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Parameter identification in electrochemical kinetics of alkaline methanol oxidation

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We present several approaches for parameter identification of electrochemical kinetic model of alkaline methanol oxidation. This process is relevant for the development of costefficient fuel cells. Experimental data comprise a set of cyclic voltammograms, measured for different fuel and alkaline concentrations. The mathematical model describes the process by a system of 6 differential equations, parametrically depending on 16 reaction constants. The main challenges here are: High stiffness of the system, creating stability problems for numerical integration, as well as high dimension and undefined range of parameter space, creating a known "curse of dimensionality" problem for numerical minimization algorithms. In our implementation, the integration of the differential equations is performed by an adaptive implicit algorithm, specially designed for stiff systems. For parameter identification we consider a combination of automatic derivative-free global minimization, traditional monte carlo and interactive parameter study. The common feature in experimental data is a strong hysteresis effect, i.e., the curves for increasing and decreasing voltages do not coincide. This effect appears in a thin subset of parameter space, representing special rare combinations of parameters. Several scenarios of the process are considered, related with different mechanisms of platinum oxide formation and various paths in carbon oxidation chain. We discover four islands of solutions, corresponding to the local minima of chi-square function. We have also found an interesting cross-relation between reaction constants, preserving chi-square. The best match belongs to the scenario with sequential mechanism of platinum oxidation, for which we present the reconstructed reaction constants.

Biography

Dr Lialia Nikitina graduated from Moscow State University, MS in 1994, PhD in 2003. Since 2004 she is a research scientist at fraunhofer institute for algorithms and scientific computing, sankt augustin, Germany. Principal research interests are mathematical modeling, numerical simulation, data analysis, multidimensional optimization. She has published more than 50 papers in reputed journals and conference proceedings.

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