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From electrons to infrastructure: Engineering concrete from the bottom up

Hamlin M. Jennings [a,*], Jeffrey W. Bullard [b]

[a] Concrete Sustainability Hub, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, USA

[b] Materials and Construction Research Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD, USA

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ABSTRACT

An approach rooted in fundamental, mechanistic models of concrete materials offers the only viable path for handling the enormous number of variables that are being introduced as new materials are added to the design space, and as new properties are mandated for a sustainable infrastructure. These models must begin at the smallest length scales relevant for concrete properties; in some cases this is the scale of electron interactions among atoms and ions. But concrete has complex chemical and structural properties that are manifested at greater length and time scales, so atomic scale models must ultimately be integrated with new models that capture behavior at mesoscopic and macroscopic scales. We refer to this methodology as the "bottom-up" approach because it proceeds from the smallest length scales. We describe this kind of modeling approach, include some recent results, and suggest some principles for collaboratively integrating multi-scale models.

Contents

1. Introduction[1]

The world's most used man-made substance, portland cement concrete, is also one of the world's most complex substances. Current worldwide annual production of portland cement stands at 2.13 billion tonnes, enough to produce some 23 billion tonnes of concrete each year. Moreover, concrete is used everywhere, including environments with extreme conditions of temperature and pressure, and it is expected to perform well over long periods of time under these diverse service conditions. Unfortunately, the massive use of concrete has a significant impact on the environment: the production of each tonne of portland cement requires about 1.6 tonnes of raw materials, primarily quartz and limestone, and releases about 0.9 tonnes of CO_2 into the atmosphere, thus being responsible for probably 5% of the world's greenhouse gas emissions [1,2]. One of the key near-term challenges for the cement industry is to reduce the greenhouse gas emissions, energy consumption, and natural resources associated with cement production by developing innovative and sustainable cement-based material solutions.

* Corresponding author.
E-mail address: hmj@mit.edu (H.M. Jennings).

[1] A number of extensive reviews have been written since the last International Congress on the Chemistry of Cement (ICCC) that have covered broadly exciting developments in the field of cement science, and this paper is not in competition with these reviews. Recently an unusually concentrated effort has been initiated at the Massachusetts Institute of Technology (MIT), with the theme of “bottom-up” engineering analysis and design, starting at the electron, atomic and molecular scales. For years the National Institute of Standards and Technology (NIST) has also been developing a similar approach, but starting at the micrometer scale. This paper focuses on the expertise and laboratory environments of the authors.

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