



## Modeling and simulation of cement hydration kinetics and microstructure development

Jeffrey J. Thomas<sup>a,\*</sup>, Joseph J. Biernacki<sup>b</sup>, Jeffrey W. Bullard<sup>c</sup>, Shashank Bishnoi<sup>d</sup>, Jorge S. Dolado<sup>e</sup>, George W. Scherer<sup>f</sup>, Andreas Luttgé<sup>g</sup>

<sup>a</sup> Schlumberger-Doll Research, Cambridge, MA 02139, USA

<sup>b</sup> Department of Chemical Engineering, Tennessee Tech University, Cookeville, TN, USA

<sup>c</sup> Materials and Construction Research Division, National Institute of Standards and Technology, Gaithersburg, MD, USA

<sup>d</sup> Department of Civil Engineering, Indian Institute of Technology Delhi, New Delhi, India

<sup>e</sup> Center for Nanomaterials Application in Construction, LABEIN-Tecnalia, Bilbao, Spain

<sup>f</sup> Department of Civil and Environmental Engineering, Princeton University, Princeton, NJ, USA

<sup>g</sup> Department of Chemistry, Rice University, Houston, TX, USA

### ARTICLE INFO

#### Article history:

Received 24 June 2010

Accepted 7 October 2010

#### Keywords:

Hydration (A)

Kinetics (A)

Microstructure (B)

Modeling (E)

### ABSTRACT

Efforts to model and simulate the highly complex cement hydration process over the past 40 years are reviewed, covering different modeling approaches such as single particle models, mathematical nucleation and growth models, and vector and lattice-based approaches to simulating microstructure development. Particular attention is given to promising developments that have taken place in the past few years. Recent applications of molecular-scale simulation methods to understanding the structure and formation of calcium–silicate–hydrate phases, and to understanding the process of dissolution of cement minerals in water are also discussed, as these topics are highly relevant to the future development of more complete and fundamental hydration models.

© 2011 Elsevier Ltd. All rights reserved.

### Contents

1.	Introduction . . . . .	1258
2.	Historical overview of kinetic models . . . . .	1258
2.1.	Single-particle models . . . . .	1258
2.2.	Nucleation and growth models . . . . .	1260
2.2.1.	Early nucleation and growth . . . . .	1260
2.2.2.	The JMAK nucleation and growth equation . . . . .	1260
2.2.3.	A numerical model for nucleation and growth on a planar surface . . . . .	1262
2.2.4.	The mathematical boundary nucleation and growth model . . . . .	1262
2.2.5.	Limitations of nucleation and growth modeling . . . . .	1262
2.3.	Hydration simulation models . . . . .	1263
2.3.1.	The Jennings + Johnson microstructure simulation model . . . . .	1264
2.3.2.	The HymoStruc model . . . . .	1264
2.3.3.	The CEMHYD3D digital hydration model . . . . .	1265
2.3.4.	The HydratiCA simulation model . . . . .	1266
2.3.5.	The $\mu\text{ic}$ microstructural modeling platform . . . . .	1266
3.	Recent advances in kinetic modeling . . . . .	1267
3.1.	Analyzing $\text{C}_3\text{S}$ hydration kinetics and the effects of $\text{CaCl}_2$ using the boundary nucleation and growth model . . . . .	1267
3.2.	Insights on early-age kinetic mechanisms using HydratiCA . . . . .	1268
3.3.	Analyzing early hydration with $\mu\text{ic}$ . . . . .	1269
4.	Molecular modeling of specific hydration steps . . . . .	1270
4.1.	Atomistic simulation methods . . . . .	1270

\* Corresponding author.

E-mail address: [jthomas39@slb.com](mailto:jthomas39@slb.com) (J.J. Thomas).