Abstract Submitted
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COSMO-3D: Introducing Steric Effects into COSMO Solvation Models[1] ERIN MCGARRITY, Delft Technical University, JAN VAN DER EERDEN[2], Condensed Matter and Interfaces-Debye Institute for Nanomaterials Science, Utrecht Unversity, Netherlands, GERARD KROOSHOF, DSM Research, Netherlands — We will present a modified COSMO-based thermodynamical model which can be used for the prediction of solvation in liquid mixtures. The method provides values for the surface-segment interactions and molecular contact areas as functions of the relative positions of all the segment pairings of the constituent molecules in a mixture. These expressions are obtained by placing the complete molecules into contact at each segment pair to determine if the molecules overlap, and using a probing particle to determine the total area of contact. The former expression can be used to discard terms from the COMSO-based segment sums which correspond to overlapping molecular configurations. The areas are used to determine the average contact energies based on Onsager's theory for dielectric screening. Our method allows us to remove three parameters from the original model without any loss of accuracy. We will show the results of our model as applied to binary mixture vapor-liquid equilibrium predictions.

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