Present Status of the Group Contribution Methods UNIFAC, Modified UNIFAC (Dortmund), and the Predictive Equations of State PSRK and VTPR. Revision and Extension

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For process development and simulation, the group contribution concept can be successfully applied for the estimation of missing pure component and mixture properties. This concept has the great advantage that only a limited number of group interaction parameters is required. With the support of a company consortium founded in 1996 at the University of Oldenburg, the group contribution model modified UNIFAC (Dortmund) for the prediction of phase equilibria and excess properties has been continuously revised and extended. Within the consortium the number of available group interaction parameters of modified UNIFAC (Dortmund) has been doubled. At the same time, the reliability of the results was greatly improved and the range of applicability was extended to ionic liquids, polyethers, aromatic ethers, nitriles, sulfides, n-formylmorpholine, mercury, polyethylenglycol, pyrrole, glycerol, thionyl, urethane, etc. A relevant prerequisite for the further development of predictive methods UNIFAC, modified UNIFAC (Dortmund), PSRK and VTPR was the direct access to the worldwide largest factual data bank for thermophysical information, DDB (Dortmund Data Bank). Today the most sophisticated group contribution equation of state is the volume translated Peng-Robinson group contribution equation of state VTPR whose limited range of applicability is currently being further developed within the UNIFAC consortium. In this poster, various aspects of our developments are given. Furthermore, the current status of the consortium developments is shown.