Capabilities and Limitations of Predictive Engineering Theories for Multicomponent Adsorption

Supporting Information

Table S1. Langmuir and Toth isotherm parameters fitted to experimental data for pure component adsorption on molecular sieves (MS-13X) and molecular sieving carbon (MSC-5A) along with absolute deviation from data.

Langmuir	**N (mmol/g)**	**b (1/Pa)**		**Pressure range (kPa)**	**AADn (%)**
Acetone MS-13X	2.2780	8.3847		0.01-17	21.2
Acetone MSC-5A	2.2907	0.0589		0.01-10	9.54
Methanol MS -13X	4.0192	0.4679		0.01-12	24.1
Methanol MSC-5A	3.3464	0.0031		0.1-15	12.4
n-Hexane MS-13X	1.3254	1.2263		0.02-17	22.0
n-Hexane MSC-5A	1.3348	0.2503		0.01-15	4.89
Benzene MS-13X	1.9876	1.1950		0.02-11	25.8
Benzene MSC-5A	1.6945	0.4481		0.02-12	17.1
Toth	**N (mmol/g)**	**b (1/Pa)**	**t**	**Pressure range (kPa)**	**AADn (%)**
Acetone MS-13X	2.7070	337.0859	0.3134	0.01-17	4.60
Acetone MSC-5A	2.7860	3.0886	0.3125	0.01-10	2.89
Methanol MS -13X	4.9244	38.8771	0.2792	0.01-12	3.98
Methanol MSC-5A	4.6766	0.0122	0.4288	0.1-15	1.33
n-Hexane MS-13X	1.5690	18.9636	0.3604	0.02-17	6.01
n-Hexane MSC-5A	1.4830	43.2047	0.3073	0.01-15	1.80
Benzene MS-13X	2.3074	56.0863	0.3107	0.02-11	7.93
Benzene MSC-5A	2.0322	5.6923	0.3773	0.02-12	3.13

Table S2. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption of molecular sieves 13X.

			IAST + Langmuir		IAST + Toth		Multicomponent Langmuir	
			ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**Adsorb.**	**NP**						
methanol-acetone	MS-13X	8	22.2	24.8	27.0	19.6	76.1	43.4
methanol-benzene	MS-13X	6	8.1	22.0	8.94	21.3	58.2	45.4
acetone-hexane	MS-13X	6	4.9	16.2	4.4	8.7	41.6	36.7
acetone-benzene	MS-13X	5	10.1	22.6	9.71	13.3	27.4	24.4
Avr. deviation (%)			11.3	21.4	12.5	15.7	50.8	37.5

Table S3. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption of molecular sieving carbon 5A.

			IAST + Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
			ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**adsorbent**	**NP**						
Methanol-acetone	MSC-5A	10	7.8	9.5	11.3	6.7	23.2	11.7
methanol-hexane	MSC-5A	8	15.1	11.0	14.3	10.3	31.7	27.9
methanol-benzene	MSC-5A	14	8.7	11.7	9.6	4.6	12.0	22.7
acetone-hexane	MSC-5A	9	35.9	19.1	36.9	21.8	8.6	7.4
Avr. deviation (%)			16.9	12.8	18.0	10.9	20.9	17.4

Table S4. Langmuir and Toth isotherm parameters fitted to pure component experimental data on activated carbon (G-2X) along with absolute deviation from data.

Langmuir	**N (mmol/g)**	**b (1/Pa)**		**Pressure range (kPa)**	**AADn (%)**
Acetone G-2X	6.3568	0.0059		0.01-17	5.2
Methanol G-2X	8.7999	6.8539e-04		0.15-18	15.0
n-Hexane G-2X	3.0771	1.0699		0.05-16	21.9
Benzene G-2X	4.9575	0.0565		0.05-14	7.6
Toth	**N (mmol/g)**	**b (1/Pa)**	**t**	**Pressure range (kPa)**	
Acetone G-2X	6.9582	0.0146	0.6106	0.01-17	1.6
Methanol G-2X	12.5641	0.0046	0.3783	0.15-18	1.7
n-Hexane G-2X	3.5030	15.1057	0.3721	0.05-16	7.3
Benzene G-2X	5.3359	0.2077	0.5179	0.05-14	7.1

Table S5. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption of activated carbon G-2X.

			IAST + Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
Adsorbates	**adsorbent**	**NP**	**ADDx**	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
methanol-acetone	G-2X	7	7.2	9.2	2.7	12.5	16.1	10.9
methanol-hexane	G-2X	3	16.9	9.6	23.3	13.4	4.9	10.2
methanol-benzene	G-2X	7	9.4	5.5	15.9	5.7	4.9	3.8
acetone-hexane	G-2X	7	16.1	4.8	19.6	7.5	15.6	18.6
acetone-benzene	G-2X	8	12.8	2.4	17.5	4.0	2.7	1.5
Avr. deviation (%)			12.5	6.3	15.8	8.6	8.8	9.0

Table S6. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption of 2-propanol-water on silica gel at 333.15K.

			IAST + Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
			ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**adsorbent**	**NP**						
isopropanol-water 5kPa	Silica gel	5	10.3	20.7	-	-	18.0	70.6
isopropanol-water 10kPa	Silica gel	5	9.4	24.2	-	-	20.0	27.6
Avr. deviation (%)			9.9	22.5	-	-	19.0	49.1

Table S7. Langmuir and Toth isotherm parameters fitted to experimental data along with absolute deviation from data.

Langmuir	**N (mmol/g)**	**b (1/Pa)**		**Pressure range (kPa)**	**AADn (%)**
n-heptane	17.2123	2.8475E-6		1.3-24	14.4
Water	49.6659	3.859E-6		9-25	5.7
Toth	**N (mmol/g)**	**b (1/Pa)**	**t**		**AADn (%)**
n-heptane	6.0252	7.761e-6	6.0617	1.3-24	14.1
water	13.537	1.318e-5	10.014	9-25	4.3

Table S8. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption of water-n-heptane on silica gel.

			IAST + Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
			ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**adsorbent**	**NP**						
water-heptane 10000Pa	silica gel	3	16.2	10.2	17.0	10.9	16.5	10.2
water-heptane 15000Pa	silica gel	3	11.6	40.7	12.7	41.8	12.2	40.8
Avr. deviation (%)			13.9	25.5	14.9	26.3	14.4	25.5

Table S9. Langmuir and Toth isotherm parameters fitted to experimental data for pure component adsorption on Cab-O-Sil silica at 293.15K along with absolute deviation from data.

Langmuir	**N (mmol/g)**	**b (1/Pa)**		**Pressure range (kPa)**	**AADn (%)**
Ethanol	2.0223	0.0019		0.03-5.6	18.9
Benzene	2.7574	9.8671e-005		0.6-9.4	10.4
Cyclohexane	8.6315	1.7352e-005		0.4-9.6	11.5
Toth	**N (mmol/g)**	**b (1/Pa)**	**T**	**Pressure range (kPa)**	**AADn (%)**
Ethanol	8.8681	0.9686	0.1529	0.03-5.6	4.9
Benzene	5.0259	6.7683e-005	0.6427	0.6-9.4	9.1
Cyclohexane	97.0284	1.5441e-006	0.5881	0.4-9.6	11.4

Table S10. Langmuir and Toth isotherm parameters fitted to experimental data for pure component adsorption on Cab-O-Sil silica at 303.15 K along with absolute deviation from data.

Langmuir	**N (*10^6 mol/m^2)**	**b (1/Pa)**		**Pressure range (kPa)**	**AADn (%)**
Ethanol	7.6530	0.0011		0.3-2.8	7.4
Benzene	4.7093	3.0415e-004		0.7-4	6.7
cyclohexane	5.7140	9.0740e-005		0.5-4.8	9.1
Toth	**N (*10^6 mol/m^2)**	**b (1/Pa)**	**t**	**Pressure range (kPa)**	**AADn (%)**
ethanol	7.7530	0.0013	0.8900	0.3-2.8	6.1
Benzene	384.1255	3.2967e-005	0.1785	0.7-4	5.6
cyclohexane	3.2535	1.4800e-004	1.5619	0.5-4.8	9.0

Table S11. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir from binary experimental data for adsorption on Cab-O-Sil.

			IAST+Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
			ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**adsorbent**	**NP**						
ethanol-benzene	cab-o-sil	8	4.2	38.9	-	-	3.4	38.5
ethanol-cyclohexane	cab-o-sil	8	6.3	33.4	-	-	3.8	31.6
Benzene-cyclohexane	cab-o-sil	9	7.2	25.1	3.9	26.0	5.9	25.2
Avr. deviation (%)			5.9	32.5	3.9	26.0	4.4	31.8

Table S12. Absolute average deviation of calculated predictions for IAST and multi-component Langmuir for adsorption at 303.15K on Cab-O-Sil.

				IAST + Langmuir		**IAST + Toth**		**Multicomponent Langmuir**	
				ADDx	**ADDn**	**ADDx**	**ADDn**	**ADDx**	**ADDn**
Adsorbates	**adsorbent**	**Pressure**	**NP**						
ethanol-benzene	cab-o-sil	Constant	8	3.9	22.6	6.6	75.1	4.2	21.5
ethanol-benzene	cab-o-sil	Varying	8	4.1	19.2	6.8	75.6	4.2	18.1
ethanol-cyclohexane	cab-o-sil	Constant	9	5.8	79.6	4.8	22.2	5.3	79.3
ethanol-cyclohexane	cab-o-sil	Varying	9	5.9	80.3	4.7	18.9	5.3	80.0
Benzene-cyclohexane	cab-o-sil	Constant	9	3.7	23.0	5.5	24.4	4.6	23.0
Benzene-cyclohexane	cab-o-sil	Varying	9	3.7	25.9	5.5	27.2	4.6	26.0