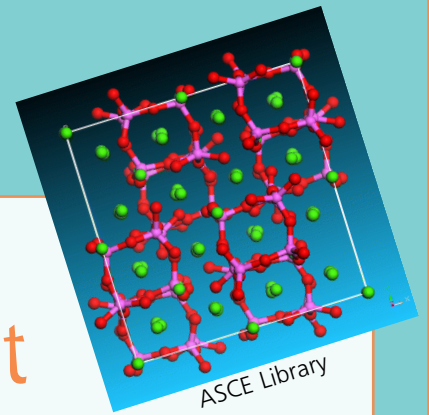


Apply It.

The math behind... Molecular Dynamics in Cement



Technical terms used:

Cement hydration, molecular dynamics (computer experiments), classical Newtonian mechanics, Hamiltonian mechanics, continuum mechanics and numerical approximations

Uses and applications:

Modifying the behavior of cement at the atomic level can lead to innovations in current cement usage. The process can decrease CO₂ emission in cement production, increase strength and other mechanical properties, increase ductility, produce self-consolidating concrete by increasing rheology, produce ultra-high performance concrete, and make sensors by introducing piezo-electric composites.

How it works:

Cement hydration describes the process where cement is mixed with water and changes into a hardened state within a certain period of time. Structural marvels from the ancient pyramids to modern-day Burj Khalifa used some form of the principles of cement hydration. Manipulating the behavior of cement on micro- or nano-scale is a challenging but a necessary task of late.

We can use molecular dynamics, one of the many "faces" of computer simulations, to help manipulate the atomic level behavior of cement, and eventually produce futuristic cements. In molecular dynamics, the position and momentum of atoms are calculated using classical Newtonian mechanics based on the interatomic potential energy. The atomic forces, positions, velocities and displacements are calculated using numerical approximations such as Verlet algorithms, velocity-Verlet algorithm or Leap-Frog scheme. The forces obtained on atomic scale are converted to "true" Cauchy stress with the help of continuum mechanics and Hamiltonian Mechanics. The initial and final displacements obtained through the molecular dynamics simulation represent the initial and (pseudo) final states of cement hydration process. Also, displacements at intermediate time-steps generate the evolution of hydrated states of cement. Thus, a complete hydration process of cement can be obtained by employing molecular dynamics technique. This innovative process can help us manipulate the behavior of cement on small scales and can even help produce futuristic cement.

Interesting facts:

Cement is the most widely used construction material and the most notorious source of carbon emission in the world. The United States alone consumed 93 million metric tons of cement in 2015, slightly less than its peak of 128 million metric tons in 2004. Cement can obtain almost 50% of its 28-day strength within 1st day of hydration, and 98% of total strength in 28 days. The computer simulation of cement hydration is important in investigating and predicting the interaction of cement with water and minerals and other composites.

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