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Use of the Saul'yev method for the digital simulation of chronoamperometry and linear sweep voltammetry at the ultramicrodisk electrode

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Abstract

The two-dimensional Saul'yev method of simulating processes at an ultramicrodisk electrode is compared with the fully implicit backward differentiation method started with a few backward implicit steps, and an alternating direction implicit method. 2D Saul'yev is convenient to program and although it is significantly slower in execution than the other two methods, it still executes in reasonable time, and yields equally good results with a suitable choice of discrete intervals, and despite its inherent propagation problem, and a certain restriction in the relationship of the spatial and temporal intervals. Saul'yev was implemented for the diffusion limited potential step experiment, as well as linear sweep voltammetry for a reversible system.

Keywords: Computational Electrochemistry; Digital Simulation; Saul'yev method; finite differences; ultramicrodisk electrode simulation

1. Introduction

There are several approaches to the digital simulation of the behaviour of the ultramicrodisk electrode (UMDE), and one way to classify them is by programming convenience. We have recently studied the question of what method achieves the highest efficiency, measured by the least computing time for a given target accuracy and concluded [1] that multi-point derivative approximations in transformed space, solving for the whole two-dimensional grid with an implicit method such as BDF,

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