Numerical study on water penetration in graphene oxide reinforced concrete by the multiscale approach

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ABSTRACT

Durability is an important property that determines the long-term behaviour of cement-based materials. In this study, graphene oxide nanoparticles (GONPs) are proposed to prevent the ingress of water in the concrete. GONPs contain a range of reactive oxygen functional groups that enable it as a suitable candidate for reaction in cementitious materials. The multiscale approach is adopted to study the unsaturated transport properties of GONPs-reinforced concrete. At the nanoscale, the most important parameters for unsaturated mass transport analysis of GONPs-reinforced calcium silicate hydrate (CSH) are determined through the molecular dynamic (MD) simulation. At the microscale, a hydrated cement model is adopted and its pernetration characteristics are calculated. At the mesoscale, a three-phase mesoscale model of concrete is presented, which considers particles, cement paste, and the interfacial transition zone (ITZ) as separate constituents to simulate the unsaturated flow under the mixed actions of capillary suction, external hydrostatic pressure, and gravity. The proposed approach is validated by comparing the numerical result with those of the available experimental data taken from this paper to verify the reliability and efficiency of multiscale model for predicting the unsaturated water transport properties. Experimental and numerical results indicate that the incorporation of a very low fraction of GONPs (0.1% by weight of cement) can effectively hinder the ingress of water molecules. It can be concluded that adding GONPs improve the transport properties of concrete which subsequently improves its durability.

KEYWORDS

Graphene oxide nanoparticles (GONPs), Concrete, Durability, Unsaturated water transport, Multiscale approach.

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1. Introduction

In the design of concrete structures both strength and durability must be considered by designers. Permeability can be considered as one of the most important parameters in controlling the strength and durability of concrete [1]. Internal and external factors such as porosity and applied pressure can affect the permeability of cement-based materials [1]. With the advancement of nanotechnology, high-performance nanofibers such as carbon nanotubes and graphene oxide nanotubes (GONPs) have been developed that can improve the performance of nanoscale cement-based materials. Studies show that GONPs improve the hydration process of cement and affect the structure of pores in the matrix [2].

Due to the importance of permeability in concrete durability and the lack of studies in this field on GONPs reinforced concrete, in the present study, water transport of unsaturated concrete reinforced by GONPs was simulated. The effect of hydrostatic pressure and different dosages of GONPs on penetration results was evaluated. Due to the complex and heterogeneous structure of concrete, in this study, multi-scale methods have been used as an approach that can extract the properties of materials based on details in small scales and apply in higher scales [3]. The process of conducting this research is as follows; Initially, a laboratory program was developed to investigate the effect of GONPs on concrete permeability and cement paste porosity. In the next section, numerical modeling of unsaturated flow was performed by considering the mechanisms of capillary suction, external hydrostatic pressure and gravity. For this purpose, three scales nano, micro and meso were used. At the nanoscale, the transfer characteristics of calcium silicate hydrate (CSH) were determined as the main component of hydration products through molecular dynamics simulation. At the micro-scale, the hydrated-cement model was prepared using µic software and used to model the permeability in the COMSOL multiphysics software. At a higher scale, the mesoscopic model of three-phase concrete including aggregate, cement paste and interfacial transition zone (ITZ) was simulated to determine the water transport characteristics. In order to validate, the results of multiscale analysis were compared with the laboratory results obtained from this paper.

2. Methodology

2.1. Experimental program

Type II Portland cement (455 Kg/m^3), gravel (900 Kg/m^3) and sand (1100 Kg/m^3) were used in the mix design. The water to cement ratio is considered 0.5 for all samples and GONPs values vary from (0-0.1)% by weight of cement (bwoc). In this study, in order to better disperse of GONPs in water, the ultrasonic bath technique as well as superplasticizers (SP); based on modified polycarboxylate; were used [4]. SP was added to the mix at the rate of 0.5% bwoc. Cube molds with dimensions of 150×150×150 mm were used for the penetration test. For validation purpose, concrete penetration tests have been performed using a "cylindrical chamber" device, which is a new method for measuring permeability [5]. Figure 1 shows the cylindrical chamber apparatus.

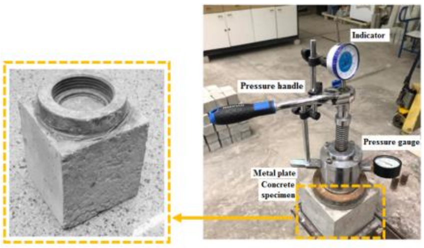

Figure 1. Penetration test setup

2.2. Multiscale theories

In the multiscale method, the properties calculated on a scale, for example at the nanoscale, are used as input parameters in higher scale modeling, for example the micro scale. For simulation of water transport in concrete, three scales nano, micro and meso were used.

At the nanoscale, the transport characteristics of CSH as the main component of hydration products, was determined through the molecular dynamics simulation and LAMMPS software. In this simulation, the tobermorite structure was used for CSH modeling. To simulate the interaction of atoms, the ClayFF and CVFF force fields were selected [6]. At the micro scale, hydrated models of cement including clinker, hydration products and capillary pores were prepared using µic software and transferred to COMSOL finite element software to simulate penetration. At a higher scale, the mesoscopic model of three-phase concrete including aggregate, cement paste and ITZ was simulated to determine the concrete transport characteristics. In order to validate, the results of numerical analysis were compared with the laboratory results obtained from this paper. In the penetration modeling section, the Richards equation is used to simulate water transport in unsaturated concrete, Equations (1) -(3).

$$\frac{\partial \theta}{\partial t} = \nabla . [D(\theta)\nabla \theta],\; C(\theta)\frac{\partial \phi}{\partial t} = \nabla . [K(\theta)\nabla \phi] \tag{1}$$

$$D(\theta) = D_0 e^{n\theta},\; D_0 = \frac{n^2 S^2}{(\Theta_s - \Theta_r)^2 . [e^n(2n-1) - n + 1]} \tag{2}$$

$$K(\theta) = K_s e^{\alpha(\theta-1)},\; K_s = f l_1^2 / (2h_p \Delta t) \tag{3}$$

3. Results and Discussion

In this section, in order to determine the permeability coefficient of hardened cement paste, K_s, which is used as an input parameter in mesoscale, the porosity and penetration test performed base on ASTM and EN480-5 respectively on cement paste samples with water to cement ratio of 0.5 and different dosages of GONPs. The permeability coefficient is calculated using equation (3), [7]. The values of α and n are considered equal to 5.86 and 6, respectively, [7].

According to the nanoscale results, compared to CSH, the water penetration depth and MSD is lower in models containing GONPs. It can be explained as follows; First, the interaction between water molecules is eliminated by the addition of GONPs and capillary absorption is impaired, and on the other hand, GONPs prevent the transfer of water molecules into the channel. Results of microscale simulation shows the cumulative water penetration is lower for all mixtures with GONPs than for the control sample. In order to validate the simulation process in this scale, specimens with dimensions of 40×40×160 mm were modeled and subjected to capillary adsorption test. According to the results, the numerical simulation results have an acceptable agreement with the experimental data.

In the mesoscale, to evaluate the efficiency of the multiscale modeling approach presented in this paper, samples with different dosages of GONPs were numerically tested and compared with the laboratory results of this study. By comparing the numerical water penetration volume results, a good agreement with the laboratory results was observed, Figure 2.

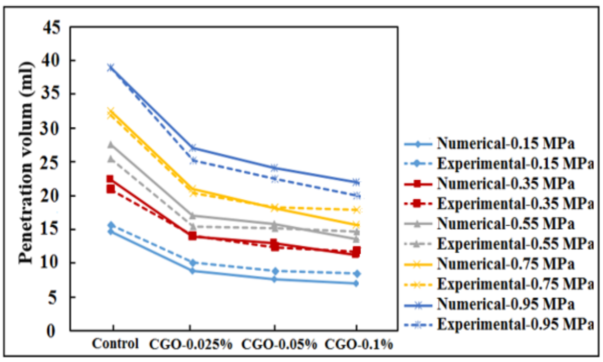

Figure 2. Results of numerical and experimental models

In the following other samples with a wider range of GONPs (up to 0.4% bwoc) and also under higher hydrostatic pressures were tested. Results show that the cumulative water penetration for all mixtures with GONPs under different hydrostatic pressures is lower than the control sample. The results also show that an increase in the amount of GONPs causes a further decrease in penetration volume.

4. Conclusion

The results are as follows:

By comparing the volume of water penetration in numerical simulation with the available experimental data, it was shown that the multiscale approach can provide an acceptable prediction of the water transport process in unsaturated concrete.

The results of simulation of water flow in unsaturated concrete at mesoscale showed that the water penetration for all mixtures with GONPs has decreased compared to the control sample. The reduction in water penetration can be attributed to the improvement of capillary pore structure and barriers formed by GONPs.

5. References

[1] Banthia, N. , Biparva, A., and Mindess, S., 2005. “Permeability of concrete under stress”. *Cement and Concrete Research*, 35(9) 1651-1655.

[2] Pan, Z., He, L., Qiu, L., Korayem, A.H., Li, G., Zhu, J.W., Collins, F., Li, D., Duan, W.H., and Wang, M.C., 2015. “Mechanical properties and microstructure of a graphene oxide–cement composite”. *Cement and Concrete Composites*, 58 140-147.

[3] Eftekhari, and M., Mohammadi, S., 2016. “Multiscale dynamic fracture behavior of the carbon nanotube reinforced concrete under impact loading”. *International Journal of Impact Engineering*, 87 55-64.

[4] Han, B., Guan, X., and Ou, J., 2009. “Application of ultrasound for preparation of carbon fiber cement-based composites”. *Mater. Sci. Technol*, 17(3) 368-372.

[5] Naderi, M., 2010. “Registration of Patent in Companies and industrial property Office, Determination of concrete, stone, mortar, brick and other construction materials permeability with cylindrical chamber method”, (in Persian).

[6] Zhang, W., Li, S., Hou, D., Geng, Y., Zhang, S., Yin, B., and Li, X., 2019. “Study on unsaturated transport of cement-based silane sol coating materials”. *Coatings*, 9(7) 427.

[7] Li, X., Chen, S., Xu, Q., and Xu, Y., 2017. “Modeling the three-dimensional unsaturated water transport in concrete at the mesoscale” *Computers & Structures*, 190 (2017) 61-74.

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