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Prediction Models for Thermal Conductivity of Cement-based Composites

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ABSTRACT
Cement-based materials are the most consumed materials in the construction industry. Low or high thermal conductive cement-based materials are of interest in applications such as

embedded floor heating systems, building envelopes or structural elements. This paper describes prediction models for thermal conductivity of cementitious composites by considering different variables such as constituent materials, porosity and moisture content. The presented prediction models may be used for thermal conductivity based mix design of cementitious materials. Based on the desired accuracy, different solutions are proposed.

Key words: Mix Design, Model, Thermal Conductivity, Cement-based Materials.

1. INTRODUCTION

Thermal conductivity is an important material property in the energy design process of buildings. While cement-based materials are the most consumed materials in the construction industry, case-tailored thermal conductivity is desirable for these materials depending on the application area. Indoor surfaces such as embedded floor heating systems or cementitious materials mixed with phase change materials, may demand high thermal conductivity. On the other hand, materials with low thermal conductivity may be of interest as a part of heat insulation or for thermal bridge calculations as well as structural elements.

Moisture content, porosity and constituent materials are the main parameters affecting thermal conductivity of cement-based materials. The thermal conductivity of water >20 times higher than thermal conductivity of the stagnant air and replacement of air by water can make a significant change in the thermal conductivity of porous materials. While changes in constituent materials and porosity may be neglected after concrete curing for thermal conductivity determination, the moisture content is expected to have considerable changes during the lifetime of most cementitious materials. This indicates that considering one certain value for thermal conductivity of such types of composites, may provide low accuracy when considering the material performance during the service life of the material. Calculating thermal conductivity as a function of main effective variables such as moisture content, porosity and constituent materials using simplified prediction models, can be a practical solution to this challenge. The thermal conductivity of dry material may be adjusted in the mix design, using the knowledge from concrete technology with regards to porosity and constituent materials. Variations in such material property due to moisture content can be estimated based on the saturation degree. Moreover, the water sorption can be controlled by modifying the pore structure as well as internal or surface hydrophobation [1, 2]. The prediction model can for example be introduced to building physics tools, where the thermal conductivity can be adjusted based on the existing climate conditions.

2. PREDICTION MODELS FOR CEMENTITIOUS COMPOSITES

2.1 Particle-matrix model based on multiphase semi-empirical equation

Determination of the thermal conductivity of the particle and the matrix phases individually, makes it possible to determine the thermal conductivity of the cementitious composites using the following two-phase model [3].

$$\lambda^{n}_{\text{composite}} = V_{\text{matrix}}\lambda^{n}_{\text{matrix}} + V_{\text{particle}}\lambda^{n}_{\text{particle}} \qquad (1)$$

where $\lambda_{\text{composite}}$, λ_{matrix} and $\lambda_{\text{particle}}$ are the thermal conductivity of the composite, the matrix and the particles, respectively. V_{matrix} and V_{particle} are the volume fractions of the matrix and the particles, respectively, and n is a constant value determined by experimental investigation. The upper and lower limits of n factor are 1 and -1 which are identical to parallel and series models, respectively.

The accuracy of the model can be modulated based on the accuracy in predicting the thermal conductivity of individual phases, which will be discussed further in this study. The expected porosity and moisture content of the cement-based materials may also be estimated and tuned by using the knowledge of concrete technology and building physics. Consequently, by introducing appropriate constituent materials, a particle-matrix model can be used for thermal conductivity based mix design of cementitious materials with desirable accuracy.

2.2 Particle-matrix model based on Hirsch model

Hirsch [4] proposed a model which may be used for predicting thermal conductivity of cement-based composites by considering the two particle and matrix phases. This model combines parallel and series models by giving them a share based on the x factor.

$$\frac{1}{\lambda_{\text{composite}}} = x\left[\frac{1}{V_{\text{particle}}\lambda_{\text{particle}} + V_{\text{matrix}}\lambda_{\text{matrix}}}\right] + (1-x)\left[\frac{V_{\text{matrix}}}{\lambda_{\text{matrix}}} + \frac{V_{\text{particle}}}{\lambda_{\text{particle}}}\right] \tag{2}$$

where x is a constant value determined by experimental investigation. In addition to the x factor, the accuracy of this model is also dependent on accurate estimation of the thermal conductivity of individual phases.

2.3 Simplified estimation using Parallel-Series bounds

While the above mentioned semi-empirical models can be used for thermal conductivity based mix design as well as estimation of thermal conductivity of cement-based composites with a reasonable accuracy, a simplified method may be used for predicting the range of this material property. These models are especially appropriated for cases were the upper or lower limits of thermal conductivity are required. Such cases could for example be the maximum heat loss through a building envelope due to moisture condensation in the pore structure of the materials or the estimating upper limit of the thermal resistance property of the cementitious materials in an embedded floor heating system due to drying. The upper limit is given by the parallel model:

$$\lambda_{\text{composite}} = V_{\text{matrix}}\lambda_{\text{matrix}} + V_{\text{particle}}\lambda_{\text{particle}} \tag{3}$$

and the series model gives the lower limit:

$$\frac{1}{\lambda_{\text{composite}}} = \frac{V_{\text{matrix}}}{\lambda_{\text{matrix}}} + \frac{V_{\text{particle}}}{\lambda_{\text{particle}}} \tag{4}$$

Thermal conductivity of particle and matrix phases can also be extracted from the literature to avoid experimental investigations.

2.4 Simplified estimation using Hashin-Shtrikman bounds

The Hashin-Shtrikman (H-S) model gives tighter bounds compared to parallel and series models. H-S lower (λ_l) and upper (λ_u) bounds for two material phases with $\lambda_1 \geq \lambda_2$, are given by [5]:

$$\lambda_l = \lambda_1 + \frac{V_2}{\frac{1}{\lambda_2 - \lambda_1} + \frac{V_1}{3\lambda_1}} \tag{5}$$

$$\lambda_u = \lambda_2 + \frac{V_1}{\frac{1}{\lambda_1 - \lambda_2} + \frac{V_2}{3\lambda_2}} \tag{6}$$

When the difference between thermal conductivity of matrix and particle phases becomes lower, the two-phase H-S bounds become tighter and a reasonable estimation of thermal conductivity of cement-based composites is readily available without experimentally investigating the composite. The same procedure may be adopted to predict the thermal conductivity of matrix or particle phases separately. For example, in the case of water-submerged hardened cement pastes (HCPs) where most of the air (low thermal conductivity), is replaced by water (thermal conductivity closer to that of solid structure of the plain HCP), the H-S bounds become tight enough to allow for a reasonable estimation of the material property (Figure 1).

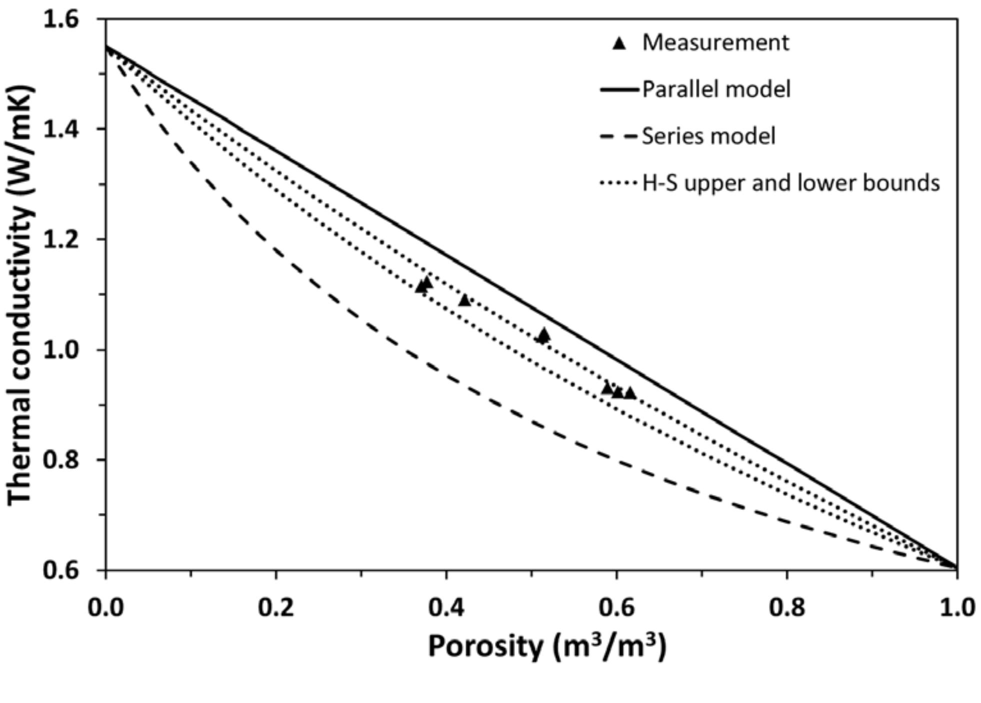

Figure 1– Measured thermal conductivity of plain HCPs submerged in water and analytical bounds [3].

2.5 Response surface method (RSM)

The Response Surface Method (RSM) method, which was developed by Box et al. [6-8] is a collection of statistical and mathematical methodologies, useful for predicting material properties considering different variables and for developing, improving, and optimizing processes. It also finds applications in the design, development, and formulation of new products, improvement of existing product designs [8], and more recently in reliability analysis. The thermal conductivity can for example be approximated with a second-order polynomial function, which for k random variables is expressed as:

$$\lambda = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum\sum_{i<1}^{k} \beta_{ij} X_i X_j \tag{7}$$

where, λ is the predicted thermal conductivity, X_i is the coded level of a design variable i, k is the total number of variables present in the problem, coefficient β_0 is a constant and β_i, β_{ii} and β_{ij} are the regression coefficients for the linear, quadratic and interaction effects, respectively.

2.6 Multi-scale model

Liu et al. [9] presented a multi-scale micromechanical model based on Mori-Tanaka scheme [10].

$$\lambda_{\mathrm{MT}} = \frac{V_{\mathrm{M}} \lambda_{\mathrm{M}} + \sum_{s=1}^{n} V_s \lambda_s A_s}{V_{\mathrm{M}} + \sum_{s=1}^{n} V_s A_s} \tag{8}$$

Where V_s and V_{M} are the volume fraction of the inclusions (can be particles) and the matrix, respectively, and λ_{MT}, λ_s and λ_{M} are the thermal conductivity values of the composite, inclusions and the matrix, respectively. By setting A_s=1, this model will function as a parallel model and considering $A_s = \lambda_{\mathrm{M}} / \lambda_s$ it will be equivalent to a series model.

This model can be deployed for considering the influences of HCP as well as fine and course aggregates in different scales. Multi-scale modelling can be an appropriate solution for high accuracy results. However, the above mentioned model has large errors in some cases such as predicting thermal conductivity of saturated materials. Further study is needed for developing this multi-scale model to increase the accuracy.

3. PREDICTING THERMAL CONDUCTIVITY OF INDIVIDUAL PHASES IN PARTICLE-MATRIX MODEL

3.1 Matrix

The main factors affecting thermal conductivity of the matrix can be considered as variables in a multiphase composite model. Baghban et al. [3] presented a three-phase model for predicting thermal conductivity of HCPs:

$$\lambda_{\mathrm{hcp}}^n = m\lambda_{\mathrm{w}}^n + \left(\varepsilon_{\mathrm{tot}} - m\right)\lambda_{\mathrm{a}}^n + \left(1 - \varepsilon_{\mathrm{tot}}\right)\lambda_{\mathrm{s}}^n \tag{9}$$

where λ_{hcp}, λ_{w}, λ_{a} and λ_{s} are the thermal conductivity of the HCP, water, air, and solid structure of the HCP, respectively. $\varepsilon_{\mathrm{tot}}$ is the total porosity, m is the saturation degree showing volumetric moisture content and n is a constant value. While λ_{w} and λ_{a} are known, a proper estimation needs to be done for λ_{s} and n based on experimental investigation.

The graph in Figure 2 illustrates the thermal conductivity of plain HCPs at different total porosities (ε_{tot}) and saturation degree (m) based on Eq. 9. λ_s is estimated as 1.55 W/mK and n is found to be 0.55 for plain hcps. Note that these two values are obtained by minimizing the calculation error of Eq. 9 to match the experimental data at different moisture states, which is in agreement with the results obtained from the laboratory (see Figure 3). λ_w and λ_a are known parameters which are considered as 0.026, 0.604 W/mK, respectively. Since thermal conductivity of solid structure of the matrix, λ_s, may vary due to changes in constituent materials such as presence of pozzolanic materials, fibres or changes in the cement chemistry, λ_s can be determined as a function of these variables by laboratory research. Furthermore, changes in the thermal conductivity of the fluid phase due to variations in the pore structure or different fluid chemistries can also be investigated by the same procedure. Other models described in previous sections can also be used for predicting thermal conductivity of each phase.

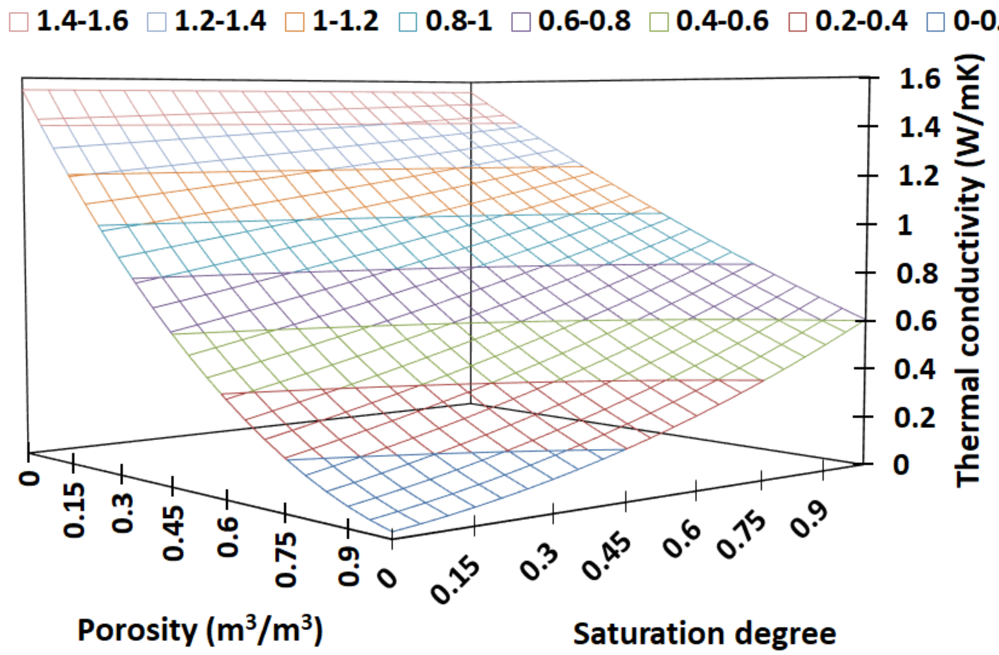

Figure 2 – Thermal conductivity of plain HCPs at different total porosities and saturation degrees calculated from Eq. 9 [3].

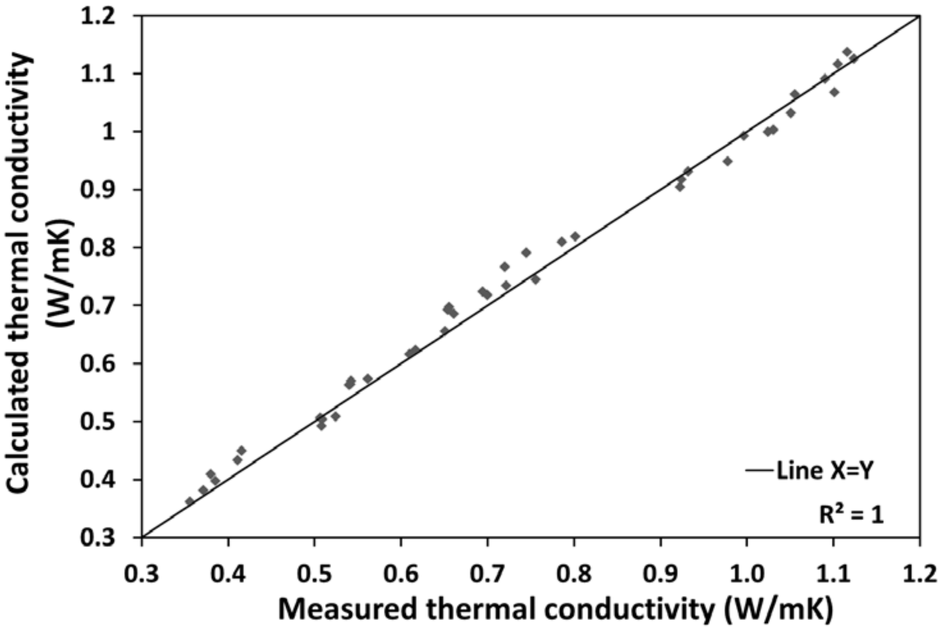

Figure 3 – Comparison of the measured and calculated thermal conductivities [3].

3.2 Particle

Stone aggregates are the most commonly used particle types in cementitious composites. These aggregates have usually a low porosity and the effect of moisture sorption may be neglected for many practical applications. On the other hand, multiphase prediction models can also be presented for the particles in case of using aggregates with considerable porosity, such as using light weight aggregates.

Fine particles in the size range of the matrix particles can be considered as a part of the matrix. Moreover, the coupling effects such as effect of interfacial transition zone can also be defined as a function of the surface area of the particles in the mix.

4. DISCUSSION

Depending on the application and intended accuracy of thermal conductivity prediction, the appropriate prediction model may be chosen. Theoretical bounds are appropriate tools to approximate the highest and lowest values. When the maximum heat loss through a building envelope due to moisture condensation in the pore structure of the material needs to be estimated or highest thermal resistivity of the cementitious materials in an embedded floor heating system due to drying is under investigation, the theoretical bounds can help to provide with the solution eliminating experiments. In this case, providing the data for thermal conductivity of individual phases in the composite is sufficient, which can usually be extracted from the existing literature with a reasonable accuracy. While parallel and series models provide the absolute upper and lower limits, H-S model can present tighter bounds. When the thermal conductivity of the phases are not so far from each other (See Figure 1), H-S bounds can even be used for estimating the thermal conductivity of the composite. Figure 4 illustrates a comparison of different prediction models for dried HCPs considering two phases of air (porosity) and solid structure, based on experimental results from Baghban et al. [3]. Since the thermal conductivity of air is more than 20 times lower than the thermal conductivity of water, the difference between H-S bounds are much higher in Figure 4 compared to Figure 1. However, the experimental data is close to the upper H-S bound for this case which can be used for predicting thermal conductivity of the composites with some over estimation. The parallel model is still farther than upper H-S bound and gives considerable difference with the experimental results.

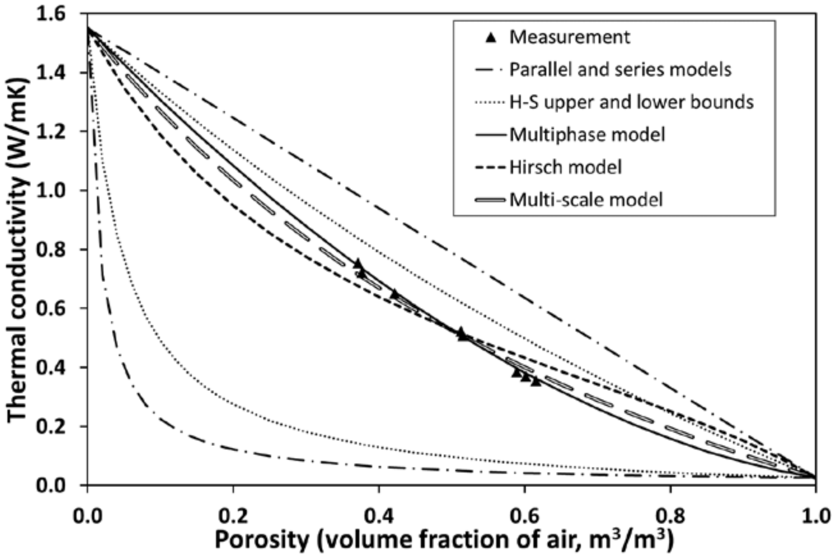

Figure 4 – Comparison of different models with the experimental results of HCPs with two phases of air and solid structure.

Multiphase semi-empirical model has shown the best fit to the experimental data in Figure 4. The three-phase model in Figure 2 generated from Eq. 9 is also based on this model which has been in alignment with the experimental results. The multi-scale model also matches for this example and has the potential for accurate prediction. However, increasing accuracy may bring up complications in the modelling, which can make this method difficult to use. On the other hand, the Hirsch model gives some error and makes this model less suitable for this case. Since RSM is an interpolation technique and not a predefined composite model, which uses statistical approaches, it is able to calculate a regression model to predict the response (in this example, thermal conductivity of the composite). The result of RSM is a polynomial of existing variables, which can easily be fitted to the experimental results in figure 4 and specially multiple variables like surfaces such as the one shown in Figure 2. Since this method is not based on a predefined composite model, providing properly distributed experimental data in the actual boundaries of the composite model can facilitate more accurate estimation of the thermal conductivity pattern. Predefined composite models are less sensitive to distribution of the experimental data.

Changes in the mix composition such as incorporating fibres, additives, different types of aggregates or moisture changes, may change the thermal conductivity pattern and prediction models should be investigated for these cases as well. In general, above-mentioned models are expected to have the potential for predicting the thermal conductivity of cementitious composites with intended accuracy.

5. CONCLUSION

In the framework of this study, different solutions for predicting thermal conductivity of cement-based composites were described. Theoretical bounds such as H-S bounds are appropriate tools to approximate the highest and lowest values. Semi-empirical models based on particle-matrix model can simply approximate this material property with a reasonable accuracy. Further investigation is needed for approximating the thermal conductivity of the individual phases under different conditions such as moisture changes and incorporation of different materials to the composite. Multi-scale modelling has the potential for accurate prediction, however, increasing accuracy may result into complications, which can render adoption of this method difficult. RSM as an interpolation technique can provide a reasonable prediction if properly distributed experimental data are available.

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