Japan Geoscience Union Meeting 2015
(May 24th - 28th at Makuhari, Chiba, Japan)

MTT40-09 会場:201A 時間:5 月 28 日 09:30-09:45

不均質反応を支配する非線形ダイナミクスのベイズ解析〜岩石形成ダイナミクスの理解に向けて〜
Bayesian analysis of nonlinear dynamics in heterogeneous reactions – toward understanding of rock-forming processes –

大森 敏明 [1*] ; 桑谷 立 [3] ; 岡本 敦 [3] ; 福島 孝治 [2]
OMORI, Toshiaki[1*] ; KUWATANI, Tatsu[3] ; OKAMOTO, Atsushi[3] ; HUKUSHIMA, Koji[2]

[1] 神戸大学, [2] 東京大学, [3] 東北大学
[1]Kobe University, [2]The University of Tokyo, [3]Tohoku University

Heterogeneous reactions, which occur at interface between two phases, play important roles in rock-forming processes. In heterogeneous reactions, dynamics are intrinsically nonlinear, because surface area governs actual reaction rates and changes temporally. In general, even static surface area, not to mention the temporal change of surface area, is very difficult to be measured. Therefore, it has still been difficult to determine kinetic parameters of heterogeneous reactions even by well-designed laboratory experiments, because we can only use nonlinear and incomplete data sets.

In this study, we develop novel methodologies which estimate kinetic parameters from nonlinear dynamics of heterogeneous reactions using a Bayesian probabilistic approach. With an increasing demand of data-driven analysis, the Bayesian estimation has been widely applied to various fields in the natural sciences including physics, medicine, brain science, and earth sciences (e.g. Watanabe et al., 2009; Naruse et al., 2009; Shouno and Okada, 2010; Omori et al., 2013; Kuwatani et al., 2014; Omori, 2014). In this study, we first formulate probabilistic models of nonlinear dynamics of heterogeneous systems based on state space model. Sequential Monte Carlo Method and EM algorithms are employed for the proposed state-space model in order to simultaneously estimate time course of heterogeneous systems and kinetic parameters underlying nonlinear dynamics. The proposed method provides a very suitable framework for inversion analysis of nonlinear dynamics from incomplete datasets.

In this study, we focus a simple heterogeneous reaction, in which the solid reactant changes to solid product via intermediate product dissolved in fluid phase. It can be regarded as one of the most fundamental and substantial heterogeneous reactions for solid-fluid interactions. Using our proposed method, the reaction rate constants of dissolution and precipitation as well as the temporal changes of solid reactants and products were successfully estimated only by the observable temporal change of the dissolved intermediate product. The proposed method can be potentially applied to actual laboratory experiments of heterogeneous kinetics in various fields of earth and planetary sciences.

キーワード: 地球惑星科学データ解析, データ駆動型アプローチ, ベイズ統計, 非線形ダイナミクス, 不均質反応, 岩石形成ダイナミクス
Keywords: data analysis in geoscience, data-driven approach, Bayesian statistics, nonlinear dynamics, heterogeneous reaction, rock-forming processes