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Isolation of determined component of the empirical dependency of binary solutions physicochemical properties

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An algorithm for separating deterministic and stochastic contribution to the empirical dependence of physicochemical properties of binary solutions on concentrations of the components based on the expansion of the function in a Fourier series has been done in this study. The result shows that the isolation of a non-additive part of dependence of physicochemical characteristics on concentration of the components in the solution allows quantitatively describe the effects of contribution to the solvation energy of a multicomponent system. In addition, the isolation of non-additive amendment gives a possibility to formulate the algorithm of analytical continuation too the formal negative values of concentrations that make no break to the function and its first and second derivatives. It was shown that the difference in speed of convergence of the Fourier expansion of deterministic and stochastic parts of the non-additive amendment allows effectively smooth the empirical dependence for sufficient data. The criteria of qualitative separation of deterministic and stochastic harmonics have been determined. The basic set of three-parameter regression of description of isobar boiling point of binary solution that gives a possibility of consideration of the main contribution to the deterministic part of the empirical information has been done. Two-stage algorithm of regressive description of dependency of boiling point of binary aqueous-organic solutions on composition has been formulated. That algorithm can reduce the amount of necessary empirical information. The calculations of the contribution and number of stochastic determined harmonics in the experimental data for aqueous-organic solutions, which have a great practical importance, have been done. For most of investigated solutions proposed regression fully describes the deterministic basis of the empirical results. For a small number of water-organic solutions a three-parameter approximation can be refined by considering deterministic harmonics. The number of deterministic harmonics for all studied solutions must not exceed two. It was found that the relative error of the proposed regressive model does not exceed 2% and can be defined only by experimental errors.

Biography

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