Abstract:
Tricalcium silicate, the main constituent of many types of cements including portland cement, white cement, and oil and well cement applications, is frequently used as a model material to study the hydration. Although theories in the literature over the past 40 years have offered considerable insights into the hydration process, reaction mechanisms, and microstructure development, a detailed quantitative representation of kinetics and transport phenomena has not been agreed upon. To help train our intuition and to test various assumptions we have built a progression of single particle models from the simple to more complex. We propose to eventually develop a rigorous multi-component model that can be used to test various hypothesis. Such models are suitable for integration with microstructure simulation tool-kits such as pic and those developed by the VCCTL and are vital inputs to other multi-scale formalisms including Population Balance Models (PBM).

Objective:
To provide a rigorous multi-component kinetic based formalism for the qualitative and quantitative study of reaction and transport mechanisms for C₃S hydration.

Reaction Mechanism:

Computational software: COMSOL
COMSOL is a multi-physics finite element computational platform for solving many types of scientific and engineering problems based on partial differential equations (PDEs).

Assumptions:
• The rate of core shrinkage is given by the dissolution rate which is proportional to the concentration of H₂SiO₄ ions.
• The rate of outer product expansion is given by the rate of reaction occurred at outer boundary.
• The diffusion coefficients are assumed to be independent of concentration of ions.
• The activities of ions are assumed to be equal to concentrations since activity coefficient were approximated to be 1 for dilute solutions, e.g. a_i = c_i.

Modeling approach:
A 1-D coordinate system is chosen and modified according to spherical geometry. A 1-D coordinate system is chosen and modified according to spherical geometry.

Center of the core
Continuous phase
Inner product
Outer product

Continuous
Subdomains:
A – Particle/core
B – Inner product
C – Outer product
D – Continuous Phase

Governing equation and boundary conditions
Diffusion equation is given by:
\[ \frac{\partial c_i}{\partial t} + \nabla \cdot (D_i \nabla c_i) = 0 \]

At boundary 2:
For H₂SiO₄ ions:
\[ N_i = K_{rea}^{inner} a_{Si} a_{H_2O} a_{SiO_4} + K_{rea}^{outer} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-} \]

For OH ions:
\[ N_i = 4 (K_{rea}^{inner} a_{Si} a_{H_2O} a_{OH}^{-}) \]

For Ca ions:
\[ N_i = 2 (K_{rea}^{inner} a_{Si} a_{H_2O} a_{OH}^{-} + 3 K_{rea}^{outer} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-}) \]

For water:
\[ N_i = 3 (K_{rea}^{inner} a_{Si} a_{H_2O} a_{OH}^{-} - K_{rea}^{outer} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-}) \]

At boundary 4:
For H₂SiO₄ ions:
\[ N_i = 0 - K_{rea}^{inner} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-} \]

For Ca ions:
\[ N_i = 2 (K_{rea}^{inner} a_{Si} a_{H_2O} a_{OH}^{-} - K_{rea}^{outer} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-}) \]

For water:
\[ N_i = 3 (K_{rea}^{inner} a_{Si} a_{H_2O} - K_{rea}^{outer} a_{Si} a_{H_2O} a_{SiO_4} a_{OH}^{-}) \]

Discussion and Conclusions:
This more elaborate continuum-based model appears to be somewhat consistent with both simpler codes as well as with the original more detailed automaton-based model from which the rate constants and physical properties were taken.

These results encourage the further development of continuum-based models. More rigorous property estimation, thermochemistry and electrochemical surface effects should be considered in turn.

References:

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