with complex physical and chemical phenomena. Considering the scale of concrete structures on one hand, and the composition of concrete on the other, it is convenient to study these phenomena on the mesoscale, while perceiving concrete as a two-phase composite consisting of cementitious mortar (matrix), coarse aggregate (inhomogeneities), and their interfaces. The most important mechanisms that cause degradation of concrete at elevated temperatures can be identified as follows:

- 1. Differential thermal expansion due to steep temperature gradients and different coefficients of thermal expansion of the constituent materials (namely, mortar and aggregate)
- 2. High internal pressures due to the release of capillary and chemically bound water, its evaporation, and movement through the porous structure (namely of mortar)

3. Thermo-chemo-mechanical changes of the constituent materials, such as dehydration of the hydrate calcium silicate (~180°C) or decomposition of the calcium hydroxide (~500°C) and of the hydrate calcium silicate ( $\sim 700^{\circ}$ C)

To be able to predict the macroscopic behavior of concrete exposed to fire and to possibly optimize its composition for better fire resistance, it would be desirable to understand the independent effects of the individual mechanisms. However, when concrete specimens of standard dimensions (on the order of 100 mm) are tested for the effects of high temperature on material behavior, e.g., strength, it is almost impossible to isolate the abovementioned phenomena. This is obvious in the case of different thermal expansion coefficients of the constituents, or in the case of their different thermochemical degradation. But to also eliminate the effects of thermal gradients, concrete specimens would have to be heated at very slow rates. Similarly, to suppress the influence of pore vapor pressure and moisture transport, prolonged drying of samples prior to testing and again very slow heating would be necessary.