Hydration of triethylenetetramine based inhibitor film accelerates the chloride-induced corrosion in concrete: a molecular dynamics study

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Abstract.
Organic corrosion inhibitors can be used to prevent chloride-induced corrosion in reinforced concrete structures. In this theoretical study Molecular Mechanics (MM) and Molecular Dynamics (MD) simulations are performed in order to better understand the interaction mechanisms with the passive film present on steel [1], in particular considering γ-FeOOH surface as solid surface which can be subject to chloride-induced corrosion process and the dimethylethanolamine (TETA) film [2]. The MD simulations are a very useful tool because they describe at atomistic level both the solid surface and organic inhibitors molecules in presence of chloride ions [2] and water molecules [3]. Hydration of organic TETA inhibitor film in presence of chloride ions always accelerate the corrosion process, as experimentally well known. In this theoretical work water molecules in fact induce chloride ions to adsorb on γ-FeOOH surface more quickly and in greater numbers respect with to the same simulations study without water molecules. This kind of organic film cannot exhibit a good behavior to prevent the chloride-induced corrosion process not displaying the so important repulsion to chloride ions. The hydration accelerates the corrosion process. This theoretical work permit to compare these results with another organic inhibitors films studied in previous work [1] in order to prevent the corrosion.

References
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