**Modeling Formation of Supported catalyst for PEM fuel cell applications**

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Supported Platinum electrocatalysts are generally used in Polymer electrolyte membrane fuel cells (PEMFC) to catalyze the hydrogen oxidation and oxygen reduction reactions. The high surface to volume ratios of supported catalysts maximizes the area of catalytic surface available for reactions. High dispersion of platinum nanoparticles on the carbon support is very important in order to minimize the loss in activity due to agglomeration of the nanoparticles. The method of preparation plays a significant role in the extent of dispersion obtained. A very common method of preparation of Platinum supported on carbon is based on a colloidal method [1]. This class of methods involves reduction of hexachloroplatinate compound with suitable reducing agents such as sodium sulfite, polyvinyl alcohol (PVA) etc. The colloidal solution is then mixed with a slurry of carbon (Vulcan XC-72®) in water. The platinum colloidal particles then adsorb on the surface of carbon thereby forming carbon particle decorated by platinum nanoparticles. The catalysts are activated by exposure to nitrogen atmosphere at medium to high temperatures.

A model is proposed to study the formation of supported catalyst from the colloidal suspension of platinum nanoparticles. A stochastic process similar to first order adsorption/desorption process is proposed. Technically this process is a Poisson process on a net covering the substrate [2]. An exponential distribution of waiting times for adsorption and desorption is assumed. The non-Euclidean geometry of spherical surfaces is taken into account. The rate constants for adsorption and desorption are calculated from Eyring's formulation based on the contributions from activation energy and energy of the local neighborhood for the platinum particles. The probabilities of adsorption and desorption are thus dependant not only on the platinum-carbon interactions but also on the energy of the platinum particle neighborhood. The energy of the neighborhood patterns is determined based on the various interactions for a given particle and its nearest neighbors. The energies of interaction are calculated based on the Hamaker coefficients that scale the free energy of interaction between particles. Hard-sphere repulsive and non Van der Waals attractive interactions are assumed. Initial size distribution for particles in colloidal suspension is obtained from Light Scattering experiments. A Metropolis-like algorithm for Monte Carlo simulations is used to study the formation of a platinum decorated carbon particle from the solution of platinum colloids. Final particle size distribution obtained from the simulations will be compared with the values obtained from Transmission electron microscopy. Temperature effects on particle size changes will also be incorporated.

The calculations can be generalized to study the formation of supported catalyst of any materials by changing the corresponding physical parameters. Such understanding in the nature of support-nanoparticle interactions and formation rates would serve as a prelude for a detailed study of support effects.

**References**

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