Multi-Scale Kinetics-Based Model for Predicting Mechanical Property Development of Concrete containing Supplementary Cementitious Materials

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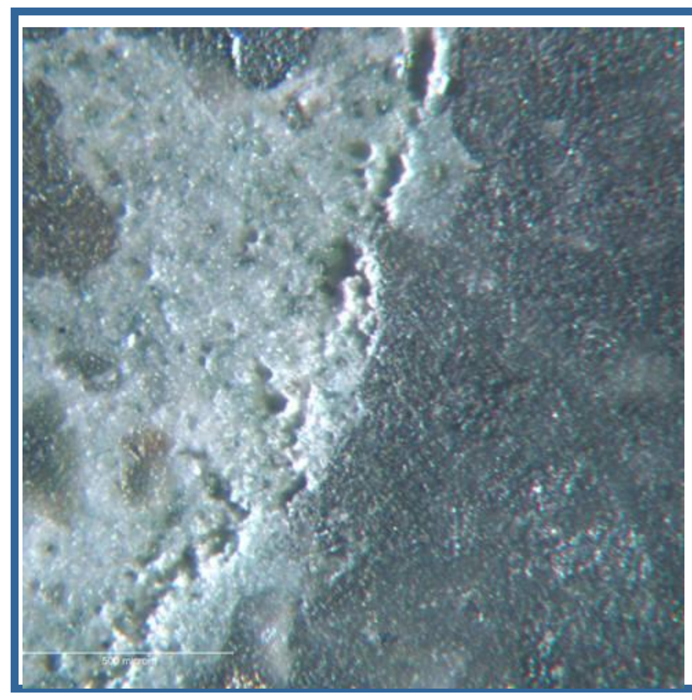
Award #0510854 NSF-CMMI

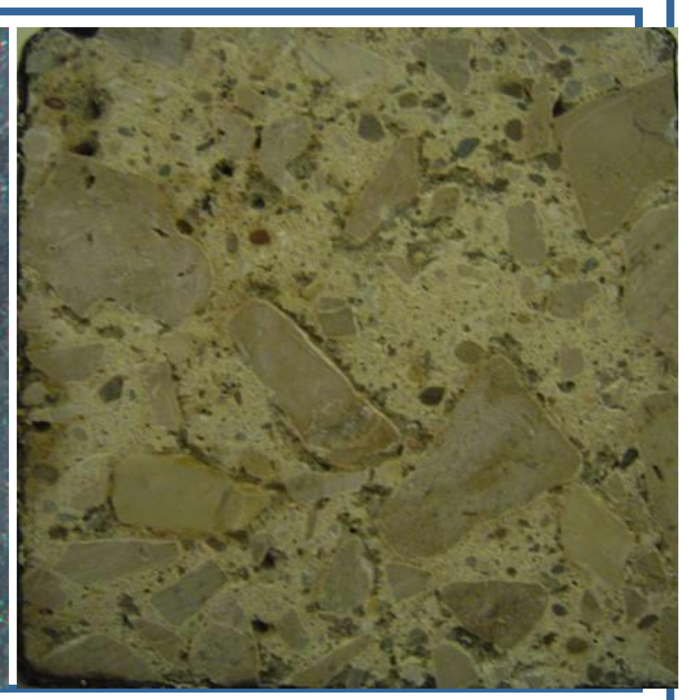
Objectives

•Develop a kinetics-based multi-component hydration model for cements and cements containing supplementary cementitious materials (SCM).

•Quantify the pozzolanic reactivity using absolute rate constants.

•Link the hydration and pozzolanic kinetics models to macro-mechanical and durability properties.





General Hydration Model Based on Nucleation-and-Growth Analysis:

Hancock and Sharp[1] proposed a classical model for analyzing reaction kinetics of enclosed systems based on nucleation-and-growth, also known as a general Avrami model for heat of hydration development Q(J/g) versus time, t (hours):

$$Q = Q_{max}\,[\,1 - \exp(-k\,t^{m})\,]$$

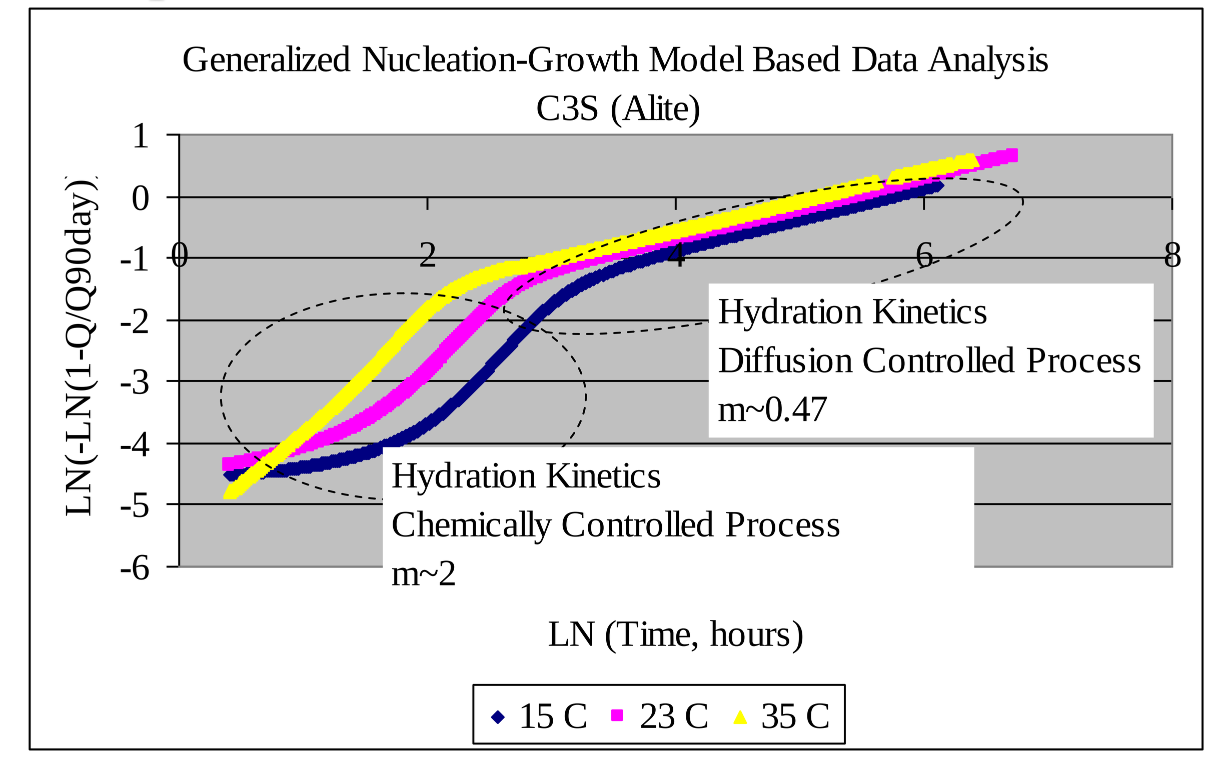
Model linearization for quantifying k & m: $Y = \ln[-\ln(1 - Q/Q_{max})] = \ln(k) + m\ln(t)$

The characteristic ranges of m are a measure of

m ~ 0.5 Diffusion controlled process

m ~ 1 Phase boundary controlled process

m ~ 2-3 Chemical controlled process



STUDY FINDINGS: Modified Hydration Model to account for Hydration Kinetics During Chemical Process Control:

Chemical Process Control: $0 < M20 < 30$ hours

Diffusion Process Control: $t > M20 = 30$ hours equivalent

Temperature effect on rate using Arrhenius type Maturity Function:

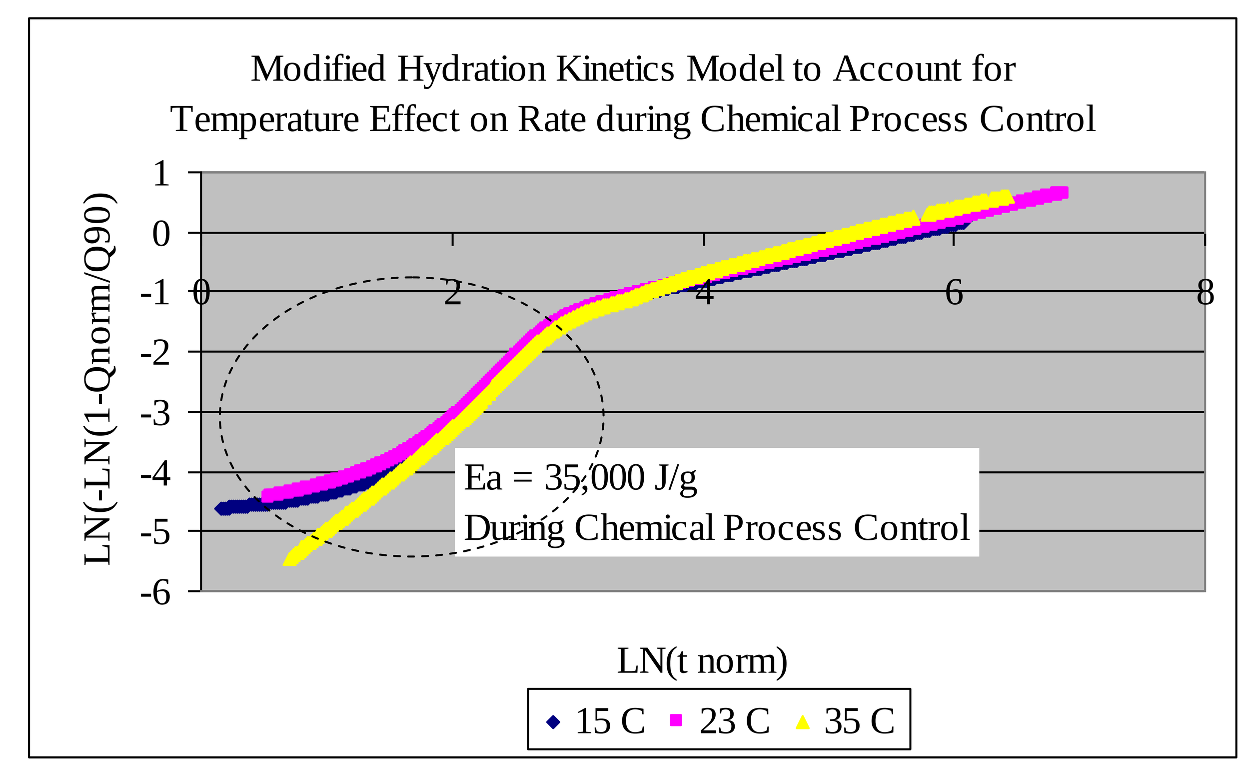
$$M20\ C\ (\text{hours}) = M20\ (\text{equivalent hours}) = \Pi\ \exp\left[\frac{E_a}{R}\left(\frac{1}{293} - \frac{1}{273+T}\right)\right]\Delta t$$

Where:

E_a=Apparent Activation Energy (J/mole); R= Gas constant (8.314 J/mole/ ^{0}C);

T = the sample temperature in ^{0}C

Δt = time, hours



Major Findings

• The kinetics based hydration model quantifies accounts for temperature effects on rate during Chemical Process Control using a Maturity Method based on the Arrhenius Equation. Study findings show that this stage is controlling hydration during the first 30 hours equivalent maturity time, while Diffusion Procress Control is dominant at later time. During this stage temperature effects vanish, except for effect on ultimate hydration.

• The interfacial transition zone, ITZ, between coarse aggregate and the hydration products of portland cement is the weak link link with respect to salt scaling resistance and thus needs to be accounted for in durability model for frost resistance. The ITZ is a region of higher capillary transport (sorptivity coefficient).

Selected References

1. J.D. Hancock and J.H. Sharp, "Method of Comparing Solid State Kinetic Data and its Application to the Decomposition of Kaolinite, Brucite, and BaCO", Journal of American Ceramic Society, Vol. 55, No. 2, p74, 1972.

2. Peng, Y., Hansen, W., Borgnakke, C., Biernacki, J.J., "Hydration Kinetics of Portland Cement Containing Supplementary Cementitious Materials, "Journal, American Ceramic Society, Special Volume "High-Performance Cement-Based Composites", pp. 149-164,2005.