Bayesian Data-driven Approach for Extracting Nonlinear Dynamics of Heterogeneous Reactions

*MASAKI ITO¹, Tatsu Kuwatani², Ryosuke Oyanagi², Toshiaki Omori¹

1. Kobe University, 2. JAMSTEC

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. In earth science, it is important to understand heterogeneous reactions in order to figure out the dynamics of rock formation near surface of the earth. We propose a Bayesian data-driven approach for estimating nonlinear dynamics of heterogeneous reactions from noisy observable data. We employ sequential Monte Carlo algorithm to partial observation problem, in order to extract hidden variables. Using our proposed method, we show that heterogeneous reactions can be estimated successfully from noisy observable data under conditions that the number of observed variables is less than that of hidden variables. Moreover, we show how our proposed method extracts substantial nonlinear dynamics of heterogeneous reactions under realistic environments.

Keywords: Heterogeneous Reactions, Data-driven Approach, Nonlinear Dynamics