

Solubility and mass transfer performance of ethane and n-butane in menthol and decanoic acid deep eutectic solvent

Yunfei Song^{1,2}

1. State Key Laboratory of Chemical Safety, Qingdao, Shandong, China
2. SINOPEC Research Institute of Safety Engineering Co., Ltd., Qingdao, Shandong, China

Table S1 The equilibrium pressure and liquid phase composition of light hydrocarbons

VOC	288.2 K		293.2 K		298.2 K	
	x	P , kPa	x	P , kPa	x	P , kPa
ethane	0.0041	8.5	0.0026	6.4	0.0024	7.9
	0.0095	19.2	0.0061	17.2	0.0046	16.1
	0.015	32.1	0.0078	22.5	0.0077	27.1
	0.0169	35.4	0.0123	33.3	0.0102	35.7
	0.0218	46.2	0.0165	47.2	0.0131	46.2
	0.0281	58.1	0.0196	54.3	0.0151	55.1
	0.0333	68	0.0246	68	0.0189	67.7
	0.0349	73.8	0.0270	75.9	0.0218	76.2
	0.0356	74.9	0.0295	81.8	0.0238	81.9
N-butane	0.038	5.5	0.0361	5.3	0.0318	5.5
	0.059	7	0.0476	7.6	0.0486	8.8
	0.085	11.5	0.0782	11.4	0.0684	11.7
	0.112	15.3	0.1041	14.9	0.0949	16.7
	0.141	19.0	0.1293	18.8	0.1468	24.0
	0.172	23	0.1565	24.3	0.1760	30.2
	0.214	29.5	0.2007	29.8	0.1952	33.5
	0.247	34.4	0.2340	33.4	0.2220	37.4
	0.278	37.5	0.2551	37.5	0.2518	42.1
	0.309	41.7	0.2837	43.5	0.2719	46.9

Table S2 statistical parameters for the linear fitting Henry's law constant

VOC	Temperature, K	<i>a</i> , kPa	<i>b</i> , kPa	<i>R</i> ²
ethane	288.2	2089.63	-0.00599	0.99869
	293.2	2790.97	-0.09799	0.99907
	298.2	3537.99	0.19034	0.9981
N-butane	288.2	136.92195	-0.22058	0.99831
	293.2	149.04808	-0.0843	0.99584
	298.2	168.62275	0.26181	0.99845

The linear fitting function is $P = ax + b$, where *a* is the Henry's law constant.

Table S3 VOC concentrations at outlet of the device with different temperatures

T min	c _{out,ethane} (μmol/mol)			T min	c _{out,N-butane} (μmol/mol)		
	288.2 K	293.2 K	288.2 K		288.2 K	293.2 K	288.2 K
2	54.20	48.36	67.05	2	0.95	0.40	1.20
4	128.45	90.54	156.49	4	1.61	0.61	1.99
6	296.27	276.21	403.54	6	4.44	1.00	4.98
8	518.68	532.08	624.37	8	10.90	2.17	13.16
10	700.50	735.49	937.85	10	27.07	2.52	30.07
12	964.60	1043.27	1235.47	12	61.95	16.87	62.68
14	1107.01	1260.93	1463.46	14	102.13	67.50	103.94
16	1268.76	1448.21	1636.54	16	155.64	130.45	167.93
18	1336.80	1549.72	1874.01	18	212.15	184.80	245.57
20	1385.86	1703.22	2036.18	20	251.11	221.04	278.22
/	/	/	/	22	290.96	259.62	320.20
/	/	/	/	24	335.81	306.04	381.05
/	/	/	/	26	391.40	351.53	409.35
/	/	/	/	28	442.18	388.01	430.70
/	/	/	/	30	427.78	414.13	452.07
/	/	/	/	32	445.03	444.48	493.63
/	/	/	/	34	478.08	468.26	520.84
/	/	/	/	36	479.67	487.98	542.63
/	/	/	/	38	555.42	489.78	575.94
/	/	/	/	40	595.56	498.97	597.05

Table S4 Statistical parameters for the nonlinear function fitting for different temperatures in the dynamic bubbling experiments

VOC	Temperature, K	<i>a</i>	<i>b</i>	<i>x</i> ₀	<i>p</i>	<i>R</i> ²
ethane	288.2	99.522	83.597	10.954	2.894	0.995
	293.2	99.756	78.723	12.381	2.783	0.995
	298.2	99.788	70.497	14.223	2.263	0.996
N-butane	288.2	100.096	93.132	24.151	2.896	0.997
	293.2	100.080	94.443	22.265	3.840	0.997
	298.2	100.091	93.174	22.713	3.069	0.995

The linear fitting function is $y=b+[a-b]/(1+(x/x_0)^p)$.

Table S5 VOC concentrations at outlet of the device with different intel VOC concentrations

T min	C _{out,ethane} (μmol/mol)			T min	C _{out,N-butane} (μmol/mol)		
	8000	9000	10000		288.2 K	293.2 K	288.2 K
2	48.12	51.32	54.20	2	0.83	0.90	0.95
4	119.63	123.39	128.45	4	1.39	1.58	1.61
6	263.64	279.21	296.27	6	3.97	4.21	4.44
8	493.36	503.56	518.68	8	10.56	10.73	10.9
10	654.29	676.87	700.50	10	25.88	26.79	27.07
12	939.58	953.21	964.60	12	58.37	59.61	61.95
14	1061.17	1099.30	1107.01	14	89.54	96.54	102.13
16	1234.55	1253.21	1268.76	16	135.42	141.22	155.64
18	1296.32	1319.86	1336.80	18	187.26	210.54	212.15
20	1311.04	1322.54	1385.86	20	222.76	240.28	251.11
/	/	/	/	22	271.37	281.13	290.96
/	/	/	/	24	301.37	313.42	335.81
/	/	/	/	26	351.66	359.91	391.4
/	/	/	/	28	374.70	390.17	442.18
/	/	/	/	30	414.53	415.30	427.78
/	/	/	/	32	410.06	439.63	445.03
/	/	/	/	34	452.68	464.72	478.08
/	/	/	/	36	480.49	482.57	479.67
/	/	/	/	38	517.51	525.10	555.42
/	/	/	/	40	553.08	560.03	595.56

Table S6 Statistical parameters for the nonlinear function fitting for different VOC concentrations of the model gas in the dynamic bubbling experiments

VOC	c_{in} ($\mu\text{mol/mol}$)	a	b	x_0	p	R^2
ethane	8000	99.362	80.936	10.734	3.139	0.994
	9000	99.376	82.995	10.577	3.187	0.994
	10000	99.522	83.597	10.955	2.894	0.995
N-butane	8000	100.09867	91.25825	26.29917	2.757	0.996
	9000	100.07333	92.57742	24.77116	2.908	0.997
	10000	100.091	93.143	24.151	2.896	0.997

The linear fitting function is $y=b+[a-b]/(1+(x/x_0)^p)$.

Table S7 VOC concentrations at outlet of the device with different flow rate of model gas

T min	c _{out,ethane} (μmol/mol)				T min	c _{out,N-butane} (μmol/mol)			
	500 ml·min ⁻¹	100 ml·min ⁻¹	50 ml·min ⁻¹	30 ml·min ⁻¹		500 ml·min ⁻¹	100 ml·min ⁻¹	50 ml·min ⁻¹	30 ml·min ⁻¹
2	1794.28	660.32	164.51	54.20	2	585.62	324.72	37.51	0.95
4	6219.83	3184.76	283.54	128.45	4	2164.32	606.84	58.64	1.61
6	9421.24	6692.80	1020.36	296.27	6	3293.05	1232.65	118.43	4.44
8	9448.28	9187.63	3821.66	518.68	8	4876.25	2075.37	255.81	10.90
10	9519.38	9261.39	7149.33	700.50	10	5531.79	2941.54	374.59	27.07
12	9666.98	9338.29	7173.95	964.60	12	5904.21	3556.37	511.90	61.95
14	9680.86	9393.28	7264.25	1107.01	14	6232.76	4062.51	660.31	102.13
16	9685.60	9440.67	7370.30	1268.76	16	6674.37	4347.74	738.03	155.64
18	9692.19	9471.07	7412.71	1336.80	18	6819.07	4456.31	916.07	212.15
20	9698.21	9494.85	7465.42	1385.86	20	7024.44	4508.67	1045.23	251.11
/	/	/	/	/	22	7095.44	4548.83	1204.14	290.96
/	/	/	/	/	24	7153.29	4586.34	1412.52	335.81
/	/	/	/	/	26	7206.37	4608.95	1552.22	391.40
/	/	/	/	/	28	7252.21	4634.71	1643.54	442.18
/	/	/	/	/	30	7314.80	4672.00	1721.88	427.78
/	/	/	/	/	32	7359.78	4689.69	1796.84	445.03
/	/	/	/	/	34	7398.64	4709.74	1857.30	478.08
/	/	/	/	/	36	7421.34	4724.65	1909.87	479.67
/	/	/	/	/	38	7426.92	4740.49	1957.33	555.42
/	/	/	/	/	40	7462.51	4763.21	1996.42	595.56

Table S8 Statistical parameters for the nonlinear function fitting for different flow rate of the model gas in the dynamic bubbling experiments

VOC	F , ml/min	a	b	x_0	p	R^2
ethane	500	82.539	3.628	3.863	7.749	0.998
	100	94.146	4.663	4.915	4.708	0.994
	50	96.397	25.953	7.966	10.730	0.995
	30	99.522	83.597	10.955	2.894	0.995
N-butane	500	101.63746	23.29395	6.29218	1.95936	0.998
	100	96.60784	52.33535	9.02372	3.39634	0.997
	50	99.68205	75.74224	21.41707	2.51925	0.998
	30	100.091	93.143	24.151	2.896	0.997

The linear fitting function is $y=b+[a-b]/(1+(x/x_0)^p)$.