Application of Geostatistics to dissolution processes observed at microscale resolutions

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Abstract

We consider the dissolution process taking place at the surface of a calcite crystal in contact with deionized water. We document the heterogeneous pattern of surface topography and ensuing reaction rates through in-situ real-time imaging obtained via atomic force microscopy. The experiments enable one to document the occurrence of various mechanisms driving the evolution of the crystal surface. Local dissolution rates are evaluated from the difference between measurements of the crystal surface at various times. Observations are then interpreted within a geostatistical framework. We analyze jointly the probability distribution of reaction rates and their associated spatial increments, taken between locations separated by any given distance (or lag). We rely on a bi-modal Gaussian mixture model to characterize the spatial distribution of reaction rates. The modes of the mixture correspond to an indicator random variable. The latter is in turn related to the processes taking place across the domain of observation. Our formulations for the probability density function of spatial increments of the rate enables us to embed a joint analysis of the (sample) probability density function of data and their increments within a unique theoretical framework that ensures consistency between these two types of information. Our results (*a*) support our ability to obtain direct observation at the microscale of such dissolution processes, (*b*) reveal a remarkable agreement between sample and modeled statistics of dissolution rates and their spatial increments, and (*c*) show that one can effectively infer distributions of quantities of interest through a joint analysis of observed values and their increments.

Short CV of Alberto Guadagnini

Vice Rector for Research and full Professor of Hydraulic and Water Engineering at Politecnico di Milano. Director of the Department of Civil and Environmental Engineering at Politecnico di Milano (2017-2022). Adjunct Professor at the Department of Hydrology and Atmospheric Sciences of the University of Arizona (USA). Main research activity is related to qualitative and quantitative aspects of flow and reactive transport in groundwater systems and underground energy resources. Key roles in EU framework projects (FP5-FP7, H2020: Coordinator, Deputy Coordinator, Project leader, Supervisory Board member, and PI of numerous research projects funded by the industrial sector). Chair of the Communication Committee of the International Society for Porous Media (Interpore). Chair of the Committee on Groundwater Hydraulics and Management of the International Association for Hydro-Environment Engineering and Research (IAHR). Chief Executive Editor of the Journal Hydrology and Earth System Sciences (EGU) and Associate Editor of the Journals Water Resources Research (AGU) and PNAS Nexus. Recipient of the Chaire Gutenberg and Prix Gutenberg 2018 (Award by Cercle Gutenberg and Région Grand-Est, France, for research on Climate change and water cycle in Upper Rhine Basin). Elected member of the European Academy of Sciences and Arts (2021).