Thermodynamic phase behavior of binary azeotropic system separation and extractive distillation process

青岛科技大学
Qingdao University of Science & Technology

The vapor-liquid equilibrium experiment was used to obtain the vapor-liquid equilibrium properties of the difficult separation system, and on this basis, the solvent extraction mechanism was studied. The mechanism of solvent separation plays a guiding role in selecting suitable solvents for industrial separation. The interaction energy, bond length and charge density distribution of p-xylene with solvent are calculated by quantum chemistry method. The quantum chemistry calculation results and experiment results showed that N-Formylmorpholine is the best solvent among the alternative solvents in the work. This work provides an effective and complete solvent screening process from phase equilibrium experiments to quantum chemical calculation.

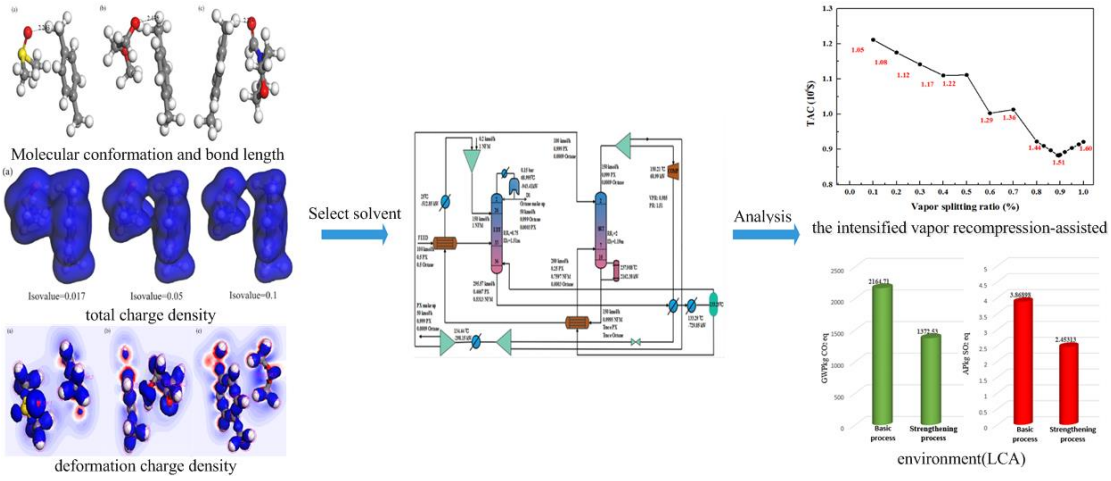

Table S2. Experimental VLE Data for The System PX(1) + Butyl butyrate(2) at 101.3 kPa[a]

T/K	x_1	y_1	γ_1	γ_2	$G^E/J \cdot mol^{-1}$	α_{12}
412.72	0.8454	0.9153	1.0323	1.2312	194.66	1.78
413.47	0.8174	0.8881	1.0315	1.2323	218.18	1.77
415.58	0.6978	0.8025	1.0329	1.2333	296.88	1.76
416.67	0.6419	0.7618	1.0358	1.2154	320.27	1.78
416.76	0.6378	0.7606	1.0385	1.2046	317.20	1.80
416.94	0.6294	0.7565	1.0418	1.1912	314.16	1.83
420.68	0.4765	0.6681	1.1040	1.0300	219.17	2.21
423.87	0.3740	0.5701	1.1079	1.0184	175.33	2.22
433.47	0.1212	0.2308	1.0958	0.9949	23.83	2.18
434.62	0.0935	0.1862	1.1148	0.9896	2.57	2.22

[a] Standard uncertainties u of T, P, x, and y are u(T)=0.10 K, u(P)=0.1 kPa, u(x)=0.0005, u(y)=0.0005.