Bayesian inversion analysis of nonlinear spatiotemporal dynamics of heterogeneous reactions in rock-water interactions

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It is essential to extract nonlinear dynamics from time-series data as an inverse problem in natural sciences. We propose a Bayesian statistical framework for extracting nonlinear spatiotemporal dynamics of surface heterogeneous reactions from sparse and noisy observable data. Surface heterogeneous reactions are chemical reactions with conjugation of multiple phases, and they have the intrinsic nonlinearity of their dynamics caused by the effect of surface-area between different phases. We employ sequential Monte Carlo algorithm and other statistical algorithm to partial observation problem, in order to simultaneously estimate the time course of hidden variables and the kinetic parameters underlying dynamics. Using our proposed method, we show that the rate constants of dissolution and precipitation reactions, which are typical examples of surface heterogeneous reactions, and the diffusion constants, as well as the spatiotemporal changes of solid reactants and products, were successfully estimated only from the observable temporal changes in the concentration of the dissolved intermediate product.

[1] Omori et al., Bayesian inversion analysis of nonlinear dynamics in surface heterogeneous reactions, Phys. Rev. E, 94, 033305 (2016)

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