

Supplementary Information

Effect of solvent composition on adsorption isotherms based on multi-component breakthrough curve analysis and application of a multi-component BET model

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This supplementary information provides additional information regarding experimentally determined loadings of single- and multi-component system, as well as additional results from the data analysis.

Table SI.1 : Equilibrium loadings of three components measured at different $x_{V,mod}$ applying frontal analysis. All c and q values are in mol/L.

$x_{V,mod}$ [-]	c_1	q_1	c_2	q_2	c_3	q_3
0.6	0.0637	1.048	0.0674	1.394	0.0529	1.288
	0.0509	0.8389	0.0537	1.102	0.0416	0.9874
	0.0389	0.6426	0.0411	0.8347	0.0314	0.7292
	0.0253	0.4163	0.0268	0.5321	0.0212	0.4812
	0.0126	0.2056	0.0134	0.2596	0.0104	0.2303
0.7	0.0971	0.7612	0.1669	1.591	0.1645	1.832
	0.0775	0.6122	0.1326	1.269	0.1315	1.454
	0.0582	0.4586	0.0994	0.9447	0.0988	1.084
	0.0389	0.3080	0.0666	0.6284	0.0659	0.7127
	0.0191	0.1517	0.0333	0.3115	0.0341	0.3695
0.8	0.1857	0.7268	0.4243	1.881	0.4249	2.237
	0.1524	0.6017	0.3405	1.535	0.3464	1.830
	0.1191	0.4756	0.2567	1.171	0.2534	1.350
	0.0873	0.3486	0.1726	0.8043	0.1670	0.8938
	0.0425	0.1723	0.0859	0.4087	0.0858	0.4581
0.9	0.2978	0.5367	1.0483	1.823	1.0511	2.095
	0.2550	0.4741	0.8374	1.556	0.8324	1.744
	0.2103	0.3973	0.6286	1.220	0.6269	1.381
	0.1722	0.3276	0.4212	0.8693	0.4277	0.9977
	0.1381	0.2632	0.2137	0.4654	0.2111	0.5133
	0.0688	0.1346	-	-	-	-
	0.0348	0.0683	-	-	-	-

Table SI.2: Summary of feed compositions of multi-component experiments. All feed concentrations c_i^F given are in mol/L.

$x_{V,mod}$ [-]	Mixture	Feed composition		
		c_1^F	c_2^F	c_3^F
0.6	Ternary	0.0206	0.0206	0.0205
		0.0038	0.0038	0.0041
		0.0450	0.0079	0.0076
		0.0079	0.0452	0.0077
		0.0077	0.0079	0.0449
		0.0329	0.0133	0.0132
		0.0129	0.0335	0.0133
		0.0130	0.0133	0.0334
0.7	Ternary	0.0516	0.0515	0.0513
		0.0039	0.0038	0.0037
		0.0224	0.0632	0.0633
		0.0974	0.0226	0.0226
		0.0302	0.0304	0.0302
		0.0153	0.0151	0.0152
	Binary	0.0516	0.0513	0
		0.0745	0.0752	0
		0.0526	0	0.0518
		0.0765	0	0.0750
0.8	Ternary	0.1126	0.1121	0.1120
		0.0039	0.0039	0.0039
		0.0561	0.1387	0.1386
		0.1787	0.0566	0.0560
		0.0377	0.0372	0.0374
		0.0757	0.0748	0.0750
	Binary	0.1648	0	0.1641
0.9	Ternary	0.2605	0.2617	0.2623
		0.0039	0.0039	0.0039
		0.1718	0.1721	0.1720
		0.0902	0.0899	0.0895

Table SI.3: Feed and intermediate states concentrations and loadings (determined from integration of recorded BTCs) of ternary experiments, all c and q values are in mol/L.

$x_{V,mod}$ [-]	Feed state						Analysis of adsorption branches								Analysis of desorption branches			
	Ternary						Sub-single		Sub-binary				Sub-single		Sub-binary			
	c_1^F	c_2^F	c_3^F	q_1^F	q_2^F	q_3^F	c_1^{P1}	q_1^{P1}	c_1^{P2}	c_2^{P2}	q_1^{P2}	q_2^{P2}	c_3^{P2}	q_3^{P2}	c_2^{P1}	c_3^{P1}	q_2^{P1}	q_3^{P1}
0.6	0.0206	0.0206	0.0205	0.351	0.415	0.473	0.0171	0.275	0.0188	0.0162	0.308	0.314	0.0244	0.550	0.0212	0.0208	0.426	0.478
	0.0038	0.0038	0.0041	0.061	0.071	0.090	0.0036	0.057	0.0037	0.0035	0.060	0.066	0.0044	0.095	0.0038	0.0042	0.073	0.091
	0.0450	0.0079	0.0076	0.745	0.156	0.170	0.0419	0.684	0.0435	0.0073	0.716	0.142	0.0090	0.196	0.0089	0.0081	0.171	0.179
	0.0079	0.0452	0.0077	0.135	0.919	0.180	0.0061	0.098	0.0075	0.0397	0.125	0.797	0.0124	0.277	0.0456	0.0077	0.926	0.180
	0.0077	0.0079	0.0449	0.135	0.163	1.066	0.0061	0.098	0.0064	0.0049	0.103	0.093	0.0469	1.107	0.0080	0.0450	0.165	1.068
	0.0329	0.0133	0.0132	0.553	0.264	0.301	0.0289	0.472	0.0309	0.0114	0.512	0.222	0.0157	0.350	0.0142	0.0136	0.279	0.308
	0.0129	0.0335	0.0133	0.219	0.674	0.305	0.0104	0.167	0.0121	0.0279	0.201	0.551	0.0180	0.399	0.0340	0.0133	0.684	0.306
	0.0130	0.0133	0.0334	0.225	0.272	0.782	0.0105	0.169	0.0113	0.0092	0.184	0.176	0.0365	0.845	0.0135	0.0337	0.275	0.787
0.7	0.0516	0.0515	0.0513	0.409	0.479	0.541	0.0488	0.382	0.0513	0.0469	0.405	0.432	0.0499	0.533	0.0462	0.0477	0.435	0.512
	0.0039	0.0038	0.0037	0.031	0.035	0.038	0.0039	0.031	0.0039	0.0038	0.031	0.035	0.0037	0.038	0.0038	0.0037	0.035	0.038
	0.0224	0.0632	0.0633	0.180	0.599	0.674	0.0208	0.163	0.0215	0.0551	0.170	0.513	0.0632	0.674	0.0602	0.0611	0.574	0.654
	0.0974	0.0226	0.0226	0.765	0.208	0.237	0.0957	0.750	0.0959	0.0216	0.752	0.199	0.0224	0.239	0.0195	0.0206	0.184	0.222
	0.0302	0.0304	0.0302	0.241	0.284	0.320	0.0283	0.222	0.0293	0.0273	0.231	0.252	0.0315	0.333	0.0293	0.0296	0.276	0.314
	0.0153	0.0151	0.0152	0.123	0.141	0.160	0.0147	0.117	0.0150	0.0139	0.119	0.128	0.0160	0.167	0.0150	0.0152	0.140	0.160
	0.1126	0.1121	0.1120	0.436	0.506	0.561	-	-	-	-	-	-	-	-	-	-	-	-
0.8	0.0039	0.0039	0.0039	0.015	0.018	0.020	-	-	-	-	-	-	-	-	-	-	-	-
	0.0561	0.1387	0.1386	0.217	0.634	0.700	-	-	-	-	-	-	-	-	-	-	-	-
	0.1787	0.0566	0.0560	0.694	0.253	0.279	-	-	-	-	-	-	-	-	-	-	-	-
	0.0377	0.0372	0.0374	0.150	0.173	0.195	-	-	-	-	-	-	-	-	-	-	-	-
	0.0757	0.0748	0.0750	0.298	0.347	0.384	-	-	-	-	-	-	-	-	-	-	-	-
	0.2605	0.2617	0.2623	0.416	0.490	0.542	-	-	-	-	-	-	-	-	-	-	-	-
0.9	0.0039	0.0039	0.0039	0.008	0.009	0.010	-	-	-	-	-	-	-	-	-	-	-	-
	0.1718	0.1721	0.1720	0.295	0.347	0.384	-	-	-	-	-	-	-	-	-	-	-	-
	0.0902	0.0899	0.0895	0.165	0.192	0.214	-	-	-	-	-	-	-	-	-	-	-	-

Table SI.4: Feed and intermediate states concentrations and loadings (determined from integration of recorded BTCs) of binary experiments, all c and q values are in mol/L.

$x_{V,mod}$ [-]	Binary system	Feed state				Analysis of adsorption branches		Analysis of desorption branches	
		Binary				Sub-single		Sub-single	
		c_1^F	c_2^F	q_1^F	q_2^F	c_1^{P1}	q_1^{P1}	c_2^{P1}	q_2^{P1}
0.7	comp1: comp2	0.0516	0.0513	0.4041	0.4754	0.0516	0.4041	0.0487	0.4537
		0.0745	0.0752	0.5828	0.6938	0.0761	0.5968	0.0666	0.6277
	comp1: comp3	0.0526	0.0518	0.4189	0.5470	0.0499	0.3912	0.0498	0.5319
		0.0765	0.0750	0.6133	0.5470	0.0727	0.5782	0.0691	0.7449
0.8	comp1: comp3	0.1648	0.1641	0.6395	0.8222	0.1705	0.6695	0.1325	0.7004

Table SI.5: Adsorption isotherm model parameters of single components at $x_{V,mod} = 0.6$ obtained using the single-site BET model with a finite number of adsorbed layers, N_L [Eq. 14], considering different N_L values for three solutes. All K values are given in L/mol and q_{sat} value is in mol/L.

$K_{S,1}$	$K_{S,2}$	$K_{S,3}$	$K_{L,1}$	$K_{L,2}$	$K_{L,3}$	$N_{L,1}$	$N_{L,2}$	$N_{L,3}$	q_{sat}	$O. F.$
3.961	4.663	5.295	2.146	3.104	3.645	2.5	2.3	3.2	4.10	0.0131