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- Misek, T., Berger, R., Schröter, J., Standard Test Systems for Liquid Extraction, Rugby, England, 1985 (for details go to: library@icheme.org.uk)

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Standard Test Systems for Liquid Extraction are:

water/acetone/toluene (high interfacial tension)
water/acetone/butyl acetate (medium interfacial tension)
water/succinic acid/n-butanol (low interfacial tension)

All data are in Misek, T. et al., 1985 (see literature list)

Reactive Test Systems for Liquid Extraction is:

$ZnSO_4$/di(2ethylhexyl) phosphoric acid in isododecane

All data are in the report of Bart, H.-J. and Slater, M.J., below or in
http://www.dechema.de/Extraktion/

Further Test Systems with a distribution coefficient near 10 are:

water/methyl isopropyl ketone/toluene (high interfacial tension)
water/methyl isopropyl ketone/butyl acetate (medium interfacial tension)

All data are in the following tables. For more info go into the original literature:
Berger, R., Hampe, M.J., Schröter, J., Neue Testsysteme für die Flüssig-flüssig-Extraktion, Chem.-Ing.-Techn. 64 (1992), 11, 1044-1046 (Microfiche MS 2083/92)

Tab. 1: Density, Kinematic Viscosity and Refractive Index of the Pure Substances (298 K)

Substance	ρ [kg/m^3]		ν [10^{-6} m^{2}s^{-1}]		n_D [-]	
	Exp.	Lit.[1]	Exp.	Lit.[1]	Exp.	Lit.[1]
MIPK[2] Merck 805966	804.5	805.1	0.6072	-	1.38805	1.3880
BuAc[3] Merck 9652	880.6	882.5	0.8267	0.8295	1.39413	1.3941
H_2O (bidist.)	998.1	998.2	1.0155	1.0038	1.331312	1.33299

[1] Weast, R.C., Lide, D.R. et al. (Ed.): Handbook of Chemistry and Physics, 70th Ed., 1989-1990, CRC Press Inc., Boca Raton, USA
[2] MIPK: Methylisopropylketone
[3] BuAc: n-Butylacetate

Tab. 2: Density, Kinematic Viscosity and Binary Diffusion Coefficients of MIPK-BuAc-Mixtures

T [K]	X_{MIPK} [-]	ρ [kg/m^3]	υ [10^{-6} m^2/s]	D [10^{-9} m^2/s]
288	0.0000	885.7	0.8830	-
	0.0211	-	-	1.812 ± 1.4 %
	0.2134	872.3	0.8298	-
	0.3964	859.5	0.7858	-
	0.5998	-	-	2.057 ± 4.7 %
	0.6028	843.8	0.7353	-
	0.7846	828.8	0.6922	-
	0.8063	-	-	2.154 ± 4.2 %
	0.9856	-	-	2.247 ± 3.9 %
	1.0000	809.4	0.6394	-
293	0.0000	880.6	0.8267	-
	0.0197	-	-	1.994 ± 1.2 %
	0.2134	867.2	0.7790	-
	0.2174	-	-	2.053 ± 0.2 %
	0.3964	854.6	0.7385	-
	0.3971	-	-	2.110 ± 5.4 %
	0.6028	838.8	0.6933	-
	0.6140	-	-	2.223 ± 2.0 %
	0.7846	823.9	0.6549	-
	0.8178	-	-	2.294 ± 0.8 %
	0.9864	-	-	2.366 ± 0.4 %
	1.0000	804.5	0.6072	-
298	0.0000	876.2	0.7763	-
	0.0213	-	-	2.154 ± 0.8 %
	0.2123	-	-	2.192 ± 0.3 %
	0.2134	862.0	0.7379	-
	0.3954	-	-	2.261 ± 1.7 %
	0.3964	849.4	0.6975	-
	0.6019	-	-	2.367 ± 5.3 %
	0.6028	833.7	0.6573	-
	0.7846	818.7	0.6204	-
	0.7851	-	-	2.444 ± 0.5 %
	0.9857	-	-	2.554 ± 3.0 %
	1.0000	799.4	0.5780	-

Tab. 3: Density, Kinematic Viscosity and Binary Diffusion Coefficients of MIPK-H_2O-Mixtures

T [K]	X_{MIPK} [-]	ρ [kg/m^3]	υ [10^{-6} m^2/s]	D [10^{-9} m^2/s]
288	0.0000	999.1	1.1481	-
	0.0019	-	-	0.844 ± 5.9 %
	0.0037	-	-	0.832 ± 5.5 %
	0.0065	995.1	1.2632	-
	0.0074	-	-	0.775 ± 2.6 %
	0.9295	-	-	1.773 ± 1.0 %
	0.9296	813.3	0.6731	-
	0.9599	-	-	2.102 ± 1.0 %
	0.9790	-	-	2.302 ± 3.7 %
	0.9793	810.5	0.6489	-
	1.0000	809.4	0.6394	-
293	0.0000	998.1	1.0155	-
	0.0009	-	-	0.953 ± 4.1 %
	0.0029	-	-	0.939 ± 5.0 %
	0.0055	-	-	0.876 ± 7.5 %
	0.0065	994.1	1.1083	-
	0.0090	-	-	0.829 ± 6.2 %
	0.9174	-	-	1.894 ± 1.6 %
	0.9272	-	-	2.027 ± 1.0 %
	0.9296	808.5	0.6365	-
	0.9554	-	-	2.331 ± 2.0 %
	0.9793	805.6	0.6155	-
	1.0000	804.5	0.6072	-
298	0.0000	997.0	0.9057	-
	0.0021	-	-	1.122 ± 7.2 %
	0.0060	-	-	1.073 ± 6.5 %
	0.0065	993.0	0.9770	1.007 ± 5.6 %
	0.9034	-	-	1.969 ± 1.2 %
	0.9296	803.4	0.6046	-
	0.9570	-	-	2.661 ± 1.1 %
	0.9717	-	-	2.869 ± 1.2 %
	0.9793	800.5	0.5860	-
	0.9803	-	-	2.986 ± 1.0 %
	1.0000	799.4	0.5780	-

Tab. 4: Density, Kinematic Viscosity and Binary Diffusion Coefficients of BuAc-H_2O-Mixtures

T [K]	X_{MIPK} [-]	ρ [kg/m^3]	υ [10^{-6} m^2/s]	D [10^{-9} m^2/s]
288	0.0000	999.1	1.1481	-
	0.0006	999.1	1.1561	0.643 ± 2.5 %
	0.9824	886.6	0.8885	-
	0.9861	-	-	2.198 ± 2.9 %
	0.9913	-	-	2.233 ± 0.5 %
	1.0000	885.7	0.8830	-
293	0.0000	998.1	1.0155	-
	0.0006	998.0	1.0189	0.777 ± 0.5 %
	0.9824	881.8	0.8311	-
	0.9859	-	-	2.448 ± 3.8 %
	0.9915	-	-	2.480 ± 4.2 %
	1.0000	880.6	0.8267	-
298	0.0000	997.0	0.9057	-
	0.0006	996.9	0.9076	0.939 ± 0.5 %
	0.9824	876.3	0.7798	-
	0.9862	-	-	2.748 ± 2.3 %
	0.9954	-	-	2.804 ± 1.6 %
	1.0000	876.2	0.7763	-

Tab. 5: Binodal Curves – System 1: Toluene (A) – Water (B) – MIPK (C)

T [K]	z_A [w/w-%]	z_B [w/w-%]	z_C [w/w-%]
283	99.97	0.03	-
	90.06	0.04	9,89
	79.50	0.22	20.29
	69.13	0.29	30.57
	59.56	0.09	39.96
	49.66	0.66	49.67
	39.61	0.90	59.50
	29.68	1.20	69.13
	19.67	1.70	78.64
	9.75	2.31	87.94
	-	2.88	97.12
	-	95.86	4.14
	0.05	98.44	1.57
	0.03	99.96	-
293	99.98	0.03	-
	94.96	0.04	5.01
	94.96	0.04	10.50
	89.41	0.08	10.54
	69.73	0.30	29.97
	65.09	0.43	34.48
	59.52	0.50	39.97
	49.65	0.77	49.58
	40.17	1.07	58.76
	29.32	1.37	69.63
	19.48	1.91	78.60
	9.66	2.48	87.86
	-	3.32	96.98
	-	95.94	4.75
	0.03	98.98	0.99
	0.06	99.98	-
303	99.97	0.04	-
	94.85	0.05	5.10
	87.46	0.21	20.53
	69.93	0.31	29.76
	58.73	0.64	40.63
	47.58	0.94	51.48
	39.34	1.21	59.45
	29.63	1.54	68.84
	20.96	1.95	77.09
	9.65	2.77	87.6
	-	3.57	96.43
	-	94.24	5.76
	0.04	99.96	-

Tab. 6: Binodal Curves – System 2: BuAc (A) – Water (B) – MIPK (C)

T [K]	z_A [w/w-%]	z_B [w/w-%]	z_C [w/w-%]
283	99.94	0.06	-
	89.66	0.17	10.17
	75.41	0.27	24.32
	65.81	0.48	33.71
	57.06	0.66	42.28
	48.18	0.91	50.91
	41.26	1.24	57.5
	29.66	1.63	68.71
	19.34	2.02	78.64
	9.89	2.49	87.62
	-	2.99	97.01
	-	95.96	4.04
293	98.91	1.09	-
	91.56	1.08	7.36
	87.24	1.15	11.61
	77.11	1.31	21.58
	58.79	1.48	39.73
	49.10	1.62	49.28
	43.95	1.90	54.15
	32.96	1.99	65.05
	19.30	2.14	78.56
	9.39	2.61	88.00
	-	3.43	96.57
	-	93.69	6.31
	0.67	99.33	-
303	98.78	1.22	-
	90.92	1.43	7.65
	77.55	1.57	20.88
	73.94	1.70	24.36
	58.79	2.06	39.15
	47.97	2.33	49.70
	35.79	2.62	61.59
	26.78	2.74	70.48
	10.96	3.21	85.83
	-	3.67	96.33
	-	94.21	5.79
	0.70	99.30	-

Tab. 7: Binodal Data (Tie Lines) – System 1: Toluene (A) – Water (B) – MIPK (C)

T [K]	x_c [ww-%]	y_c [ww-%]
283	0.11	0.84
	0.26	2.20
	0.56	5.37
	1.19	12.79
	1.84	22.80
	2.54	31.76
293	0.04	0.43
	0.12	1.52
	0.32	4.14
	0.82	11.14
	1.85	25.95
303	0.08	0.86
	0.22	2.73
	0.61	9.12
	0.8	11.47
	0.88	13.12
	1.74	29.95
	2.39	43.63
	2.72	49.03

Tab. 8: Binodal Data (Tie Lines) – System 2: BuAc (A) – Water (B) – MIPK (C)

T [K]	x_c [ww-%]	y_c [ww-%]
283	0.10	0.99
	0.20	1.91
	0.23	2.73
	0.46	4.70
	0.53	6.10
	1.04	11.75
	1.16	12.84
	2.32	27.75
	2.60	32.39
293	0.06	0.52
	0.39	4.76
	0.72	9.63
	0.89	11.80
	0.95	12.53
	1.73	22.54
	2.07	26.99
	2.26	29.46
303	0.10	1.36
	0.29	4.19
	0.76	11.22
	1.38	21.69
	1.93	31.50
	2.18	36.10

Tab. 9: Physical Properties at Equilibrium (Density, Dynamic Viscosity and Interfacial Tension) – System 1: Toluene (A) – H_2O (B) – MIPK (C)

T [K]	x_C [ww-%]	ρ_x [kg/m^3]	ρ_y [kg/m^3]	Δ_p [kg/m^3]	η_x [mPas]	η_y [mPas]	σ [mN/m]
283	0.00	999.9	877.0	123.7	1.308	0.660	36.2
	0.11	999.3	875.5	123.8	1.270	0.618	28.3
	0.26	999.2	874.6	124.6	1.267	0.643	22.0
	0.56	998.6	872.4	126.2	1.267	0.627	17.1
	1.19	997.9	868.0	129.9	1.308	0.600	11.3
	1.84	997.2	864.0	133.2	1.317	0,584	8.9
	2.54	996.3	856.9	139.4	1.357	0.575	8.4
293	0.00	998.2	866.9	131.3	1.005	0.582	35.3
	0.12	998.1	866.4	131.7	0.975	0.553	28.7
	0.32	997.7	864.2	133.5	0.962	0.549	23.7
	0.82	997.2	862.2	135.0	0.982	0.542	21.6
	1.85	996.1	853.8	142.3	1.004	0.523	10.1
303	0.00	995.7	857.7	138.0	0.801	0.520	35.0
	0.08	995.4	857.2	138.2	0.699	0.468	30.1
	0.22	995.3	855.6	139.7	0.698	0.465	26.90
	0.61	995.1	851.2	134.9	0.708	0.458	23.60
	0.80	994.7	849.8	144.9	0.717	0.455	20.40
	0.88	994.5	848.8	145.7	0.718	0.453	20.10
	1.74	993.4	839.4	154.0	0.746	0.450	16.10
	2.39	992.4	832.3	160.1	0.745	0.454	13.40
	2.72	992.2	828.2	164.1	0.734	0.454	12.70

Tab. 10: Physical Properties at Equilibrium (Density, Dynamic Viscosity and Interfacial Tension) – System 2: BuAc (A) – H_2O (B) – MIPK (C)

T [K]	x_C [ww-%]	ρ_x [kg/m^3]	ρ_y [kg/m^3]	Δ_p [kg/m^3]	η_x [mPas]	η_y [mPas]	σ [mN/m]
283	0.00	999.7	891.9	107.8	1.308	0.851	14.1
	0.10	999.4	891.8	107.6	1.362	0.771	12.6
	0.20	999.2	890.6	108.6	1.365	0.768	12.5
	0.23	999.2	890.5	108.7	1.372	0.765	12.5
	0.46	998.9	888.2	110.7	1.381	0.758	12.2
	0.53	998.8	887.9	110.9	1.377	0.754	12.1
	1.04	998.0	882.6	115.4	1.410	0.737	11.3
	1.16	998.1	882.1	116.0	1.414	0.731	11.1
	2.32	996.5	871.2	125.3	1.468	0.696	9.0
	2.60	996.3	868.2	128.1	1.474	0.684	8.3
293	0.00	998.2	880.0	118.2	1.005	0.731	11.9
	0.06	998.9	884.3	114.6	0.975	0.700	--
	0.39	997.9	879.4	118.5	0.992	0.683	11.7
	0.72	997.3	875.1	122.2	0.998	0.671	11.7
	0.89	997.2	874.0	123.2	0.999	0.665	11.6
	0.95	997.1	873.0	124.1	1.010	0.661	11.7
	1.73	996.0	864.9	131.1	1.024	0.636	10.6
	2.07	995.7	861.3	134.4	1.028	0.625	9.7
	2.26	995.5	859.4	136.1	1.038	0.616	9.7
303	0.00	995.7	872.1	123.6	0.801	0.642	12.5
	0.10	995.7	871.7	124.0	0.773	0.604	13.0
	0.29	995.4	869.5	125.9	0.773	0.595	12.9
	0.76	994.9	863.7	131.2	0.784	0.578	12.3
	1.38	993.6	855.0	138.6	0.796	0.557	11.0
	1.93	993.0	848.1	144.6	0.808	0.541	10.3
	2.18	992.5	843.4	149.1	0.814	0.536	9.7

Tab. 11: Binodal and Tie Line Data – System 2: BuAc (A) – H_2O (B) – MIPK (C)

T [K]	x_A [ww-%]	x_B [ww-%]	x_C [ww-%]	y_A [ww-%]	y_B [ww-%]	y_C [ww-%]
288	0.69	99.31	0.00	99.05	0.95	0.00
	0.69	99.01	0.30	95.48	1.07	3.45
	0.68	98.85	0.47	93.65	1.12	5.23
	0.68	98.71	0.61	91.94	1.11	6.95
	0.68	98.56	0.76	90.23	1.15	8.62
	0.67	98.42	0.91	88.47	1.18	10.35
	0.67	98.32	1.01	86.84	1.19	11.96
	0.66	98.18	1.17	85.26	1.24	13.50
	0.64	98.03	1.33	83.43	1.25	15.32
	0.63	97.90	1.47	81.67	1.28	17.04
	0.60	97.63	1.76	78.42	1.35	20.23
	0.57	97.26	2.17	72.87	1.44	25.70
	0.53	96.87	2.60	69.41	1.51	29.07
	0.53	96.82	2.65	66.62	1.53	31.84
	0.53	96.82	2.65	66.63	1.56	31.81
	0.51	96.59	2.90	63.54	1.64	34.81
	0.43	95.79	3.78	50.48	1.89	47.63
	0.37	95.01	4.63	38.10	2.16	59.73
	0.28	94.42	5.31	31.50	2.51	65.99
	0.28	94.42	5.31	28.78	2.42	68.80
	0.11	93.76	6.13	17.38	2.66	79.96
	0.22	93.41	6.57	12.22	2.88	84.89
			6.98	2.26	3.07	94.67
			7.47	0.17	3.26	96.58

Tab. 11: continued

293	0.61	99.39	0.00	98.93	1.08	0.00
	0.61	99.11	0.28	95.39	1.18	3.44
	0.61	98.96	0.43	93.52	1.21	5.27
	0.60	98.83	0.56	91.88	1.24	6.88
	0.60	98.58	0.82	88.54	1.31	10.15
	0.60	98.44	0.96	86.56	1.38	12.05
	0.59	98.34	1.07	85.25	1.38	13.37
	0.58	98.20	1.21	83.33	1.42	15.25
	0.58	98.14	1.28	81.87	1.45	16.68
	0.56	97.84	1.60	77.83	1.54	20.62
	0.53	97.48	1.99	72.84	1.64	25.52
	0.51	97.25	2.24	69.17	1.74	29.09
	0.49	97.10	2.40	66.70	1.77	31.53
	0.47	96.89	2.63	62.87	1.85	35.29
	0.39	96.05	3.56	51.49	2.17	46.34
	0.33	95.32	4.35	38.98	2.54	58.48
	0.32	95.22	4.46	36.34	2.66	60.99
	0.30	94.88	4.83	31.34	2.74	65.93
	0.28	94.71	5.01	30.41	2.84	66.75
	0.15	94.17	5.68	19.67	3.19	76.93
	0.07	93.84	6.10	14.22	3.45	82.32
	0.01	93.61	6.38	5.35	3.21	91.44
	0.00	93.55	6.45	0.96	3.40	95.64
298	0.57	99.43	0.00	98.82	1.18	0.00
	0.56	99.05	0.39	93.43	1.33	5.25
	0.55	98.69	0.76	88.22	1.36	10.42
	0.54	98.36	1.10	83.38	1.45	15.17
	0.52	98.05	1.43	77.95	1.52	20.53
	0.50	97.64	1.86	72.31	1.64	26.05
	0.47	97.24	2.29	67.38	1.76	30.86
	0.46	97.09	2.45	63.40	1.85	34.75
	0.42	96.52	3.06	50.96	2.09	46.94
	0.33	95.80	3.87	38.61	2.43	58.95
	0.25	95.28	4.47	28.98	2.72	68.30
	0.20	94.95	4.85	19.70	2.99	77.31
	0.08	94.27	5.65	13.88	3.51	82.61
	0.05	94.05	5.90	8.32	3.84	87.84
			6.65	3.29	4.07	92.64
				0.00	3.62	96.38

Tab. 12: Physical Properties at Equilibrium (Density, Dynamic Viscosity and Interfacial Tension) – System 2: BuAc (A) – H_2O (B) – MIPK (C)

T [K]	x_C [ww-%]	ρ_X [kg/m^3]	ρ_Y [kg/m^3]	υ_X [mm^2/s]	υ_Y [mm^2/s]	σ [mN/m]
288	0.30	998.1	885.4	1.189	0.889	
	0.47	998.0	884.8	1.223	0.891	11.2
	0.61	999.9	883.5	1.225	0.881	
	0.76	997.5	882.3	1.229	0.895	
	0.91	997.0	880.7	1.236	0.872	
	1.01	996.9	878.9	1.242	0.884	
	1.17	996.9	878.6	1.247	0.871	
	1.33	986.5	875.9	1.256	0.87	10.0
	1.47	996.1	874.4	1.253	0.864	
	1.76	995.8				
	2.17	994.7	868.8	1.277	0.844	9.1
	2.60	994.7	865.5	1.287	0.837	
	2.65	983.8	863.7	1.297	0.831	
	2.65	995.5	863.4	1.294	0.823	
	2.90	995.1	860.2	1.312	0.815	8.6
	3.78	994.1	852.5	1.349	0.793	
	4.63	992.9	842.1	1.385	0.77	6.5
	5.31	990.3	840.9	1.381	0.766	
	5.31	991.7	837.5	1.411	0.753	
	6.13	990.9	831.8	1.431	0.742	5.9
	6.57	990.5	827.7	1.456	0.734	
	6.98	990.1	823.7	1.494	0.371	4.9
	7.47		817.1		0.734	

Tab. 12: continued

293	0.28	997.6	880.0			
	0.43	996.7	878.2			11.3
	0.56	997.4	878.2			
	0.82	997.4	874.1			11.0
	0.96	996.7	873.6			
	1.07	996.5	872.4			
	1.21	996.4	871.1	1.063	0.831	10.4
	1.28	996.4	869.8			
	1.60	996.2	867.6	1.078	0.813	9.9
	1.99	995.6	863.2	1.081	0.799	9.5
	2.24	995.2	860.6	1.115	0.793	
	2.40	994.9	858.2	1.126		
	2.63	994.7	858.2	1.141	0.781	8.1
	3.56	993.9	852.2	1.170	0.764	7.4
	4.35	992.3	842.9	1.200	0.751	
	4.46	992.5	835.8			
	4.83	991.9	835.0	1.174		
	5.01	991.6	836.2	1.234	0.740	5.7
	5.68	991.2	829.9	1.244	0.740	
	6.10	990.9	825.8	1.256	0.725	5.4
	6.38	990.3	817.8	1.259	0.688	
	6.45		814.3		0.686	
298	0.39	995.5	873.5	0.949	0.788	11.6
	0.76	995.0	869.2	0.948	0.770	
	1.10	994.8	864.9	0.958	0.759	10.5
	1.43	994.7	861.8	0.975	0.752	
	1.86	994.4	856.5	0.985	0.738	9.6
	2.29	994.0	853.2	0.992	0.729	
	2.45	993.8	850.2	1.001	0.723	8.9
	3.06	992.1	841.9	1.014	0.705	
	3.87	991.7	834.2	1.035	0.689	7.2
	4.47	991.0	827.9	1.054	0.800	
	4.85	990.7	824.9	1.064	0.670	6.2
	5.65	990.8	822.7	1.088	0.687	
	5.91	990.2	820.4		0.688	5.5
	6.65		817.6		0.656	

EUROPEAN FEDERATION OF CHEMICAL ENGINEERING
WORKING PARTY ON DISTILLATION, ABSORPTION AND EXTRACTION

STANDARD TEST SYSTEM FOR REACTIVE EXTRACTION - ZINC/D2EHPA

Hans-Jörg Bart
Mike J. Slater

CONTENTS

Preface

The EFCE Working Party on "Distillation, Absorption and Extraction" has initiated and recommended the use of standard test systems, all published by the Institution of Chemical Engineers (London). It started in 1969 with "Recommended Test Mixtures for Distillation Columns" with a second edition in 1990 in the distillation field. This was followed 1978 and in a slightly modified second edition 1985 entitled "Standard Test Systems for Liquid Extraction" by T. Misek, R. Berger and J. Schröter in the extraction field. The statements of T. Misek in the preface of the first edition are still valid:

The recommendation of using only a few selected systems in liquid extraction studies is aimed at providing a comparable basis for these studies, and at achieving deeper knowledge of these systems, so that the above disadvantages can be avoided. Thus, in addition to testing extraction equipment in the laboratory and pilot plant, the recommended systems should also be used for studying the basic components of the extraction processes, e.g. formation and motion of drops, transfer of heat and mass, coalescence, interphase phenomena, etc.. Hopefully, the work of different authors could then become comparable and the explanation of anomalous phenomena, deviations and strange behaviour will be possible.

However, the focus of the above publications is with physical systems and thus in the mid eighties the needs of a standard reactive reaction system was discussed between S. Hartland, T. Misek, J. Schröter, H.F. Svendsen and us. As a result the metal ion extraction process of zinc with the cation exchanger D2EHPA (di-(2ethylhexyl)phosphoric acid) was choosen due to price, easy availability and handling and because of its widespread large scale use in industrial hydrometallurgy. Similar to the previous publications the text of the work has been kept as brief as possible. However, due to the chemistry involved, besides equilibria also chemical rate constants are given derived from kinetically controlled mass transfer experiments.

Kaiserslautern, March 2001 — Bradford, March 2001

H.-J. Bart — M. J. Slater

1.1 Theoretical Background

An introduction to reactive extraction is given in several handbooks (Handbook of Solvent Extraction, 1983; Principles and Practice of Solvent Extraction, 1992; Science and Practice of Liquid-Liquid Extraction, 1992; Liquid-Liquid Extraction Equipment, 1994). Functions were sought to describe the physical properties (density, viscosity, interfacial tension) in a sufficiently precise manner. Equilibria can be predicted with activity coefficient models freely available from the internet and kinetic correlations have been developed suitable for computational use.

The reactive test system consists of the components $ZnSO_4$ and H_2SO_4 in the aqueous phase and the cation exchanger D2EHPA[1] diluted in isododecane as organic phase. The final choice of isododecane as diluent was due to savety and cost reasons. The effects of other diluents on equilibria and kinetics is discussed elsewhere (Wachter et al. 1993, Bart et al. 1994, Sainz-Diaz et al. 1996, Klocker et al. 1997, Hancil & Slater 1990, Mansur et al. 2002a,b,c).

1.2 General Description of the System

Solvent extraction processes which use liquid ion exchangers and fundamental research with respect to their compounds still dominate the proceedings of the International Solvent Extraction Conferences (ISEC). This wide application of reactive extraction has been the reason for the demand for a reactive test system to be added to the physical extraction systems described by Misek (1978, 1985). In 1987 (Slater 1987, Bart et al. 1987) a discussion was initiated on the characterisation of such a reactive test system. An extended summary on the problems with reactive systems when extracting zinc from a sulphuric acid solution by D2EHPA dissolved in a diluent, is given by Bart et al. (1994). Further information on treating reactive extraction systems and their equilibria can be found in Rydberg et al. (1992) and Slater (1994). The basic equilibrium reaction in the system is as follows, where (R_2H_2) is the D2EHPA dimer which is dominant in aliphatic diluents (Kolarik 1976, 1982):

$$Zn^{++} + \frac{n}{2}(R_2H_2) \leftrightarrow ZnR_2(RH)_{n-2} + 2H^+ \qquad (1)$$

The equilibrium can be shifted and thus the ion exchanger regenerated with an acid. The equilibrium constant K for the zinc extraction is then

$$K = \frac{[\overline{ZnR_2(RH)_{n-2}}]\cdot[H^+]^2}{[Zn^{2+}]\cdot[\overline{R_2H_2}]^{n/2}} \qquad (2)$$

where the bar denotes the organic phase compounds. As can be seen, in contrast to physical extraction systems, the distribution coefficient depends on the pH-value, on the ion exchanger concentration and the complex formation stoichiometry n. However, FTIR analytical measurements confirm n to be equal 3 and Karl-Fischer-titration reveal no water to be co-extracted with the complex into the organic phase at low Zn^{++} and low fraction loading of D2EHPA (Sainz-Diaz et al. 1996). This is in contrast to the extraction of nickel or cobalt (Neumann 1990) for example where water is co-extracted and even inverse micellation can occur. The concentration domain of the test system is shown in Table 1.

The organic phase loaded with zinc (even in the presence of sodium) behaves nearly ideally and both phases can be considered as mutually insoluble. Since most of the reactive solvent extraction processes deal with metal ions, the focus was on a system with a heterogeneous (interfacial) reaction. The limiting case of a homogeneous reaction is not considered with this test system.

[1] D2EHPA: di-(2ethylhexyl)phosphoric acid

Table 1: Concentration domain of the test system

substance	$ZnSO_4$	H_2SO_4	D2EHPA
moles p. litre	$5 \cdot 10^{-5}$ to $5 \cdot 10^{-2}$	0 to 0.01	0.005 to 0.2
grammes p. litre	0.008 to 8	0 to 0.98	1.61 to 64.4
mass percent	0.0008 to 0.8	0 to 0.098	0.22 to 8.7

2 System Properties and Behaviour of the System Constituents

2.1 Preparation of the System

The extraction system is investigated between 8 g/L and 8 mg/L $ZnSO_4$ (see Table 1) which is typical for metal extractions. The temperature range is between 283 K and 303 K (see Appendix B).

The aqueous phase consists of analytical grade sulphuric acid and zinc sulphate dissolved in distilled water. D2EHPA (CAS-No.: 298-07-7) is diluted in isododecane (CAS-No.: 93685-81-5 / 31807-55-3) which is polymerized from isobutylene leading to a high purity (> 98 %) 2,2,4,6,6-pentamethylheptane (CAS-No.: 13475-82-6) commonly called isododecane. Suppliers of isododecane are e.g. FLUKA or Gefachem-Prochemie/Leverkusen and of D2EHPA are e.g. BDH-Chemicals, Merck, Fluka, Daihachi, Union Carbide, Morton Thiokol, Bayer, Albright and Wilson, etc.. D2EHPA purification methods are described by Hancil et al. (1990) and Sainz-Diaz et al. (1996) and it can be used as delivered, if the mono-acid content is less than 0.5 % (see 2.3).

2.2 Safety and Emergency Instructions

2.2.1 Safety Instructions

Sulphuric acid, D2EHPA and the resulting organic and aqueous phase mixture irritate skin and eyes (use gloves, goggles!). All liquids are virtually colourless and odourless and the organic components are immiscible with water. Isododecane causes minor irritation but is flammable, evaporates slowly, forms explosive mixtures with air, is heavier than air and can be electrostatically charged during filling/pumping (see also Table 2).

Table 2: Fire and safety properties

	D2EHPA	Isododecane	H_2SO_4	$ZnSO_4$
Status	liquid	liquid	liquid	solid
boiling point or distillation range K	n.a[1]	449-914	> 550	n.a.
melting point K	223	192	258	600
flash point K	471	318	n.a.	n.a.
ignition temperature K	> 550	683	n.a.	n.a.
vapor pressure mbar at 298 K	n.a.	1	n.a.	n.a.
solubility in water g/L at 298 K	< 1	< 0.1	very good	good
pH-value	ca. 3	neutral	acidic	neutral
lower % vol.	n.a.	0.5	n.a.	n.a.
upper % vol.	n.a.	4.0	n.a.	n.a.
LD_{50} oral (nat) mg/kg	4940	> 2000	-	2200
LC_{50} inhalative (rat) mg/L (1 h)	-	> 21.3	-	-
skin irritation (rabbit)	strong	no	strong	-

[1] ... not applicable

2.2.2 Emergency Instructions

Transport exposed persons outdoors and loosen clothes. Remove any wetted part of the clothes, thoroughly rinse the skin with water and soap. When the eyes are exposed, rinse with water for 10 to 15 minutes. In such a case or after oral consumption, call a physician.
Fire: Extinguish with water, fog, powder, carbon dioxide powder or foam.

2.3 Analytical Methods

H_2SO_4 concentrations can easily be checked with a pH-meter. The purity grade of the extractant D2EHPA can be determined by a potentiometric acid-base titration with 0.1 molar NaOH with about 1 % D2EHPA in isopropanol. The inflection point at pH 7.1 is for D2EHPA and 10.8 for the mono-acid (Sainz-Diaz et al. 1996).

2.3.1 Zn-Analysis by AAS

The zinc concentration in the organic and the aqueous phase is best detected by Atomic Absorption Spectrometry (AAS) at a wavelength of 213 nm. The samples have to be diluted in order to meet the required concentration range (usually < 12 mg/L). For both phases commercial analytical standards are available; alternatively the organic phase can be acid stripped and analysed. However, the switch from aqueous to organic AAS analysis needs a considerable time of washing the burner system either with water or acetone/isododecane. It is recommended to strip the organic phase with acid (see 2.3.2) and balance the organic concentrations.

2.3.2 Zn-Analysis by Titration with Sodium EDTA

The zinc concentration can be detected by titration with sodium salts of ethylenediaminetetraacetic acid (Titriplex® III; Merck). Klocker describes the procedure of the analysis (Klocker, H. 1996b). The initial 0.1 mol/L solution has to be diluted 1:20 with distilled water, in order to analyse small zinc concentrations. For indicator buffer tablets from Merck were used as well as zinc standard solutions (1000 ppm) for calibration.

Buffer tablets were diluted in 100 mL in distilled water. 50 mL of that stock solution were transferred to a beaker. After adding 0.5 mL of ammonia, 0.5-8 mL of the sample solution is added and the shift from red over grey to green is titrated. The amount of ammonia used has to be raised when analysing acid samples (1.5 mL). Because of a distinct colour shift good reproducibility is given. According this method zinc concentrations greater than 5 mM can be determined with high accuracy. For organic samples a re-extraction is necessary, since titration with EDTA only works in aquatic environments. For re-extraction the organic phase is contacted with 1 mol/L sulfuric acid (phase ratio 1:1) for about 1 hour.

2.4 Recovery of the System

During extraction zinc is removed and protons are set free (see equ. (1)). The organic phase can be re-used after stripping the zinc with 2.5 molar sulphuric acid twice and at least twice washing with water to neutrality at a phase ratio equal to one. The aqueous raffinate cannot be re-used after neutralization with NaOH and admixture of $ZnSO_4$. However, the resulting compound Na_2SO_4 is not included in the test system, since it shows a significant influence on the zinc distribution coefficient (see Fig. 1). When discharging either the aqueous or organic phase, one has to consider local governmental regulations since both phases are toxic for fish and bacteria.

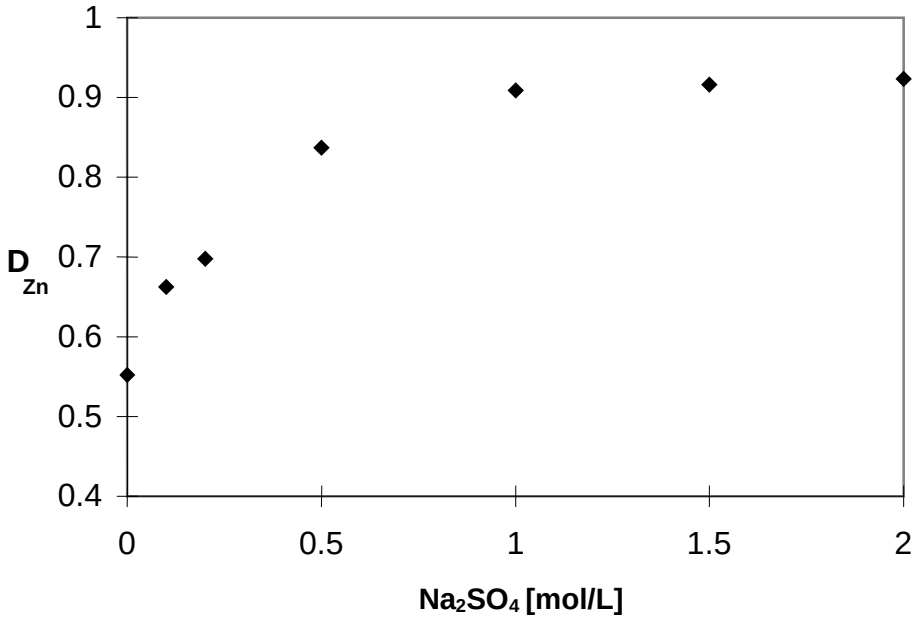

Figure 1: Influence of sodium sulphate on the zinc distribution coefficient;
$[ZnSO_4]_{start}$ = 0.05 mol/L, $[D2EHPA]_{start}$ = 0.1 mol/L, pH_{start} = 7

2.5 Physical Properties

The change of aqueous viscosity due to a shift of pH and zinc concentrations is negligible, however the influence on density is given with equ. (3). D2EHPA is of medium viscosity and has a density of 960 kg/m^3. The following correlations are valid at 298 K. The interfacial tension is not very sensitive to pH but slightly sensitive to the aqueous zinc concentration. A compendium of all measured values (including data at 283 and 303 K) is given in Appendix B.

$$\rho_{aqu} = 165.5 \cdot [ZnSO_4] + 997.2 \quad [\pm 2.28\ kg/m^3] \tag{3}$$

$$\rho_{org} = 75.7 \cdot [D2EHPA] + 745.4 \quad [\pm 96.2\ g/m^3] \tag{4}$$

$$\nu_{org} = 1.0801 \cdot [D2EHPA] + 1.6365 \quad [\pm 3.39 \cdot 10^{-3}\ \ mm^2/s] \tag{5}$$

$$\sigma = 17.23 \cdot [D2EHPA]^{-0.094} \quad [\pm 1.95\ mN/m] \quad [Zn]_{aqu} < 0.001\ \ mol/L \tag{6}$$

$$\sigma = 18.31 \cdot [D2EHPA]^{-0.088} \quad [\pm 1.36\ mN/m] \quad 0.001 < [Zn]_{aqu} < 0.01\ \ mol/L \tag{7}$$

$$\sigma = 18.61 \cdot [D2EHPA]^{-0.092} \quad [\pm 1.00\ mN/m] \quad [Zn]_{aqu} > 0.01\ \ mol/L \tag{8}$$

3 Equilibria

The equilibria were measured with D2EHPA from Baysolvex (Bayer) with 0.5 % mono-acid and 2.2 % (mass) neutral impurities (mainly 2-ethylhexanol) without further purification. Using the distribution coefficient D_{Zn}, equation (2) can be rewritten as

$$K = D_{Zn} \cdot \frac{[H^+]^2}{[\overline{R_2H_2}]^{n/2}} \qquad (9)$$

The complex stoichiometry, n, is usually found by slope analysis of a logarithmic plot of equ. (9), which then reads as follows:

$$\log D_{Zn} = \frac{n}{2} \cdot \log([\overline{R_2H_2}]) + 2pH + \log K \qquad (9b).$$

This slope and thus n can be derived from Fig. 2.

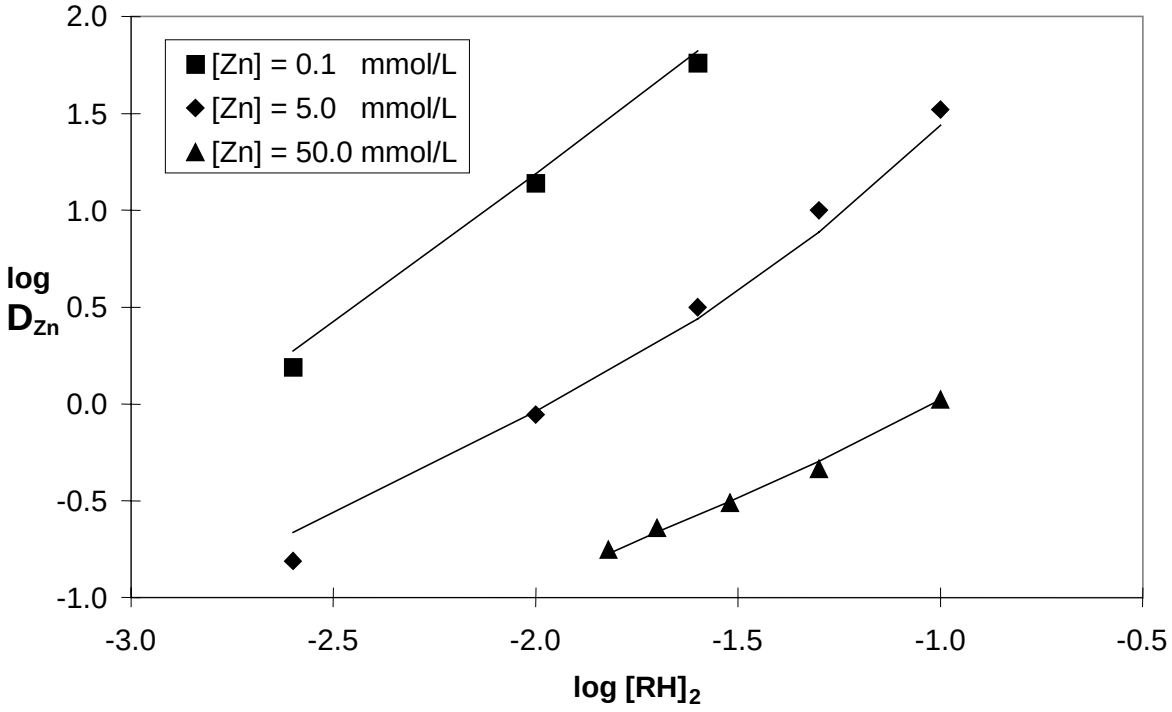

Figure 2: Log D_{Zn} versus log $[D2EHPA]_2$ for different initial zinc concentrations

The line at the lowest zinc concentration (0.0001 mol/L) gives a slope of 1.5 which is equivalent to the FTIR-measurement of n = 3 (Sainz-Diaz et al. 1996). The highest zinc concentration (0.05 mol/L) yields a slope of 1.0 or n = 2 which according to FTIR is not valid. The proposed way to consider these effects in Fig. 2 is by using activity coefficients with a uniform stoichiometry in the considered concentration range. This leads to the reaction equation

$$Zn^{2+} + 1.5\,\overline{R_2H_2} \leftrightarrow \overline{ZnR_2RH} + 2H^+ \qquad (10)$$

with the equilibrium constant:

$$K_{1,3} = \frac{[\overline{ZnR_2RH}]\cdot[H^+]^2}{[Zn^{2+}]\cdot[\overline{R_2H_2}]^{1.5}} \cdot \frac{\gamma_{\overline{Zn}}\cdot\gamma_H^2}{\gamma_{Zn}\cdot\gamma_{\overline{R_2H_2}}^{1.5}} \qquad (11)$$

To calculate the activity coefficients γ_i, the Pitzer-model (Pitzer, 1973, 1975, 1977, 1978, 1979) is used for the aqueous phase and the Hildebrand-Scott-solubility parameter (Hildebrand and Scott, 1950) is used for the organic phase. The Pitzer-, Masson- and solubility parameters are taken from literature (Klocker et al. 1996a), (Baes and Moyer 1988), (Clegg et al. 1994), (Moyer et al. 1993). With the software of Baes et al. (1990), the solubility parameter of the organic complex and the equilibrium constant can be estimated. The quality of the fit is expressed by the agreement factor σ (see equ. (16)). The program is freely available in the internet (http://www.ornl.gov/divisions/casd/csg/sxlsqi/). In this context, a selection of 66 experiments out of 102 (listed in appendix B) was used to simulate the extraction equilibria The parameters needed to run the program are given in Tables 3 to 5. Figures 3 and 4 depict the good description of the equilibrium data by the model.

Table 3: Pitzer parameters of the system $ZnSO_4/H_2SO_4$ at 298 K -Klocker et al. (1996a)

interaction	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^ϕ or $C^{\phi(0)}$	$C^{\phi(1)}$	α_1	α_2	ω
Zn^{2+}-SO_4^{2-}	0.16724	3.49906	-40.5911	0.036746	-12.9451	1.4	12	3.3
Zn^{2+}-HSO_4^-	0.56879	2.61593	-	-0.046724	-	2.0	-	-
H^+ - SO_4^{2-}	0.06421	0.225902	-	0.031126	-	2.0	-	-
H^+ - HSO_4^-	0.22297	0.460016	-	-0.002660	-	2.0	-	-

Zn^{2+}-H^+	Θ	0
Zn^{2+}-H^+-SO_4^{2-}	Ψ	0
Zn^{2+}-H^+-HSO_4^-	Ψ	0
SO_4^{2-}-HSO_4^-	Θ	-0.135342
Zn^{2+}-SO_4^{2-}-HSO_4	Ψ	0.0731378
H^+-SO_4^{2-}-HSO_4^-	Ψ	0.0278059

Table 4: Masson parameters (298 K), molecular weight (MW) and molecular volume Φ^V (298 K) of ions in the organic phase (Moyer et al. 1993)

ion	MW [g/mol]	Φ_j^0 [cm³/mol]	S_j	$\Phi^V_{Zn,org}$ [cm³/mol]
H^+	1.0079	0	0	0.0
Zn^{2+}	65.38	-22.27	4.66	-4.2
SO_4^{2-}	96.0636	13.98	8.64	
HSO_4^-	97.0715	37.88	2.18	

Table 5: Molecular weight (MW), molar volume V_i (298 K) and solubility parameter δ (298 K) of D2EHPA and isododecane (Klocker 1996b), (Baes 1988)

species	MW [g/mol]	V_i [cm^3/mol]	δ_i [$cal^{1/2}cm^{-3/2}$]
D2EHPA (monomeric)	322.43	332.61	8.76
Isododecane	170.34	228.42	7.031

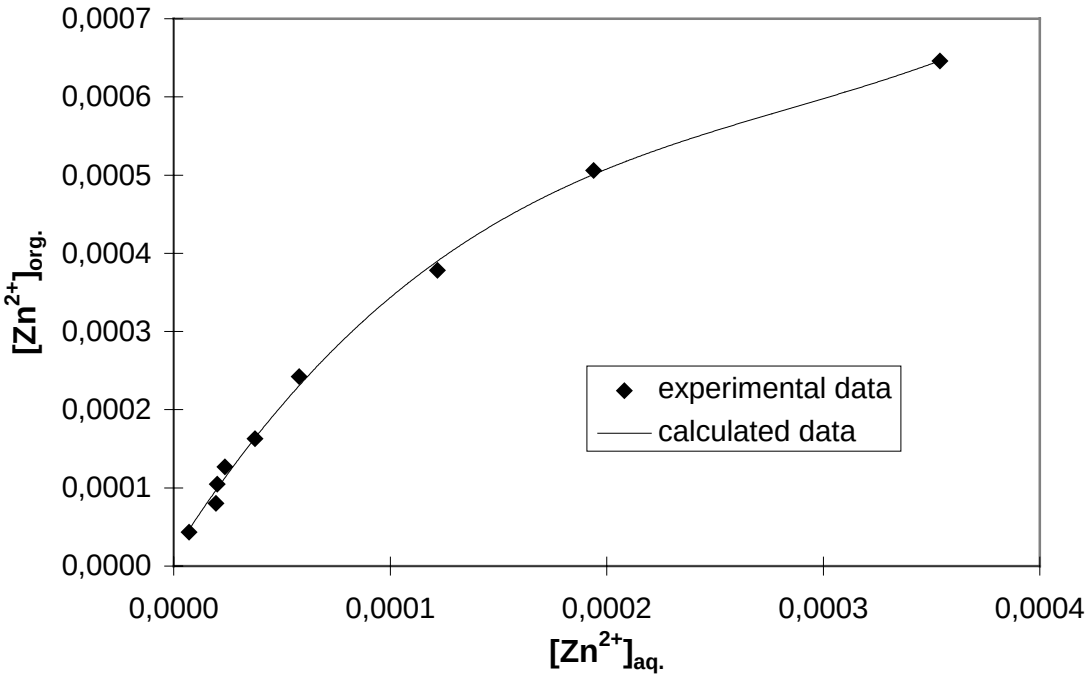

Figure 3: Experiments A 48-A 57; $[Zn^{2+}]_{org.}$ versus $[Zn^{2+}]_{aq.}$; $[Zn^{2+}]_{start}$ = 0.05 – 1.0 mmol/L, $[D2EHPA]_{start}$ = 10 mmol/L, $[H_2SO_4]_{start}$ = 2.0 mmol/L

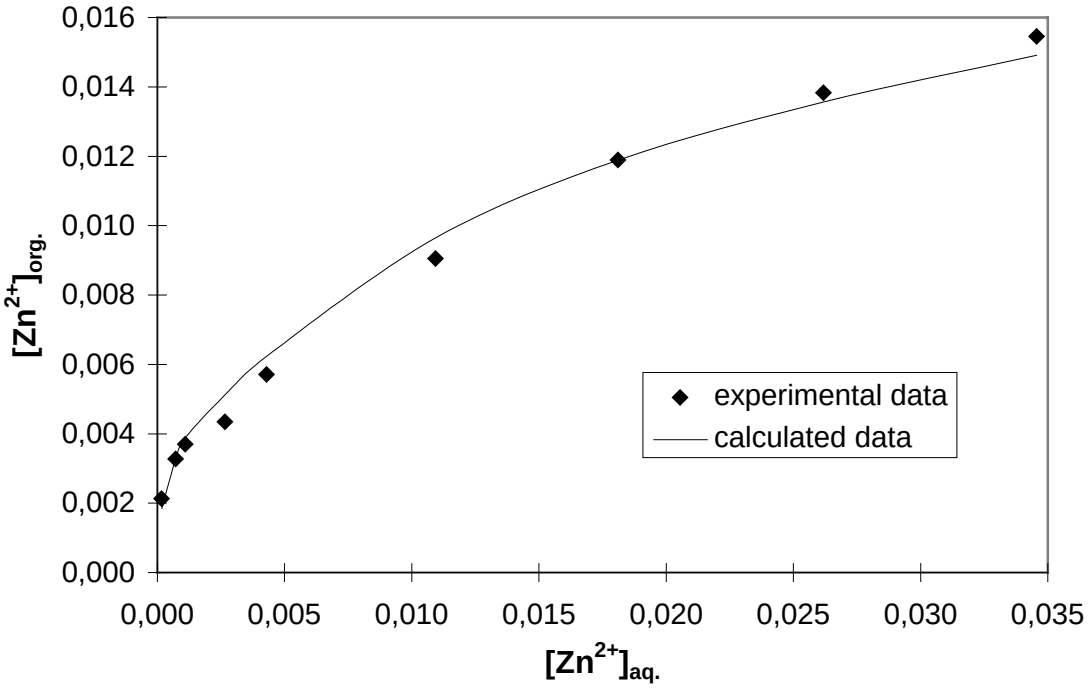

Figure 4: Experiments A 58-A 66; $[Zn^{2+}]_{org.}$ versus $[Zn^{2+}]_{aq.}$; $[Zn^{2+}]_{start}$= 2.0 – 50.0 mmol/L, $[D2EHPA]_{start}$ = 0.1 mol/L, $[H_2SO_4]_{start}$ = 0.01 mol/L

As can be seen from Table 6, there is practically no difference in the complex stoichiometry and equilibrium values when using another aliphatic diluent such as n-heptane instead of isododecane as long as the species concentration range is according to Table 1.

Table 6: Estimated equilibrium parameters

species	$\log_{10} K_{1,3}$	δ [$cal^{1/2}cm^{-3/2}$]	σ
$\overline{ZnR_2(RH)}$ in isododecane	-1.1863	9.3040	1.2194
$\overline{ZnR_2(RH)}$ in n-heptane	-0.9441	9.086	1.6479

If someone does not want to use the full model, equation 11 can be used to estimate the equilibrium concentrations by assuming all activity coefficients as γ_i = 1. For aqueous equilibrium concentrations lower than 50 µmol/L, where the D2EHPA-concentration can be assumed as constant, the ideal calculations predict the organic zinc concentration within 20% relative error, δ. Fig. 5 shows that the predictions become much worse for higher concentrations.

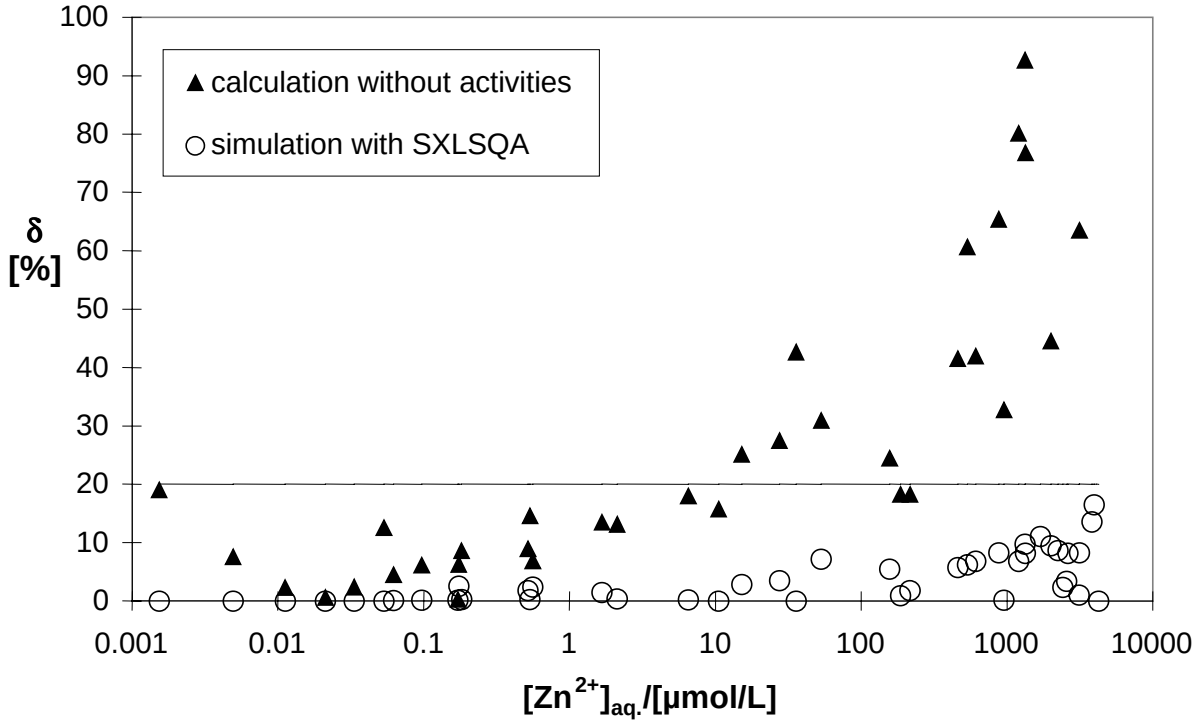

Figure 5: Relative error, δ, of simulation based on activities and of estimation based on concentrations showing dependence on aqueous zinc concentration in equilibrium

4 Mass Transfer

4.1 Reaction Kinetics

In reactive extraction, the overall mass transfer is accomplished through diffusion and reaction kinetics due to the chemistry given in equ. (1). The reaction kinetics parameters can be estimated by fitting models which have mixed kinetics when there is no diffusional influence on mass transfer. The work is usually done in a Lewis-type mass transfer cell with constant plane interfacial area. The kinetics domain can be found when increased turbulence in the bulk phase minimises the diffusional contribution to the interfacial initial zinc flux. Such experiments have been carried out in a Nitsch-type cell (Nitsch 1989). A chemical kinetics model of Cianetti and Danesi (1983) was adopted (Klocker et al. 1997) with the following rate-determining equations:

$$Zn^{2+} + 2\,(RH)_{ad} \xleftrightarrow{k_{v,1},\,k_{r,1}} (ZnR_2)_{ad} + 2\,H^+ \tag{12}$$

$$(ZnR_2)_{ad} + 1.5\,\overline{R_2H_2} \xleftrightarrow{k_{v,2},\,k_{r,2}} \overline{ZnR_2(RH)} + 2\,(RH)_{ad} \tag{13}$$

The rate laws for these reactions combined with the law of Langmuir to describe the adsorption of ion exchanger molecules lead to the following mass transfer expression:

$$-\frac{d[Zn^{2+}]}{dt} = \frac{\kappa_v \cdot [\overline{R_2H_2}]^{1.5} \cdot [Zn^{2+}] - \kappa_r \cdot [H^+]^2 \cdot [ZnR_2(RH)]}{[\overline{R_2H_2}]^{1.5} + C_1 \cdot [H^+]^2} \cdot \left(\frac{\sqrt{[\overline{R_2H_2}]}}{C_2 + \sqrt{[\overline{R_2H_2}]}} \right)^2 \tag{14}$$

The complete derivation of equation (14) can be found in appendix A and in related literature (Bart 2001a). The two constants C_1, C_2 and the overall forward kinetic constant κ_v have to be determined from experimental data. With the value of κ_v known, κ_r can be calculated using the equilibrium constant $K_{1,3}$ (see equation 11):

$$\kappa_r = \frac{\kappa_v}{K_{1,3}}; \qquad K_{1,3} = 10^{-1.1863}\ \text{mol}^{1/2}\,\text{L}^{-1/2} = 2.059\ \text{mol}^{1/2}\text{m}^{-3/2} \tag{15}$$

A typical time/concentration diagram according to equ. (14) is given in Fig. 6. The model parameters for the diluents n-heptane and isododecane are in Table 7. As can be seen, the kinetic data do not depend on the diluent since there is a rather good agreement factor σ (N_E is the number of experimental data and N_P the number of adjustable parameters and σ_i denotes the experimental error) as defined as:

$$\sigma = \left[\sum_{i=1}^{N_E} \left(\frac{1}{\sigma_i^2} \left(y_i - y_{i,calc} \right)^2 \frac{1}{N_E - N_P} \right) \right]^{0.5} \tag{16}$$

Table 7: Results of simulation; experiments with low zinc concentration

experiments at low zinc concentration	κ_v [s^{-1}]	κ_r [$mol^{-1/2}m^{3/2}s^{-1}$]	C_1 [$mol^{-1/2}m^{3/2}$]	C_2 [$mol^{1/2}m^{-3/2}$]	σ
B1-B10 in isododecane	$2.3801 \cdot 10^{-4}$	$1.1559 \cdot 10^{-4}$	1.2379	0.5962	1.47
F8-F28 in n-heptane -Klocker (1996b)	$3.262 \cdot 10^{-4}$	$9.065 \cdot 10^{-5}$	1.126	0.591	1.72

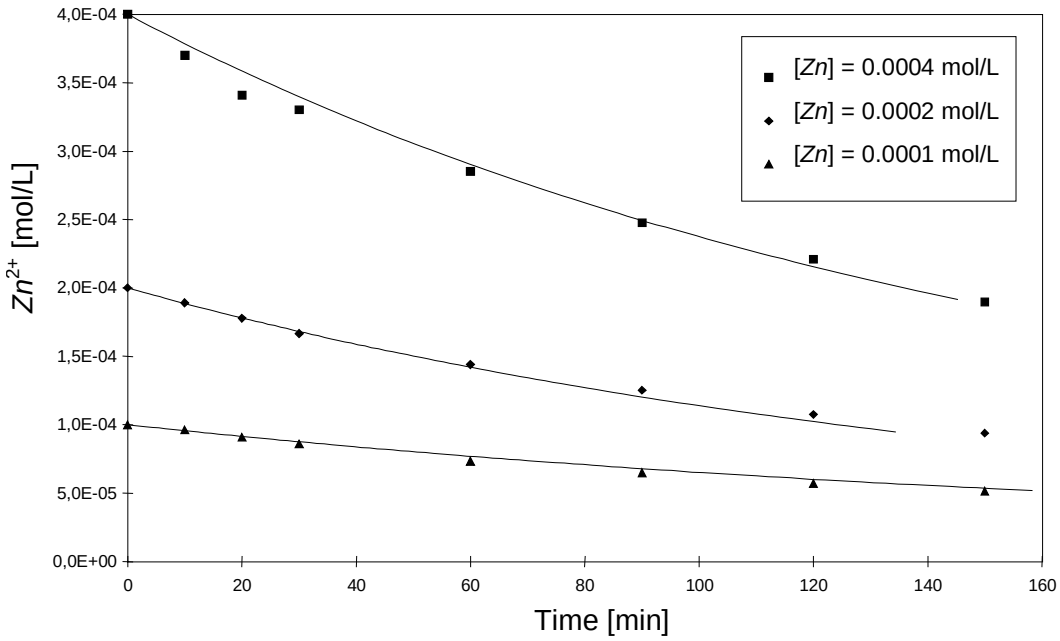

Figure 6: Concentration/time diagram with varied initial zinc concentrations (solid lines according to equ. (14))

4.2 Mass Transport

The reaction kinetics of equation (14) describe the stirred cell experiments at low zinc concentrations very well. However, for higher zinc values (≥ 0.01 mol/L), diffusional resistance has also to be considered. Here, differences due to the different viscosities of the n-heptane and isododecane system are evident. In order to calculate the mass transfer in the mixed regime (Klocker et al. 1997) or to use standard mass transfer correlations (Slater 1994) the diffusion coefficients at infinite solution needed for the aqueous phase (Newman 1991) are in Table 8. The organic ones are calculated after Wilke and Chang (1955) and the molar attraction theory of Le Bas (Reid et al. (1988), Le Bas (1915) enables the calculation of the molar volumes needed (Table 9).

Table 8: Fick diffusion coefficients of ions in aqueous solutions at infinite dilution (298 K).

ion	diffusion coefficient [m^2/s]
Zn^{2+}	$0.71 \cdot 10^{-9}$
H^+	$9.312 \cdot 10^{-9}$
SO_4^{2-}	$1.065 \cdot 10^{-9}$
HSO_4^-	$1.33 \cdot 10^{-9}$

Table 9: Diffusion coefficients after Wilke and Chang (1955)

binary system	V_1 [cm^3/mol]	M_2 [g/mol]	η_2 [mPa·s]	$D° = Đ$ [m^2/s]
R_2H_2 in Isododecane	806.4	170.34	1.2191	$4.25732 \cdot 10^{-10}$
$ZnR_2(RH)$ in Isododecane	1191.1	170.34	1.2191	$3.36898 \cdot 10^{-10}$
$ZnR_2(RH)$ in R_2H_2	1191.1	644.86	39.7	$2.014 \cdot 10^{-11}$

Effects found during the mass transfer into or out of droplets and droplet swarms also have to be considered. Whereas very small drops behave as rigid spheres with molecular diffusion controlling the mass transfer, circulation within the drop starts with rising drop diameter. For internally well-mixed large drops, molecular diffusion is not of any importance for the dispersed phase. Surface active components like the ion exchanger D2EHPA have an influence on the internal circulation of the droplets and thus on the mass transfer.

Slater (1994) gives an overview on the numerous mass transfer correlations found in literature. Simulations (Klocker et al. 1997) showed that transport resistances in the given system are mainly on the organic side in the Lewis-type mass transfer cell. Mörters (2001) came to the same conclusions with droplets and droplet swarms (Bart 2001b) which is also discussed further in detail (Mörters, Bart 2001).

The stripping reaction is not considered as suitable for test system purposes because of high concentrations of acid needed but the reaction has recently been considered in detail by Mansur et al. (2002a,b).

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Notation

A	specific interfacial area	[m²/m³]
a, b, n	stoichiometric constants	[-]
C_1	constant 1 in kinetic law	[$mol^{-1/2}m^{3/2}$]
C_2	constant 2 in kinetic law	[$mol^{1/2}m^{-3/2}$]
D	diffusion coefficient	[m²/s]
d	droplet diameter	[mm]
$K_{1,3}$	equilibrium constant	[$mol^{1/2}m^{-3/2}$]
$K_{0,1}$	equilibrium constant for dimerization of D2EHPA	[$mol^{1/2}m^{-3/2}$]
k	mass transfer coefficient	[m/s]
$k_{v,1}$	forward kinetic constant of reaction 1	[$m^6mol^{-2}s^{-1}$]
$k_{r,1}$	backward kinetic constant of reaction 1	[$m^6mol^{-2}s^{-1}$]
$k_{v,2}$	forward kinetic constant of reaction 2	[$m^{4.5}mol^{-3/2}s^{-1}$]
$k_{r,2}$	backward kinetic constant of reaction 2	[$m^6mol^{-2}s^{-1}$]
$\tilde{M}$	molar weight	[g/mol]
S_j	Masson parameter	[-]
t	time	[s]
V_i	molar volume	[cm³/mol]
α_L	Langmuir constant	[mol/m^3]
α_i, $\beta^{(i)}$, C^ϕ, ω, Θ, Ψ	Pitzer parameter	[-]
γ_L	Langmuir constant	[mol/m³]
γ_i	activity coefficient	[-]
δ	solubility parameter	[$cal^{1/2}cm^{-2/3}$]
Φ^V	molecular volume	[cm³/mol]
η	dynamic viscosity	[mPas]
κ_r	overall backward reaction kinetic constant	[$m^{3/2}mol^{-1/2}s^{-1}$]
κ_v	overall forward reaction kinetic constant	[s^{-1}]
ν	viscosity	[mm²/s]
ρ	density	[kg/m³]
σ	interfacial tension	[mN/m]

Subscripts

0	initial
ad	adsorbed
aqu	aqueous
d	dispersed phase
org	organic
*	equilibrium

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Appendix A: Development of the Kinetic Model

The kinetic model is based on the assumption that the following two reaction steps are rate-determining:

reaction 1: $$Zn^{2+} + 2(RH)_{ad} \xleftrightarrow{k_{v,1},k_{r,1}} (ZnR_2)_{ad} + 2H^+ \qquad (A.1)$$

reaction 2: $$(ZnR_2)_{ad} + 1.5\overline{R_2H_2} \xleftrightarrow{k_{v,2},k_{r,2}} \overline{ZnR_2(RH)} + 2(RH)_{ad} \qquad (A.2)$$

The rate law for reaction 1 is:

$$-\frac{d[Zn^{2+}]}{dt} = k_{v,1} \cdot [Zn^{2+}] \cdot [(RH)_{ad}]^2 - k_{r,1} \cdot [(ZnR_2)_{ad}] \cdot [H^+]^2 \qquad (A.3)$$

The rate law for reaction 2 is:

$$-\frac{d[(ZnR_2)_{ad}]}{dt} = k_{v,2} \cdot [(ZnR_2)_{ad}] \cdot [\overline{R_2H_2}]^{1.5} - k_{r,2} \cdot [\overline{ZnR_2(RH)}] \cdot [(RH)_{ad}]^2 - \\ - k_{v,1} \cdot [Zn^{2+}] \cdot [(RH)_{ad}]^2 + k_{r,1} \cdot [(ZnR_2)_{ad}] \cdot [H^+]^2 \qquad (A.4)$$

With the assumption that the interfacial zinc complex is adsorbed quasistationary:

$$-\frac{d[(ZnR_2)_{ad}]}{dt} = 0 \qquad (A.5)$$

equations (A.3) to (A.5) lead to:

$$-\frac{d[Zn^{2+}]}{dt} = [(RH)_{ad}]^2 \cdot \frac{k_{v,1} \cdot [Zn^{2+}] \cdot [\overline{R_2H_2}]^{1.5} - \frac{k_{r,1} \cdot k_{r,2}}{k_{v,2}} \cdot [H^+]^2 \cdot [ZnR_2(RH)]}{[\overline{R_2H_2}]^{1.5} + \frac{k_{r,1}}{k_{v,2}} \cdot [H^+]^2} \qquad (A.6)$$

$(RH)_{ad}$ can be described with the law of Langmuir:

$$[(RH)_{ad}] = \frac{\alpha_L \cdot \frac{[\overline{RH}]}{\gamma_L}}{1 + \frac{[\overline{RH}]}{\gamma_L}} \qquad (A.7)$$

The equilibrium of the dimerisation reaction of monomeric D2EHPA-molecules

$$\frac{1}{2}[\overline{R_2H_2}] \leftrightarrow \overline{RH} \qquad \text{with equilibrium constant } K_{0,1} \qquad (A.8)$$

leads to:

$$[\overline{RH}] = K_{0,1} \cdot [\overline{R_2H_2}]^{0.5} \quad \text{(A.9)}$$

With the introduction of the constant

$$C_2 = \frac{\gamma_L}{K_{0,1}} \quad \text{(A.10)}$$

equations (A.7) and (A.9) can be written as

$$[(RH)_{ad}] = \alpha_L \frac{[\overline{R_2H_2}]^{0.5}}{C_2 + [\overline{R_2H_2}]^{0.5}} \quad \text{(A.11)}$$

After the introduction of the constant

$$C_1 = \frac{k_{r,1}}{k_{v,2}} \quad \text{(A.12)}$$

and the two overall reaction kinetic constants

$$\kappa_v = \alpha_L^2 \cdot k_{v,1} \quad \text{(A.13)}$$

and

$$\kappa_r = \alpha_L^2 \cdot \frac{k_{r,1} \cdot k_{r,2}}{k_{v,2}} \quad \text{(A.14)}$$

which are connected via the equilibrium constant

$$K_{1,3} = \frac{\kappa_v}{\kappa_r} \quad \text{(A.15)}$$

the combination of equations (A.6) and (A.11) leads to the mass transfer expression

$$-\frac{d[Zn^{2+}]}{dt} = \frac{\kappa_v \cdot [\overline{R_2H_2}]^{1.5} \cdot [Zn^{2+}] - \kappa_r \cdot [H^+]^2 \cdot [ZnR_2(RH)]}{[\overline{R_2H_2}]^{1.5} + C_1 \cdot [H^+]^2} \cdot \left(\frac{\sqrt{[\overline{R_2H_2}]}}{C2 + \sqrt{[\overline{R_2H_2}]}} \right)^2 \quad \text{(A.16)}$$

Appendix B: Equilibrium Data and Physical Properties (Density, Dynamic Viscosity and Interfacial Tension)

$[ZnSO_4]$	$[H_2SO_4]$	[D2EHPA]	$[Na_2SO_4]$	T	$[ZnSO_4]_{aq}$	$[Zn]_{org.}$	$density_{org}$	$density_{aq}$	$viscosity_{org}$	$viscosity_{aq}$	$pH\text{-}value_{aq}$	σ
mol/L	mol/L	mol/L	mol/L	K	mol/L	mol/L	$10^3 kg/m^3$	$10^3 kg/m^3$	mm^2/s	mm^2/s	-	mN/m
start	start	start	start	-	eq.[1]	eq.	eq.	eq.	eq.	eq.	eq.	eq.
0.0001	0	0.005	0	298	8.2569E-07	9.9174E-05	0.74582	0.9972	1.607	0.897	3.66	25.56
0.0001	0	0.01	0	298	4.7401E-07	9.9526E-05	0.74613	0.99733	1.598	0.889	3.64	25.28
0.0001	0	0.015	0	298	2.3300E-07	9.9767E-05	0.74667	0.99733	1.650	0.950	3.59	24.98
0.0001	0	0.02	0	298	1.0200E-07	9.9898E-05	0.74694	0.99734	1.630	0.950	3.58	24.43
0.0001	0	0.03	0	298	5.7430E-08	9.9943E-05	0.7476	0.99729	1.679	0.950	3.62	23.52
0.0001	0	0.04	0	298	2.4400E-08	9.9976E-05	0.74839	0.99735	1.673	0.950	3.58	23.16
0.0001	0	0.06	0	298	1.0000E-08	9.9990E-05	0.74988	0.99731	1.702	0.939	3.50	21.50
0.0001	0	0.1	0	298	1.0000E-08	9.9990E-05	0.75281	0.99712	1.722	0.941	3.41	20.24
0.0001	0	0.2	0	298	1.0000E-08	9.9990E-05	0.76063	0.99745	1.814	0.939	3.32	15.41
0.005	0	0.005	0	298	3.9653E-03	1.0347E-03	0.74576	0.99797	1.644	0.951	2.78	28.96
0.005	0	0.01	0	298	3.0988E-03	1.9012E-03	0.74629	0.998	1.647	0.976	2.53	27.55
0.005	0	0.015	0	298	2.4057E-03	2.5943E-03	0.74668	0.99791	1.669	0.964	2.42	26.60
0.005	0	0.02	0	298	1.9776E-03	3.0224E-03	0.74711	0.99789	1.675	0.963	2.35	26.19
0.005	0	0.03	0	298	1.2895E-03	3.7105E-03	0.74778	0.99772	1.677	0.961	2.27	25.07
0.005	0	0.04	0	298	9.3782E-04	4.0622E-03	0.74865	0.99778	1.689	0.958	2.22	24.72
0.005	0	0.06	0	298	5.0968E-04	4.4903E-03	0.75016	0.99782	1.710	0.957	2.17	24.19
0.005	0	0.1	0	298	1.8502E-04	4.8150E-03	0.75324	0.99756	1.748	0.949	2.19	22.42
0.005	0	0.2	0	298	4.0775E-04	4.5923E-03	0.76093	0.9978	1.861	0.942	2.20	20.65
0.05	0	0.005	0	298	4.9847E-02	1.5291E-04	0.74593	1.00501	1.646	0.998	2.76	28.76
0.05	0	0.01	0	298	4.5872E-02	4.1284E-03	0.74639	1.00503	1.636	0.922	2.55	27.99
0.05	0	0.015	0	298	4.4750E-02	5.2497E-03	0.74689	1.00486	1.610	0.926	2.41	28.07
0.05	0	0.02	0	298	4.2712E-02	7.2885E-03	0.74728	1.00482	1.616	0.977	2.30	27.96
0.05	0	0.03	0	298	4.2508E-02	7.4924E-03	0.74807	1.00479	1.770	0.940	2.12	26.89
0.05	0	0.04	0	298	4.0673E-02	9.3272E-03	0.74898	1.00464	1.680	0.970	2.05	25.20
0.05	0	0.06	0	298	3.8226E-02	1.1774E-02	0.75076	1.00448	1.702	0.963	1.86	24.49
0.05	0	0.1	0	298	3.4251E-02	1.5749E-02	0.75433	1.00382	1.739	0.957	1.73	23.20
0.05	0	0.2	0	298	2.4363E-02	2.5637E-02	0.7623	1.0031	1.849	0.989	1.57	19.84
0.0001	0.0005	0.005	0	298	1.7533E-05	8.2467E-05	0.74574	0.9973	1.644	0.940	2.96	27.05

$[ZnSO_4]$	$[H_2SO_4]$	[D2EHPA]	$[Na_2SO_4]$	T	$[ZnSO_4]_{aq}$	$[Zn]_{org.}$	$density_{org}$	$density_{aq}$	$viscosity_{org}$	$viscosity_{aq}$	$pH\text{-}value_{aq}$	σ
mol/L	mol/L	mol/L	mol/L	K	mol/L	mol/L	$10^3 kg/m^3$	$10^3 kg/m^3$	mm^2/s	mm^2/s	-	mN/m
start	start	start	start	-	eq.	eq.	eq.	eq.	eq.	eq.	eq.	eq.
0.0001	0.0005	0.02	0	298	2.4465E-06	9.7554E-05	0.74692	0.99737	1.659	0.941	2.95	22.57
0.0001	0.0005	0.05	0	298	2.2426E-06	9.7757E-05	0.74928	0.99746	1.676	0.935	2.94	22.43
0.0001	0.0005	0.1	0	298	6.1162E-08	9.9939E-05	0.75276	0.99705	1.725	0.857	3.00	20.04
0.0001	0.0005	0.2	0	298	2.0387E-08	9.9980E-05	0.76026	0.99732	1.807	0.850	2.93	18.95
0.005	0.0005	0.005	0	298	4.1081E-03	8.9195E-04	0.74592	0.99821	1.597	0.849	2.60	27.92
0.005	0.0005	0.02	0	298	2.3547E-03	2.6453E-03	0.74707	0.99801	1.655	0.956	2.31	24.74
0.005	0.0005	0.05	0	298	9.2762E-04	4.0724E-03	0.74936	0.99786	1.674	0.939	2.15	23.59
0.005	0.0005	0.1	0	298	7.9511E-04	4.2049E-03	0.75313	0.99783	1.725	0.944	2.11	22.26
0.005	0.0005	0.2	0	298	1.4271E-04	4.8573E-03	0.76056	0.99786	1.837	0.940	2.20	19.94
0.05	0.0005	0.005	0	298	5.0765E-02	0.0000E+00	0.74584	1.00567	1.643	0.957	2.79	29.05
0.05	0.0005	0.02	0	298	4.6585E-02	3.4149E-03	0.74725	1.00525	1.636	0.959	2.33	27.57
0.05	0.0005	0.05	0	298	3.9653E-02	1.0347E-02	0.74975	1.00447	1.645	0.967	1.98	25.80
0.05	0.0005	0.1	0	298	3.2212E-02	1.7788E-02	0.75405	1.00385	1.739	0.997	1.76	23.67
0.05	0.0005	0.2	0	298	2.3445E-02	2.6555E-02	0.76203	1.00303	1.845	0.952	1.59	21.89
0.0001	0.001	0.005	0	298	4.4037E-05	5.5963E-05	0.74572	0.99735	1.647	0.950	2.72	28.50
0.0001	0.001	0.02	0	298	6.7278E-06	9.3272E-05	0.74691	0.99749	1.657	0.950	2.71	25.84
0.0001	0.001	0.05	0	298	3.0581E-06	9.6942E-05	0.74908	0.99752	1.677	0.945	2.68	22.91
0.0001	0.001	0.1	0	298	2.9052E-06	9.7095E-05	0.75361	0.99752	1.755	0.908	2.71	21.20
0.0001	0.001	0.2	0	298	2.6504E-06	9.7350E-05	0.76027	0.99757	1.849	0.897	2.73	19.59
0.005	0.001	0.005	0	298	4.3323E-03	6.6769E-04	0.74593	0.99826	1.634	0.894	2.55	28.79
0.005	0.001	0.02	0	298	2.6606E-03	2.3394E-03	0.74705	0.99806	1.695	0.957	2.29	25.26
0.005	0.001	0.05	0	298	1.0092E-03	3.9908E-03	0.74937	0.99793	1.690	0.961	2.13	24.22
0.005	0.001	0.1	0	298	2.9052E-04	4.7095E-03	0.75311	0.9979	1.771	0.963	2.08	22.37
0.005	0.001	0.2	0	298	1.2844E-04	4.8716E-03	0.76051	0.9979	1.865	0.966	2.12	19.93
0.05	0.001	0.005	0	298	5.2701E-02	0.0000E+00	0.74602	1.00564	1.645	0.983	2.67	29.62
0.05	0.001	0.02	0	298	4.8471E-02	1.5291E-03	0.74725	1.00526	1.653	0.972	2.23	27.83
0.05	0.001	0.05	0	298	4.0979E-02	9.0214E-03	0.7498	1.0046	1.717	0.990	1.92	25.18
0.05	0.001	0.1	0	298	3.3435E-02	1.6565E-02	0.75405	1.00395	1.764	0.983	1.73	23.56
0.05	0.001	0.2	0	298	2.9256E-02	2.0744E-02	0.7621	1.00313	1.852	0.986	1.55	21.70
0.0001	0.01	0.005	0	298	1.0418E-04	0.0000E+00	0.7458	0.99819	1.647	0.957	1.81	29.71
0.0001	0.01	0.02	0	298	1.0291E-04	0.0000E+00	0.74677	0.99805	1.674	0.971	1.88	25.68
0.0001	0.01	0.05	0	298	4.9694E-05	5.0306E-05	0.74908	0.99815	1.685	0.957	1.86	23.72

$[ZnSO_4]$	$[H_2SO_4]$	[D2EHPA]	$[Na_2SO_4]$	T	$[ZnSO_4]_{aq}$	$[Zn]_{org.}$	$density_{org}$	$density_{aq}$	$viscosity_{org}$	$viscosity_{aq}$	$pH\text{-}value_{aq}$	σ
mol/L	mol/L	mol/L	mol/L	K	mol/L	mol/L	$10^3kg/m^3$	$10^3kg/m^3$	mm^2/s	mm^2/s	-	mN/m
start	start	start	start	-	eq.[1]	eq.	eq.	eq.	eq.	eq.	eq.	eq.
0.0001	0.01	0.1	0	298	2.4924E-05	7.5076E-05	0.7528	0.9982	1.725	0.948	1.87	21.99
0.0001	0.01	0.2	0	298	1.0550E-05	8.9450E-05	0.76026	0.99816	1.867	0.908	1.88	20.62
0.005	0.01	0.005	0	298	5.0856E-03	0.0000E+00	0.74583	0.9989	1.646	0.911	1.88	29.21
0.005	0.01	0.02	0	298	4.4037E-03	5.9633E-04	0.74697	0.99888	1.623	0.904	1.85	26.41
0.005	0.01	0.05	0	298	2.9893E-03	2.0107E-03	0.7492	0.99872	1.694	0.968	1.82	24.25
0.005	0.01	0.1	0	298	1.6922E-03	3.3078E-03	0.75302	0.99866	1.741	0.964	1.77	22.37
0.005	0.01	0.2	0	298	9.5821E-04	4.0418E-03	0.76044	0.99859	1.841	0.957	1.74	20.31
0.05	0.01	0.005	0	298	5.0357E-02	0.0000E+00	0.74584	1.00625	1.644	0.975	2.02	29.14
0.05	0.01	0.02	0	298	4.8318E-02	1.6820E-03	0.74708	1.00594	1.666	0.987	1.92	27.11
0.05	0.01	0.05	0	298	4.2202E-02	7.7982E-03	0.74954	1.00545	1.690	0.986	1.76	25.11
0.05	0.01	0.1	0	298	3.5168E-02	1.4832E-02	0.75355	1.0048	1.742	0.978	1.62	23.37
0.05	0.01	0.2	0	298	2.7523E-02	2.2477E-02	0.76099	1.004	1.844	0.975	1.49	21.57
0.05	0.0005	0.1	0.1	298	3.0071E-02	1.9929E-02	0.7575	1.01557	1.764	0.956	1.94	23.73
0.05	0.0005	0.1	0.2	298	2.9460E-02	2.0540E-02	0.75359	1.02732	1.748	1.001	2.04	23.51
0.05	0.0005	0.1	0.5	298	2.7217E-02	2.2783E-02	0.75383	1.06305	1.760	1.076	2.18	22.79
0.05	0.0005	0.1	1	298	2.6198E-02	2.3802E-02	0.75364	1.12016	1.764	1.381	2.31	21.79
0.05	0.0005	0.1	1.5	298	2.6096E-02	2.3904E-02	0.75399	1.17354	1.766	1.681	2.39	21.64
0.05	0.0005	0.1	2	298	2.5994E-02	2.4006E-02	0.75376	1.22631	1.767	2.113	2.42	21.60
0	0.0005	0	0	283	0.0000E+00	0.0000E+00	0.76202	1.00394	2.125	1.416	3.00	40.09
0.05	0.0005	0	0	283	5.0765E-02	0.0000E+00	0.76185	1.01238	2.124	1.461	3.30	39.68
0	0.0005	0.2	0	283	0.0000E+00	0.0000E+00	0.77726	1.00398	2.422	1.425	3.05	18.69
0.05	0.0005	0.2	0	283	2.3344E-02	2.6656E-02	0.77884	1.00962	2.444	1.458	1.65	19.81
0	0.0005	0	0	293	0.0000E+00	0.0000E+00	0.74823	0.99658	1.650	0.912	3.01	41.71
0.05	0.0005	0	0	293	5.0968E-02	0.0000E+00	0.7448	1.00443	1.785	1.120	3.29	37.80
0	0.0005	0.2	0	293	0.0000E+00	0.0000E+00	0.75891	0.99613	2.013	1.087	3.03	19.60
0.05	0.0005	0.2	0	293	1.5902E-02	3.4098E-02	0.76002	1.00166	2.024	1.113	1.56	21.21
0	0.0005	0	0	303	0.0000E+00	0.0000E+00	0.7411	0.99566	1.554	0.891	3.12	40.19
0.05	0.0005	0	0	303	5.1784E-02	0.0000E+00	0.74111	1.00393	1.552	0.912	3.41	34.37
0	0.0005	0.2	0	303	0.0000E+00	0.0000E+00	0.75513	0.99432	1.720	0.888	2.99	19.92
0.05	0.0005	0.2	0	303	2.4363E-02	2.5637E-02	0.75704	1.00096	1.740	0.899	1.68	22.11
0	0.0005	0	1	283	0.0000E+00	0.0000E+00	0.77009	1.12262	2.125	1.325	3.99	42.87
0.05	0.0005	0	1	283	4.9439E-02	5.6065E-04	0.76359	1.1327	2.145	2.059	3.97	39.92

$[ZnSO_4]$	$[H_2SO_4]$	[D2EHPA]	$[Na_2SO_4]$	T	$[ZnSO_4]_{aq}$	$[Zn]_{org.}$	$density_{org}$	$density_{aq}$	$viscosity_{org}$	$viscosity_{aq}$	$pH\text{-}value_{aq}$	σ
mol/L	Mol/L	mol/L	mol/L	K	mol/L	mol/L	$10^3 kg/m^3$	$10^3 kg/m^3$	mm^2/s	mm^2/s	-	mN/m
start	Start	start	start	-	eq.	eq.	eq.	eq.	eq.	eq.	eq.	eq.
0	0.0005	0.2	1	283	0.0000E+00	0.0000E+00	0.76872	1.12015	2.448	1.880	3.10	23.54
0.05	0.0005	0.2	1	283	1.5545E-02	3.4455E-02	0.77031	1.12047	2.459	1.908	2.17	18.64
0	0.0005	0	1	293	0.0000E+00	0.0000E+00	0.74847	1.11735	1.798	1.548	3.97	36.63
0.05	0.0005	0	1	293	5.1274E-02	0.0000E+00	0.7484	1.12474	1.794	1.589	3.91	42.41
0	0.0005	0.2	1	293	0.0000E+00	0.0000E+00	0.76272	1.11564	2.035	1.512	3.10	23.55
0.05	0.0005	0.2	1	293	1.7125E-02	3.2875E-02	0.76478	1.11991	2.049	1.536	2.12	19.15
0	0.0005	0	1	303	0.0000E+00	0.0000E+00	0.74143	1.10905	1.543	1.227	3.98	26.99
0.05	0.0005	0	1	303	5.0255E-02	0.0000E+00	0.74113	1.11916	1.546	1.256	3.94	37.14
0	0.0005	0.2	1	303	0.0000E+00	0.0000E+00	0.75555	1.11236	1.728	1.209	3.10	19.26
0.05	0.0005	0.2	1	303	1.4781E-02	3.5219E-02	0.75776	1.11537	1.741	1.249	2.09	20.32

[1] eq .... equilibrium

Appendix C: Kinetics Data (298 K)

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
0	2.01E-06	2.00E-04	0.00E+00	0.01	0.0007	0.001
600	1.79E-06	1.89E-04	1.08E-05			
1200	1.61E-06	1.78E-04	2.22E-05			
1800	1.45E-06	1.67E-04	3.32E-05			
3600	1.10E-06	1.44E-04	5.61E-05			
5400	8.58E-07	1.25E-04	7.48E-05			
7200	6.90E-07	1.08E-04	9.24E-05			
9000	5.66E-07	9.38E-05	1.06E-04			
0	4.01E-06	4.00E-04	0.00E+00	0.01	0.0009	0.001
600	3.52E-06	3.70E-04	3.00E-05			
1200	3.10E-06	3.41E-04	5.90E-05			
1800	2.76E-06	3.30E-04	6.97E-05			
3600	2.02E-06	2.85E-04	1.15E-04			
5400	1.54E-06	2.48E-04	1.52E-04			
7200	1.21E-06	2.21E-04	1.79E-04			
9000	9.76E-07	1.90E-04	2.10E-04			
0	1.02E-06	1.00E-04	0.00E+00	0.01	0.0011	0.002
600	8.95E-07	9.62E-05	3.77E-06			
1200	7.95E-07	9.05E-05	9.48E-06			
1800	7.11E-07	8.58E-05	1.42E-05			
3600	5.26E-07	7.32E-05	2.68E-05			
5400	4.04E-07	6.46E-05	3.54E-05			
7200	3.21E-07	5.71E-05	4.29E-05			
9000	2.60E-07	5.14E-05	4.86E-05			
0	9.96E-07	1.00E-04	0.00E+00	0.01	0.0016	0.003
600	8.06E-07	9.38E-05	6.22E-06			
1200	6.65E-07	8.89E-05	1.11E-05			
1800	5.59E-07	8.50E-05	1.50E-05			
3600	3.57E-07	7.58E-05	2.42E-05			
5400	2.48E-07	7.01E-05	2.99E-05			
7200	1.82E-07	6.59E-05	3.41E-05			
9000	1.39E-07	6.28E-05	3.72E-05			
0	3.59E-07	1.04E-04	0.00E+00	0.01	0.002104	0.004
600	3.47E-07	1.02E-04	1.66E-06			
1200	3.36E-07	1.01E-04	3.29E-06			
1800	3.26E-07	9.81E-05	5.94E-06			
3600	2.96E-07	9.05E-05	1.35E-05			
5400	2.71E-07	8.69E-05	1.72E-05			
7200	2.49E-07	7.99E-05	2.41E-05			
9000	2.29E-07	7.56E-05	2.84E-05			
0	3.38E-07	1.00E-04	0.00E+00	0.002	0.0006	0.001
600	3.16E-07	9.89E-05	1.12E-06			
1200	2.97E-07	9.68E-05	3.16E-06			

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
1800	2.79E-07	9.44E-05	5.61E-06			
3600	2.34E-07	9.05E-05	9.48E-06			
5400	1.99E-07	8.56E-05	1.44E-05			
7200	1.71E-07	8.13E-05	1.87E-05			
9000	1.49E-07	7.87E-05	2.13E-05			
0	5.20E-07	1.00E-04	0.00E+00	0.003	0.0006	0.001
600	4.92E-07	9.77E-05	2.35E-06			
1200	4.67E-07	9.44E-05	5.61E-06			
1800	4.43E-07	9.19E-05	8.05E-06			
3600	3.83E-07	8.22E-05	1.78E-05			
5400	3.34E-07	7.69E-05	2.31E-05			
7200	2.93E-07	6.95E-05	3.05E-05			
9000	2.60E-07	6.48E-05	3.52E-05			
0	8.04E-07	1.00E-04	0.00E+00	0.004	0.0006	0.001
600	7.28E-07	9.42E-05	5.81E-06			
1200	6.62E-07	9.01E-05	9.89E-06			
1800	6.05E-07	8.50E-05	1.50E-05			
3600	4.72E-07	7.48E-05	2.52E-05			
5400	3.78E-07	6.63E-05	3.37E-05			
7200	3.10E-07	5.95E-05	4.05E-05			
9000	2.58E-07	5.44E-05	4.56E-05			
0	1.05E-06	1.00E-04	0.00E+00	0.006	0.0006	0.001
600	9.36E-07	9.30E-05	7.03E-06			
1200	8.37E-07	8.62E-05	1.38E-05			
1800	7.52E-07	8.18E-05	1.82E-05			
3600	5.63E-07	6.99E-05	3.01E-05			
5400	4.38E-07	5.89E-05	4.11E-05			
7200	3.50E-07	5.04E-05	4.96E-05			
9000	2.86E-07	4.46E-05	5.54E-05			
0	1.76E-06	1.00E-04	0.00E+00	0.02	0.0006	0.001
600	1.44E-06	9.22E-05	7.85E-06			
1200	1.19E-06	8.44E-05	1.56E-05			
1800	1.01E-06	7.40E-05	2.60E-05			
3600	6.49E-07	6.14E-05	3.86E-05			
5400	4.53E-07	5.10E-05	4.90E-05			
7200	3.34E-07	4.06E-05	5.94E-05			
9000	2.56E-07	3.53E-05	6.47E-05			
0	7.15E-05	5.00E-03	0.00E+00	0.06	0.007	0.004
600	5.79E-05	4.32E-03	6.78E-04			
1200	4.78E-05	3.92E-03	1.08E-03			
1800	4.02E-05	3.71E-03	1.29E-03			
3600	2.57E-05	3.04E-03	1.96E-03			
5400	1.78E-05	2.64E-03	2.36E-03			
7200	1.31E-05	2.28E-03	2.72E-03			
9000	1.00E-05	2.07E-03	2.93E-03			

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
0	2.50E-05	5.00E-03	0.00E+00	0.06	0.008	0.006
600	2.37E-05	4.67E-03	3.31E-04			
1200	2.26E-05	4.54E-03	4.64E-04			
1800	2.15E-05	4.35E-03	6.47E-04			
3600	1.87E-05	4.00E-03	1.00E-03			
5400	1.64E-05	3.59E-03	1.41E-03			
7200	1.45E-05	3.32E-03	1.68E-03			
9000	1.29E-05	3.07E-03	1.93E-03			
0	4.93E-05	5.00E-03	0.00E+00	0.06	0.009	0.008
600	4.12E-05	4.43E-03	5.66E-04			
1200	3.49E-05	4.21E-03	7.90E-04			
1800	2.99E-05	3.95E-03	1.06E-03			
3600	2.01E-05	3.47E-03	1.53E-03			
5400	1.44E-05	3.17E-03	1.83E-03			
7200	1.08E-05	2.94E-03	2.06E-03			
9000	8.43E-06	2.67E-03	2.33E-03			
0	2.55E-05	5.00E-03	0.00E+00	0.06	0.011	0.012
600	2.35E-05	4.61E-03	3.93E-04			
1200	2.17E-05	4.48E-03	5.25E-04			
1800	2.01E-05	4.33E-03	6.68E-04			
3600	1.62E-05	3.91E-03	1.09E-03			
5400	1.34E-05	3.70E-03	1.30E-03			
7200	1.12E-05	3.43E-03	1.57E-03			
9000	9.54E-06	3.23E-03	1.77E-03			
0	2.83E-05	5.00E-03	0.00E+00	0.06	0.015	0.02
600	2.36E-05	4.66E-03	3.42E-04			
1200	2.00E-05	4.52E-03	4.84E-04			
1800	1.72E-05	4.36E-03	6.37E-04			
3600	1.15E-05	4.14E-03	8.61E-04			
5400	8.24E-06	3.95E-03	1.06E-03			
7200	6.19E-06	3.78E-03	1.22E-03			
9000	4.82E-06	3.62E-03	1.38E-03			
0	1.59E-05	5.00E-03	0.00E+00	0.006	0.0055	0.001
600	1.20E-05	4.77E-03	2.29E-04			
1200	9.32E-06	4.69E-03	3.11E-04			
1800	7.46E-06	4.63E-03	3.72E-04			
3600	4.31E-06	4.56E-03	4.43E-04			
5400	2.80E-06	4.49E-03	5.15E-04			
7200	1.97E-06	4.41E-03	5.86E-04			
9000	1.46E-06	4.33E-03	6.68E-04			
0	5.36E-05	5.00E-03	0.00E+00	0.01	0.0055	0.001
600	3.56E-05	4.78E-03	2.19E-04			
1200	2.54E-05	4.59E-03	4.13E-04			
1800	1.90E-05	4.40E-03	5.96E-04			
3600	9.63E-06	4.21E-03	7.90E-04			
5400	5.80E-06	4.02E-03	9.84E-04			

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
7200	3.88E-06	3.92E-03	1.08E-03			
9000	2.77E-06	3.83E-03	1.17E-03			
0	2.97E-05	5.00E-03	0.00E+00	0.015	0.0055	0.001
600	2.48E-05	4.76E-03	2.40E-04			
1200	2.11E-05	4.53E-03	4.74E-04			
1800	1.81E-05	4.51E-03	4.94E-04			
3600	1.22E-05	4.20E-03	8.00E-04			
5400	8.78E-06	3.99E-03	1.01E-03			
7200	6.61E-06	3.84E-03	1.16E-03			
9000	5.16E-06	3.63E-03	1.37E-03			
0	4.95E-05	5.00E-03	0.00E+00	0.02	0.0055	0.001
600	3.79E-05	4.51E-03	4.94E-04			
1200	2.99E-05	4.26E-03	7.39E-04			
1800	2.42E-05	4.09E-03	9.12E-04			
3600	1.43E-05	3.77E-03	1.23E-03			
5400	9.43E-06	3.53E-03	1.47E-03			
7200	6.68E-06	3.34E-03	1.66E-03			
9000	4.98E-06	3.17E-03	1.83E-03			
0	7.10E-05	5.00E-03	0.00E+00	0.03	0.0055	0.001
600	5.27E-05	4.45E-03	5.45E-04			
1200	4.07E-05	4.09E-03	9.12E-04			
1800	3.24E-05	3.89E-03	1.11E-03			
3600	1.85E-05	3.49E-03	1.51E-03			
5400	1.19E-05	3.16E-03	1.84E-03			
7200	8.31E-06	2.90E-03	2.11E-03			
9000	6.13E-06	2.70E-03	2.30E-03			
0	7.48E-05	5.00E-03	0.00E+00	0.04	0.0055	0.001
600	5.91E-05	4.30E-03	6.98E-04			
1200	4.79E-05	3.93E-03	1.07E-03			
1800	3.96E-05	3.63E-03	1.37E-03			
3600	2.45E-05	3.08E-03	1.92E-03			
5400	1.66E-05	2.71E-03	2.29E-03			
7200	1.20E-05	2.28E-03	2.72E-03			
9000	9.08E-06	2.12E-03	2.88E-03			
0	6.15E-05	5.00E-03	0.00E+00	0.06	0.0055	0.001
600	5.12E-05	4.37E-03	6.27E-04			
1200	4.33E-05	4.06E-03	9.43E-04			
1800	3.71E-05	3.80E-03	1.20E-03			
3600	2.48E-05	3.16E-03	1.84E-03			
5400	1.77E-05	2.82E-03	2.18E-03			
7200	1.33E-05	2.48E-03	2.52E-03			
9000	1.03E-05	2.21E-03	2.79E-03			
0	8.15E-05	5.00E-03	0.00E+00	0.1	0.0055	0.001
600	6.59E-05	4.33E-03	6.68E-04			
1200	5.45E-05	3.89E-03	1.11E-03			

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
1800	4.57E-05	3.62E-03	1.38E-03			
3600	2.92E-05	2.88E-03	2.12E-03			
5400	2.03E-05	2.44E-03	2.56E-03			
7200	1.49E-05	2.00E-03	3.00E-03			
9000	1.14E-05	1.76E-03	3.24E-03			
0	4.95E-04	5.00E-02	0.00E+00	0.1	0.0525	0.005
600	3.33E-04	4.70E-02	3.01E-03			
1200	2.39E-04	4.54E-02	4.64E-03			
1800	1.80E-04	4.32E-02	6.78E-03			
3600	9.22E-05	4.10E-02	9.02E-03			
5400	5.59E-05	4.05E-02	9.53E-03			
7200	3.75E-05	3.86E-02	1.14E-02			
9000	2.68E-05	3.80E-02	1.20E-02			
0	1.92E-04	5.00E-02	0.00E+00	0.1	0.055	0.01
600	1.72E-04	4.84E-02	1.58E-03			
1200	1.56E-04	4.79E-02	2.09E-03			
1800	1.42E-04	4.68E-02	3.21E-03			
3600	1.09E-04	4.43E-02	5.66E-03			
5400	8.62E-05	4.32E-02	6.78E-03			
7200	7.00E-05	4.08E-02	9.23E-03			
9000	5.79E-05	4.00E-02	1.00E-02			
0	1.83E-04	5.00E-02	0.00E+00	0.1	0.06	0.02
600	1.54E-04	4.84E-02	1.58E-03			
1200	1.31E-04	4.75E-02	2.50E-03			
1800	1.13E-04	4.69E-02	3.11E-03			
3600	7.66E-05	4.39E-02	6.07E-03			
5400	5.53E-05	4.33E-02	6.68E-03			
7200	4.18E-05	4.26E-02	7.39E-03			
9000	3.27E-05	4.23E-02	7.70E-03			
0	1.07E-03	5.00E-02	0.00E+00	0.06	0.051	0.002
600	3.51E-04	4.60E-02	4.03E-03			
1200	1.72E-04	4.40E-02	5.96E-03			
1800	1.02E-04	4.37E-02	6.27E-03			
3600	3.57E-05	4.27E-02	7.29E-03			
5400	1.80E-05	4.22E-02	7.80E-03			
7200	1.08E-05	4.02E-02	9.84E-03			
9000	7.21E-06	4.13E-02	8.72E-03			
0	5.42E-04	5.00E-02	0.00E+00	0.1	0.051	0.002
600	3.72E-04	4.44E-02	5.56E-03			
1200	2.71E-04	4.38E-02	6.17E-03			
1800	2.06E-04	4.28E-02	7.19E-03			
3600	1.08E-04	4.05E-02	9.53E-03			
5400	6.62E-05	3.81E-02	1.19E-02			
7200	4.47E-05	3.66E-02	1.34E-02			
9000	3.22E-05	3.63E-02	1.37E-02			

117	molar flow rate	$[Zn^{2+}]_{aq}$	$[Zn^{2+}]_{org}$	[D2EHPA]	$[SO_4^{2-}]$	$[H^+]$
s	$mmol/m^2s$	mol/L	mol/L	mol/L	mol/L	mol/L
0	4.72E-04	5.00E-02	0.00E+00	0.2	0.051	0.002
600	3.90E-04	4.41E-02	5.86E-03			
1200	3.27E-04	4.14E-02	8.61E-03			
1800	2.79E-04	4.01E-02	9.94E-03			
3600	1.84E-04	3.50E-02	1.50E-02			
5400	1.30E-04	3.25E-02	1.75E-02			
7200	9.69E-05	2.99E-02	2.01E-02			
9000	7.50E-05	2.80E-02	2.20E-02			