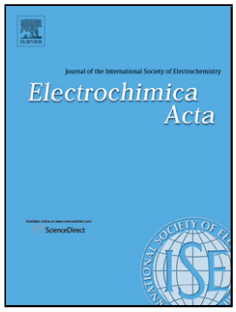

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Author: V.V. Malev

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REFORMULATION OF CHARGE TRANSFER AND MATERIAL BALANCE EQUATIONS OF POLARON-CONTAINING POLYMER FILMS

V.V. Malev [a, b)]

[a)] *Department of Chemistry, St. Petersburg State University, Universitetsky prospect 26, 198504, St. Petersburg, Russian Federation*
[b)] *Institute of Cytology, Russian Academy of Sciences, Tikhoretsky prospect 6, 194064, St. Petersburg, Russian Federation*

Abstract: As known, polaron quasi-particles of conducting polymers contain from 3 to 6 monomer fragments (repeat units) of polymer chains. This is the reason why the widely accepted approach to treating the polaron conductance assumes that the reduced forms of polarons have the same number of repeat units as included into polarons and, moreover, treats such reduced formations as separate quasi-particles. The latter obviously means that charge transfer from a polaron to a neighboring reduced quasi-particle proceeds with simultaneous transformations of all the fragments of these quasi-particles. In other words, the distance of charge transfer in such transitions is assumed to be exactly equal to the polaron size. In contrast to such treatment, the main feature of the proposed approach is a polaron flux reformulation, which assumes a unit polaron translocation to be of a one monomer size independently of number m of monomer fragments included into polaron quasi-particles. As a result, material balance equations of polaron-conducting films take a more complicated form than that accepted in the existing approach. It is shown that, at equilibrium conditions, the obtained equations, as it must be, lead to the relationships being in accordance with thermodynamic ones. At the same time, a proper analysis reveals some differences between quantitative results that follow from the proposed and traditional approaches for both quasi-equilibrium and non-equilibrium conditions. Possible directions of the further development of the represented approach are shortly discussed.

Keywords:
Polymer chains, charge transfer, polaron, cyclic voltammetry, impedance.