

Deconvolution of Distribution Functions Using Fourier Transform 푸리에 변환을 이용한 분포함수의 결정

Hyun-Kon Song, Jong H. Jang, Seung M. Oh

School of Chemical Engineering and Research Center for Energy Conversion
and Storage, Seoul National University

Most of initiative basic equations describing a phenomenon are built based on a simplified model involving the heart of the phenomenon. Although they give us information on the core of the phenomenon, the basic equations or models have been upgraded into more feasible ones for real systems by making up for the weak points of too simplified assumption. When a microscopic event (the kernel $q(x,y)$) is governed by a basic equation and the variable y in the basic equation is distributed on the distribution function $n(y)$, the macroscopic event that we observe resultantly (the observed function $p(x)$) is described by the Fredholm integral equation of the first kind (the integral of $[q(x,y) n(y)]$ with respect to y).

In this work, the distribution function $n(y)$ involved in the Fredholm equation was deconvoluted by discrete Fourier transform (DFT). The Fredholm equation was transformed into the convolution form by introducing proper variables. The observed function $p(x)$ or p_n and the kernel $q(x)$ or q_n were Fourier-transformed into the corresponding Fourier coefficient, P_k and Q_k , respectively. Fourier transformed distribution function N_k was obtained from the ratio of P_k to Q_k . Noise were removed by low-pass filtering the power spectral density $|N_k|$ in Fourier space. Then, the distribution function $n(y)$ or n_n was obtained from the noise-free N_k through inverse DFT.

Several examples were tested: Freundlich adsorption isotherm, faradaic or resistive systems for EIS (Randle model involving CPE instead of capacitance and Fractal model) and non-faradaic or capacitive systems for EIS (experimental and simulated data). The "continuous periodicity" was required for the observed data p_n and the kernel q_n . In the case of continuous distribution functions (e.g. Randle model), the distribution functions were obtained very successfully even from noisy data. For the discontinuous cases (e.g. fractal model), the noise reduction process in the deconvolution led to damping of distribution functions.