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Modeling phase partitioning of ethanol and methanol with BTEX compounds in water

K. Lee (1)

(1) Civil Engineering, West Virginia University Institute of Technology, Montgomery WV, 25136, USA (kenneth.lee@mail.wvu.edu)

This research studies the equilibrium phase partitioning behavior of ethanol and methanol in a two-phase system consisting of water and a BTEX compound. A previously developed computer program is enhanced to generate ternary phase diagrams for analysis of each alcohol-water-BTEX mixture combination. The activity coefficients are estimated using the UNIFAC model. The simulated ternary phase diagrams show that for each water-BTEX pair considered in this study, the area of the single-phase region is smaller in the presence of methanol. Furthermore, relatively similar phase partitioning behavior is observed for every BTEX compound in the presence of the same alcohol. This research illustrates the implications of pollutant phase partitioning on subsurface contamination resulting from high alcohol content fuel mixtures.