THE APPLICATION OF POPULATION BALANCE MODELS FOR THE PREDICTION OF RHEOLOGICAL PROPERTIES IN FRESH CEMENT PASTES

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ABSTRACT. Concrete is the largest material volume used in the world as well as one of the basis of the worldwide infrastructure. Due to this critical importance and the environmental issues associated with the large masses involved, it has been attracting increasing research attention since the last decades. For hardened concrete, civil engineers already possess a series of engineering tools that allow them to satisfactorily predict properties of interest (e.g. deformation, stress, etc.) as a function of material characteristics. However, when this material is encountered in a fluid state, the picture is completely different: only some empirical tests are capable of relating some material variables (e.g. concrete composition) with relevant properties (i.e. flow speed, flow spread, etc.). Although this practice is longstanding, the increasing complexity of concrete mixtures - introduced by the growing use of mineral additions, chemical admixtures and non-traditional cement chemistries - has invoked the need for developing mechanistic models.

The size range of the particles found in a typical concrete can encompass several orders of magnitude, which implies that numerous kinds of interactions and phenomena are involved. Additionally, the presence of particle clustering introduces a complex set of relationships between rheological behaviour and the evolution of particle size distribution (PSD) in time. Consequently, an adequate description of these microstructural details is deemed as a valuable tool towards the construction of rheological models with predictive capabilities under a wide range of process and material conditions.

The Population Balance Model (PBM) framework is appropriate to capture the relevant dynamics of the granulate distributions in their environmental phase. This framework is based on partial integro-differential equations and it is therefore capable of capturing both the discrete and continuous evolutionary processes that affect the particle state. As a result, PBM can be employed to track the changes in the number of entities under relevant conditions. Subsequently, this information can be used to derive the expected macroscopic behavior.Through a bottom-up approach, an initial description of fluid cement pastes is expected to serve as a stepping stone towards the adequate comprehension of full concrete mixtures. In this contribution, the implementation of a PBM based rheological model for fresh cement pastes is presented. The population balance equation was numerically solved by discretizing the continuous particle size domain in a number of classes. The scheme chosen to achieve this is known as the Cell Average Technique (CAT). The specific equations, the impact of discretization on the predicted rheological properties and other numerical considerations are discussed.

Keywords: Cement, rheology, microstructure.

Mathematics Subject Classifications (2010): 35L65, 35Q70, 35R09 ,45K05, 65M22.

REFERENCES

[1] N. Roussel, A. Lematre, R. J. Flatt, and P. Coussot. Seady state flow of cement suspensions: A micromechanical state of the art. *Cement and Concrete Research*, 40(1):77-84, 2010.

[2] M. Mohtaschemi, A. Puisto, X. Illa, and M. J. Alava. Rheology dynamics of aggregating colloidal suspensions. *Soft Matter*, 10(17):2971,2014 2008.

[3] D. Ramkrishna. *Population Balances. Theory and applications to particulate systems in engineering.* Academic Press, 2000.

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