

スパースモデリングによる不均質反応非線形ダイナミクスの推定

Sparse Modeling of Nonlinear Dynamics in Heterogeneous Reactions

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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 propose a sparse modeling approach for extracting nonlinear dynamics of surface heterogeneous reactions from sparse and noisy observable data. We employ sparse modeling algorithm and sequential Monte Carlo algorithm to partial observation problem, in order to simultaneously extract substantial reaction terms and surface models from a number of candidates. Using our proposed method, we show that the rate constants of dissolution and precipitation reactions, which are typical examples of surface heterogeneous reactions, necessary surface models and reaction terms underlying observable data were successfully estimated only from the observable temporal changes in the concentration of the dissolved intermediate product.

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