Preventing concrete bridges from falling apart

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Extremes of temperature, rain, exposure to corrosive substances—all of these environmental factors contribute to the degradation of concrete. Specifically, a gas present in our environment, called hydrogen sulphide, turns into sulphuric acid, a corrosive substance, when combined with rainwater.

In a new study published in *EPJ B*, Matthew Lasich from Mangosuthu University of Technology, Durban, South Africa, examines the adverse consequences of the adsorption of natural gas constituents found in our environment—and mixtures of several such gases -into one of the materials that make up concrete: cement hydrate. Lasich found that the preservation of concrete infrastructure from the corrosive effects would require a pre-treatment targeting the adsorption sites in cement hydrate, where the majority of hydrogen sulphide molecules become attached. However, this approach could prove difficult because of their wide distribution.

What makes concrete vulnerable to natural gas adsorption is its porous nature. Its structure is made up of a cement matrix binding together aggregates of particles of sand. In this study, the authors perform a nanoscale analysis based on Monte Carlo simulation to mimic the migration of gas molecules into the cement hydrate structure.

They first recorded the adsorption level across various temperatures for methane, ethane, ethene, and ethyne to determine the uptake of each gas species in cement hydrate. This allowed them to study the effect of molecular size and molecular shape on the sorption of gases in cement hydrate. They then performed a similar analysis for natural gas constituents including nitrogen, carbon dioxide, and, most importantly, hydrogen sulphide.

Their simulations suggest that a specific combination of molecular size and surface area is required for good uptake into cement hydrate.

While hydrogen sulphide adsorbed most favourably of all gases considered in this study, ethyne adsorbed more favourably than methane, despite being a 'heavier' molecule, because its molecular shape lent itself better to the task.

More information: Matthew Lasich, Sorption of natural gas in cement hydrate by Monte Carlo simulation, *The European Physical Journal B* (2018). DOI: 10.1140/epjb/e2018-90339-6

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