Planning cement materials for a sustainable future

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Binders and cements are crucial materials in past and modern human activities. Critical issues to be addressed for a sustainable use of cements include the global generation of CO_2 during mass production of Portland clinkers, the use of recycled materials in the formulations, and the development of alternative, durable and environmentally-compatible binders. Ultimately, the proper life cycle assessment (LCA) of the mass produced cements must be considered in order to save georesources, although this is a rather challenging task [1].

The expanding use of geopolymers [2, 3] and alkali-activated binders [4] for building applications follow this trend, although further progress is urgently needed in determining the chemico-physical, mechanical, and durability properties of alternative materials. Some of the systems currently under investigation will be reviewed, with emphasis on advantages and pitfalls.

[1] Huntzinger & Eatmon (2009) *J. Cleaner Production* **17**, 668-675. [2] van Deventer *et al* (2012) *Miner. Eng.* **29**, 89–104. [3] van Deventer *et al* (2010) *Waste Biomass Valoriz.* **1**, 145–155. [4] Shi *et al* "*Alkali-activated cements and concretes*". Taylor & Francis, 2006.

The stochastic treatment of mineral surface reaction kinetics

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There is increasing divergence in approaches describing the geochemical kinetics of mineral surface reactions. The first approach, for which there is long-standing traditional support and a large number of observational data, assumes that the most systems are essentially deterministic, i.e., imposing a given set of initial conditions or a perturbation will always produce the same result at a later time. The well-known mathematical representation of this approach is a set of coupled ordinary differential equations: the change in a given chemical species' concentration as a function of environmental conditions, constrained by heuristically determined parameters (rate constants, overall activation energies, etc.). In contrast, the second approach, supported by more recent work [1], argues that the intrinsic variability of certain mineral-fluid systems preclude such a deterministic treatment. Although well-documented, this intrinsic variability is not well understood. At the moment, neither the presence or absence of significant variations in rate under specific conditions has a consistent explanation. Furthermore, even if deterministic outcomes could be represented by probabilistic functions (by assuming fluctutations are negligible), the deterministic approach provides no explicit defense for this assumption [2].

As an initial step, we wish to assess the amplitude of intrinsic rate variation, and thus need to examine the history of dissolving surfaces over time. We present preliminary results of (1) a large number of direct observations of a fixed area of a dissolving mineral surface at constant undersaturation over time, and (2) model simulations of a similar surface, in which contributions of surface defect density, distance to grain boundaries, and other parameters can be varied. These observations of real mineral surfaces and their virtual equivalents permit comparison of the rate's distribution over the surface and its deviation from an arbitrary mean value. This resulting statistical treatment may be a precursor to a generalized stochastic model of mineral surface reactions, and resolution of otherwise inconsistent observations of reaction rate.

[1] Fischer *et al* (2012) *Geochim. Cosmochim. Acta* **98** 177–185. [2] Gillespie, D. T. (1976) *J. Comp. Phys.* **22**, 403–434.

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