

Summary

This thesis aimed to predict the pore solution and the formation of hydrates during the hydration of PC blended cements with slag and fly ash. A combined kinetic and thermodynamic approach was elaborated by creating a series of thermodynamic equilibria relying on the reactivity of the starting materials with the Gibbs free energy minimization program GEMS to simulate the hydration process.

In the case of PC binary cements, kinetics of hydration were obtained based on relevant studies from the literature whereas in the case of PC ternary cements, kinetics of hydration were assessed by using a model that correlates the pH of the pore solution to the reactivity of the materials.

Predictions were obtained for both PC binary and ternary blended cements at different substitution levels of PC. A set of virtually designed fly ash and slags were created so as to reflect the diverse characteristics (i.e. reactivity and composition) of these materials, as reported in the literature. The sensitivity of several parameters such as reactivity, composition and sorption mechanisms between pore solution and hydrates was also performed based on the up-to-date literature. In the case of PC ternary cements, additional sensitivity analysis was necessary for assessing the performances of the reactivity model, used for predicting the kinetics of hydration of fly ash and slag in PC ternary cements, which are still left unestablished by the current state of the literature.

The predictions on PC binary cements were compared with the up-to-date literature and allowed to understand the individual roles played by the characteristics of the starting materials.

In PC ternary cements, the predicted characteristics of the hydration share similarities with PC binary cements (e.g. portlandite depletion, dilution of the pore solution, formation of strätlingite at high PC replacement levels...). Depending on the type of prediction, the characteristics of either fly ash or slag play a dominant role in the simulations.

Keywords: PC binary cements; PC ternary cements; slag; fly ash; kinetic modelling; thermodynamic modelling; pore solution; hydration products; alkalinity; phase hydrate assemblage