Maximum entropy approach to characterization of random media

E. V. Vakarin

UMR 7575 LECA ENSCP-UPMC, 11 rue P. et M. Curie, 75231 Cedex 05, Paris, France
e-mail: vakarin@ccr.jussieu.fr

Characterization of complex disordered media (porous matrices, random networks, etc.) is usually based on an analysis of indirect probes. This is realized through a contact of the medium and a system with a well-defined response function $\theta(\mu|\sigma)$ conditional to the medium state σ. Thus one deals with an inversion of the following integral

$$\theta(\mu) = \int d\sigma f(\sigma)\theta(\mu|\sigma),$$

where $\theta(\mu)$ is an experimental result, $f(\sigma)$ is the desired distribution of some relevant quantity, σ. In many cases the inversion of this integral with respect to $f(\sigma)$ is an "ill-posed" mathematical problem. Therefore, current approaches involve either sophisticated regularization procedures, or a fitting with multiple adjustable parameters. The problem is complicated by the absence of a unique solution and strong sensitivity to the input deviations.

Based on a combination of the statistical thermodynamics and the maximum information principle [1] we propose a complementary approach to this problem. The distributions are calculated through a maximization of the Shannon entropy functional conditioned by the available data $\theta(\mu)$. The scheme is shown to provide an explicit solution and a systematic link between the distribution and the input ($\theta(\mu)$, and $\theta(\mu|\sigma)$). The gained amount of information is shown to be directly related to the probe thermodynamic state $\theta(\mu)$. Several illustrative examples, relevant to adsorption probes are discussed.

[1] E. T. Jaynes, Phys. Rev. **106**, 620 (1957)