

AN ABSTRACT OF A THESIS

MODELING THE KINETIC AND TRANSPORT EFFECTS IN THE REACTIONS BETWEEN CALCIUM HYDROXIDE AND FLY ASH USING CELLULAR AUTOMATA

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Master of Science in Chemical Engineering

Concrete materials have been advanced in such a way that they will be engineered by using sophisticated materials science-based mathematical simulations. These simulations, however, require detailed knowledge of the chemical and physical changes that occur during cement hydration and during exposure to the environment. The demand for concrete is increasing every year due to rapid development of constructed infrastructure around the world. Consequently, large-scale industrial production of cement results in high amounts of CO₂ released into the atmosphere.

Certain materials, such as fly ash, can be mixed with cement to reduce the amount of CO₂ produced while improving durability, strength, and various other properties of concrete. Several hypotheses have been proposed to account for the observed previous experimental results of the reaction between calcium hydroxide and fly ash. For example, the effect from pH consistency and transport distance (particle proximity) between particles.

This research project has three objectives. First, to determine if different weight ratios of fly ash to calcium hydroxide will have an effect on the pH of the react sample. Second, to determine if addition of inert, silica carbide will effect the calcium hydroxide consumption rate by affecting particle proximity, and finally, to study and simulate the reaction between fly ash and calcium hydroxide by using pixel base simulation (cellular automaton) to explore the mechanistic aspects of the reaction process.

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CERTIFICATE OF APPROVAL OF THESIS

MODELING THE KINETIC AND TRANSPORT EFFECT IN POZZOLANIC REACTION USING CELLULAR AUTOMATA

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