NUMERICAL MODEL FOR CHEMICAL KINETICS OF ALKALI SILICA REACTOIN IN THE CLOSED REACTIVE SYSTEM

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ABSTRACT

The deterioration induced by alkali silica reaction (ASR) is initiated by complicated heterogeneous chemical reactions. This paper describes development of a numerical model for the chemical kinetics of alkali silica reaction in the closed reactive system consisting of mixture of reactive silica mineral, calcium hydroxide and alkali hydroxide solution. The focus of the first part of the paper is on formulating the kinetic rate law for silica dissolution from the reactive silica minerals as a function of several factors, including pH, temperature, concentration of alkalis in solution and type of the reactive silica mineral. This kinetic rate law is then incorporated in the commercial modeling software (Geochemist's workbench®) in an attempt to simulate the ASR process.

The unknown parameters required in the model were calibrated using the sets of experimental data. Once calibrated, the model generated reasonably accurate predictions of the distribution of species in the reacting system and captured several distinct features of experimental data (i.e. depletion of calcium hydroxide levels and timing of the onset of ASR). Both experimental data and the results from the model were in general agreement with the ASR gel formation mechanism proposed by Hou et al. [1]. This mechanism suggest that, in calcium rich environment, the alkali silica gel does not form until the supply of the local calcium hydroxide has been exhausted by formation of the non-swelling calcium silica hydrates.

Though the application of the proposed model is limited to the closed ASR system, it may offer the possibility of the establishment of the unified theory which can help to bridge the gap between fundamental (chemical) mechanisms of ASR and the mechanical responses of concrete.

Keywords
Alkali-silica reaction, kinetic modeling