KYUSUP LEE, Seoul National University

Application of a New Solution Method for Fredholm Integral Equation to Geminate Recombination of Hole-Electron Pair

We have proposed a new approximate solution method for the Fredholm integral equation of the second kind with nonzero kernel function. The new solution method has been found to be very useful in the problems of diffusion-influenced chemical kinetics. Here, we consider the effects of external electric field and anisotropic long-range reactivity on the recombination dynamics of a geminate charge pair. A closed-form analytic expression for the ultimate separation probability of the pair is presented. In previous theories, analytic expressions for the separation probability were obtained only for the case where the recombination reaction can be assumed to occur at a contact separation. For this case, Noolandi and Hong obtained an exact solution, but their expression for the separation probability was too complicated to evaluate. Hence an approximate analytic expression proposed by Braun has been widely used. However, Braun's expression overestimates the separation probability when the electric field is large. In this work, we present an approximate analytic expression that is accurate enough for all parameter values. In addition, the expression is also applicable when the interaction between the geminate charge pair is described by screened Coulombic potential, and the recombination reaction has an anisotropic and long-range reactivity. We also provide the expression for the separation probability when the initial separation between the geminate charge pair is larger than the contact distance.