Bayes' Theorem, Fick's Law and Multicomponent Diffusion

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"Now, even in a Newtonian system, in which time is perfectly reversible, questions of probability and prediction lead to answers asymmetrical as between past and future, because the questions to which they are answers are asymmetrical."

Norbert Wiener (*Cybernetics*, M.I.T. Press, 1961)

Mechanical concepts have formed the basis of a number of recent publications on diffusion. Diffusion models based on mechanical interactions between diffusing species must certainly satisfy the laws of mechanics. Observed diffusion behavior, however, is typically a macroscopic manifestation of a myriad of microscopic motions. In this sense, the purpose of diffusion models is to predict future macroscopic behavior from information about the present and prior states of a material system. Since our information regarding the microstates within the macroscopic system is always incomplete, these predictions are ultimately of the probablistic, rather than the mechanistic, variety.

Our own industrial applications of diffusion theory include efforts to model the drying behavior of coated webs. We often obtain accurate drying predictions using the diffusion models

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proposed by Zielinski and Hanley ("Practical Friction-Based Approach to Modeling Multicomponent Diffusion," *AIChE J.*, **45**, 1 (1999)) and by Alsoy and Duda ("Modeling of Multicomponent Drying of Polymer Films," *AIChE J.*, **45**, 896 (1999)), despite the seemingly restrictive mechanical assumptions upon which they are based. Our appreciation and understanding of the performance of these theories shifted dramatically when we came upon a paper by the late Edwin T. Jaynes ("Clearing Up Mysteries – The Original Goal," in *Maximum-Entropy and Bayesian Methods,* J. Skilling (ed.), Kluwer, 1 (1989)).

Jaynes is best known as the creator of the Maximum Entropy Principle ("Information Theory and Statistical Mechanics, *Phys. Rev.*, **106**, 620 (1957)), which connects macroscopic behavior to probability distributions for microstates. Jaynes was also a strong advocate for applying Bayesian probability theory as logic. He believed that probability represents degree of belief commensurate with an individual's state of information. In the paper referenced above, Jaynes used Bayes' Theorem:

$$p(h \mid D, I) = \frac{p(h \mid I)p(D \mid h, I)}{p(D \mid I)}$$

to derive Fick's First Law. In Bayes' Theorem, p represents probability; h represents a hypothesis; D represents the data; and I represents other information. Terms to the right of the vertical bar within parentheses are known. The first term in the numerator on the right is the *prior probability* of the hypothesis. The second term in the numerator on the right is the *likelihood* function, which gives the probability of the data given that the hypothesis is true. The denominator serves to normalize the distribution. In Jaynes' derivation, it is the prior information in Bayes' Theorem that breaks the symmetry of self-diffusion in dilute solutions to yield Fick's First Law.

The purpose of the present paper is to extend Jaynes' derivation of Fick's Law from Bayes' Theorem in a way that connects Zielinski and Hanley's and Alsoy and Duda's mechanical theories to predictive probability concepts. Understanding their basis in probability theory as logic may help explain the success of these theories in applications to systems that clearly violate their respective mechanical foundations. More importantly, a probabilistic approach may point the way to more robust multicomponent diffusion models.