597f Modeling and Simulation of the Formation of Carbon Molecular Sieves by Carbon Deposition: Non-Linear Stochastic Approach

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Carbon molecular sieves (CMSs) are increasingly being applied to the purification and separation of gaseous and liquid mixtures, e.g., in the separation of nitrogen or oxygen from air; often, CMSs serve as catalysts or catalyst supports. Carbon adsorbents, or activated carbons, with relatively uniform pore-size distributions are suitable as substrates to manufacture CMSs; such carbon adsorbents can be produced from various sources including biomass. The CMS formation entails the modification of the original structure of activated carbons' internal surfaces by means of some chemical or physical methods to augment the adsorbing capacity. One of the methods deposits fine carbon particles on the mouths of activated carbons' pores. These carbon particles are generated by decomposing a gaseous carbon source under specific conditions of temperature and pressure. The CMS formation proceeds randomly: The pores on the activated carbons' surfaces are discrete, mesoscopic in size and irregular in shape, and the carbon particles in the gas phase move erratically. In addition, the resultant random and erratic fluctuations are intensified at the initial and final stages of CMS formation. Thus, it is highly desirable, or even necessary, to analyze and model the CMS formation by carbon deposition according to the statistical framework or a stochastic paradigm. Specifically, the CMS formation is analyzed and modeled here as a pure-birth process with a non-linear and mechanistic intensity of transition. The resultant model gives rise to the master equation of the pure-birth process as well as the governing equations for the mean and variance of the random variable characterizing the CMS formation. The complexity in solving the master equation is circumvented by resorting to a rational approximation method, system-size expansion; this yields the analytical expressions for the mean, variance, and coefficient of variation. The model is validated by comparing the analytical expressions with available experimental data. *Keywords*: Carbon molecular sieves, Kinetics, Markov processes, Mathematical modeling, Porous materials