A Cellular Automata model for the release of corrosion inhibitors from primer coatings

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Primer coatings containing active corrosion inhibitors are commonly used to protect metallic materials from corrosion. The process of transport and leaching of active species is fundamental to the functioning of this type of coatings. However, the mechanism of release and the effect of the structural characteristics of a coating on the overall process are still not completely understood. A 3D Cellular Automata model is presented to study this phenomenon. The model simulates the dissolution of soluble pigment particles and the diffusion of dissolved species from a primer coating exposed to an aqueous solution. Furthermore, the generation of virtual coatings with controlled parameters allows the investigation of the influence of the microstructure of pigmented coatings on the process of release. The results of simulations show a good agreement with available experimental data and the effect of parameters such as the pigment volume concentration or the particle size distribution on the leaching kinetic is reported. Together with the simplicity and versatility of the approach, these results prove the feasibility of a Cellular Automata model to study the release of corrosion inhibitors and improve the understanding of the relationship between microstructure and properties of organic coatings.