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Numerical benchmark campaign of COST Action TU1404 – microstructural modelling

Supplementary material
Model 5 - VCCTL

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1 Introduction

In this document the input files for the Model 5 - VCCTL used in the numerical benchmark [1] are listed as a supplementary material. The input files of the model are attached as a separate file.

2 Input files for VCCTL

File cost.cal

This text file contains experimentally measured (isothermal calorimetry) heat flux as a function of time. The program takes this input to convert the number of iterations into a physical time.

File cost.psd

This is a text file containing particle size classes obtained experimentally. This information is used in the parking algorithm that creates the initial particle distribution.

File cost.pfc

Text file containing the volume and surface fraction of the four clinker phases, estimated from Bogue composition and Blaine fineness.

Files cost.c3s cost.c4af cost.sil cost.alu

These text files contain 2-point autocorrelation functions, calculated from the volume and surface fraction of the four clinker phases. These functions are used by the program to spatially distribute the clinker phases within individual cement particles.

Other input parameters, inserted directly in the graphical user interface, include: amount of gypsum and secondary phases (e.g. calcite), w/c ratio, curing temperature.

References

[1] M. Wyrzykowski, et al., Numerical benchmark campaign of COST Action TU1404 – microstructural modelling. RILEM Technical Letters (2017) 2: 99-107. http://dx.doi.org/10.21809/rilemtechlett.2017.44

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