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APPENDICES

Appendix A Equilibrium Time Determination

Table A.1 Mercury concentration as a function of time

Time			Hg (ppb)	
Hour	Min	Total (min)	Methylcyclohexane	Toluene
0	0	0	0	0
1	0	60	187.4	-
1	0	60	184.1	146.28
1	25	85	-	187.35
3	0	180	175.42	212.69
3	0	180	-	229.84
10	0	600	147.24	-
10	0	600	128.79	-
12	0	720	161.25	241.45
12	0	720	-	211.83
15	0	900	196.03	199.75
15	0	900	175.71	230.86
18	0	1080	-	210.84
20	4	1204	171.82	-
23	0	1380	-	248.62
24	15	1455	189.23	-
24	50	1490	200.32	-
25	10	1510	175.36	-
25	27	1527	179.31	-
25	45	1545	-	202.85
26	0	1560	-	223.48
26	24	1584	-	227.65
26	42	1602	-	213.52

Table A.1 (Cont'd)

Time			Hg (ppb)	
Hour	Min	Total (min)	Methylcyclohexane	Toluene
28	5	1685	194.6	-
35	20	2120	-	208.22
44	45	2685	195.21	-

Appendix B Solubility Study of Single Solvent and Simulated Crude Oil

Table B.1 Mercury solubility data in hydrocarbons at 5°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
Cyclohexane	-	-	-	-	-	-
Methylcyclohexane	189.23	175.36	179.31	181.30	7.15	3.94
Toluene	223.48	227.65	244.30	248.73	7.26	3.28
o-Xylene	256.41	245.47	244.30	248.73	6.68	2.69
Ethylbenzene	-	-	-	-	-	-

Table B.2 Mercury solubility data in hydrocarbons at 15°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
Cyclohexane	809.45	842.45	864.59	838.36	27.75	3.31
Methylcyclohexane	347.77	349.58	349.57	348.97	1.04	0.30
Toluene	313.03	339.90	324.49	325.81	13.48	4.14
o-Xylene	335.53	331.09	351.99	339.54	11.011	3.24
Ethylbenzene	-	-	-	-	-	-

Table B.3 Mercury solubility data in hydrocarbons at 25°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	% CV
Cyclohexane	1386.67	1392.67	1301.58	1360.31	50.95	3.75
Methylcyclohexane	780.31	744.49	764.52	763.11	17.95	2.35
Toluene	829.12	836.23	827.26	830.37	4.73	0.57
o-Xylene	916.83	949.44	901.63	922.63	24.43	2.65
Ethylbenzene	-	-	-	-	-	-

Table B.3 Mercury solubility data in hydrocarbons at 40°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	% CV
Cyclohexane	2437.56	2610.21	2450.95	2499.57	96.05	3.84
Methylcyclohexane	1796.08	1748.85	1724.15	1756.36	36.55	2.08
Toluene	1878.32	1853.32	1833.49	1855.04	22.46	1.21
o-Xylene	2262.62	2283.73	2210.52	2252.29	37.68	1.67
Ethylbenzene	-	-	-	-	-	-

Table B.5 Mercury solubility data in simulated crude oil at various temperatures

Temperature (°C)	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
5	248.00	245.62	232.72	242.11	8.22	3.40
15	270.45	280.45	274.45	275.12	5.03	1.83
25	526.72	524.44	520.53	523.90	3.13	0.60
40	1424.97	1472.70	1505.09	1467.59	40.30	2.75

Appendix C Hysteresis Study on Single Solvent and Simulated Crude Oil

Table C.1 Hysteresis data on hydrocarbons at 5°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
Cyclohexane	-	-	-	-	-	-
Methylcyclohexane	178.68	199.29	188.66	188.88	10.31	5.46
Toluene	262.79	236.75	244.50	248.01	13.37	5.39
o-Xylene	246.59	246.78	247.38	246.98	0.40	0.16
Ethylbenzene	-	-	-	-	-	-

Table C.2 Hysteresis data on hydrocarbons at 15°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
Cyclohexane	902.39	947.82	930.33	926.85	22.91	2.47
Methylcyclohexane	366.10	374.15	349.24	363.16	12.71	3.50
Toluene	338.82	327.78	348.83	338.48	10.53	3.11
o-Xylene	481.35	495.01	473.06	483.14	11.08	2.29
Ethylbenzene	-	-	-	-	-	-

Table C.3 Hysteresis data on hydrocarbons at 25°C

Solvent	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	% CV
Cyclohexane	1281.75	1277.58	1314.93	1291.42	20.47	1.58
Methylcyclohexane	820.91	860.03	895.83	858.68	37.84	4.41
Toluene	1000.84	1085.54	1046.43	1044.27	42.39	4.06
o-Xylene	1005.94	1043.54	943.36	997.61	50.61	5.07
Ethylbenzene	-	-	-	-	-	-

Table C4 Hysteresis data on simulated crude oil at various temperatures

Temperature (°C)	Mercury concentration (ppb)					
	R1	R2	R3	\bar{X}	SD	%CV
5	269.91	283.68	264.22	272.60	10.01	3.67
15	382.69	349.55	339.33	357.19	22.67	6.35
25	391.03	393.73	373.26	386.01	11.12	2.88

Appendix D The Assumption of Hysteresis Manner in PathwayII

The 10% variation of mercury solubility in single solvent systems and simulated crude oil was shown at each temperature both increasing and decreasing temperature.

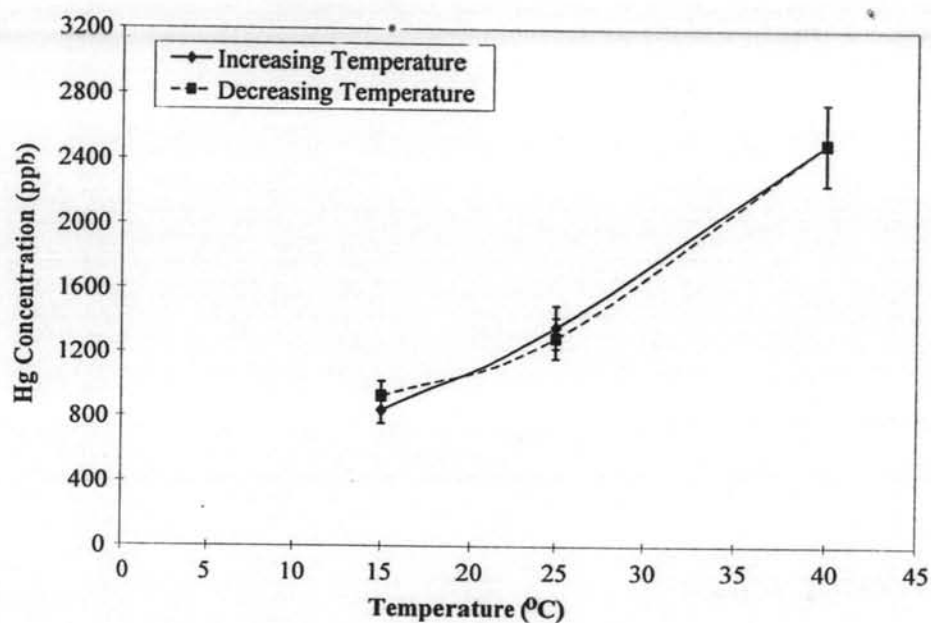


Figure D1 Hysteresis study in cyclohexane at the temperature range of 5-40°C.

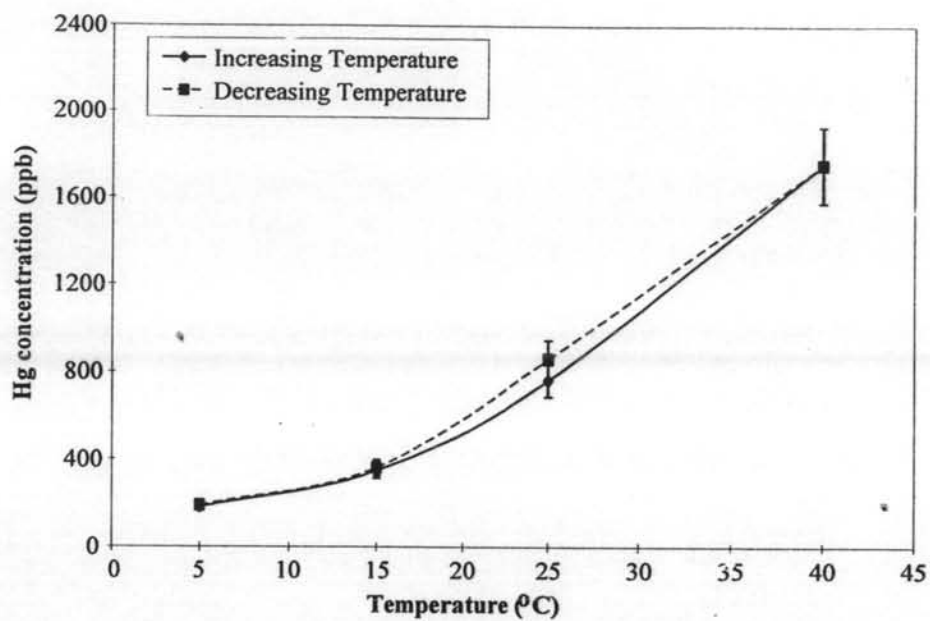


Figure D2 Hysteresis study in methylcyclohexane at the temperature range of 5-40°C.

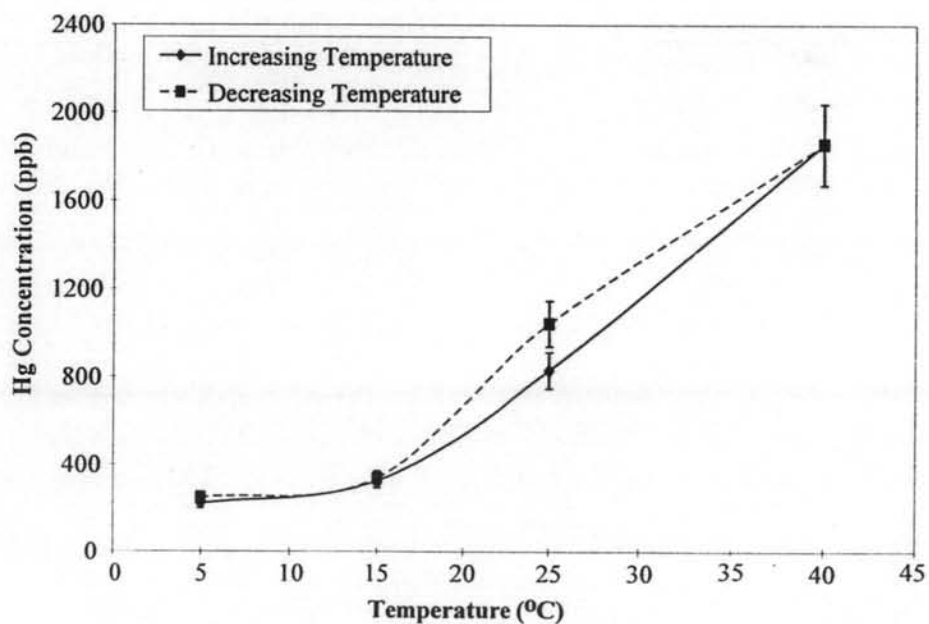


Figure D3 Hysteresis study in toluene at the temperature range of 5-40°C.

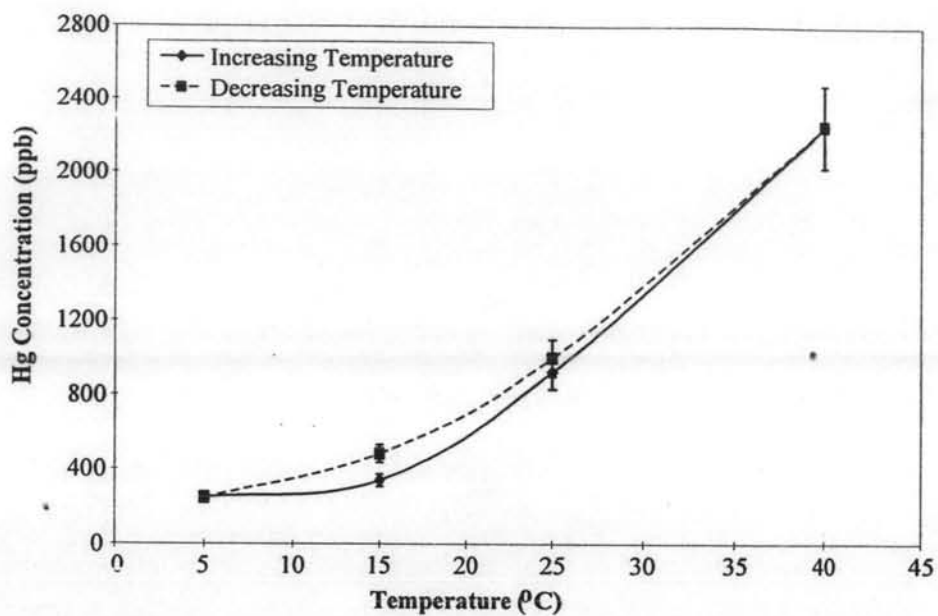


Figure D4 Hysteresis study in *o*-xylene at the temperature range of 5-40°C.

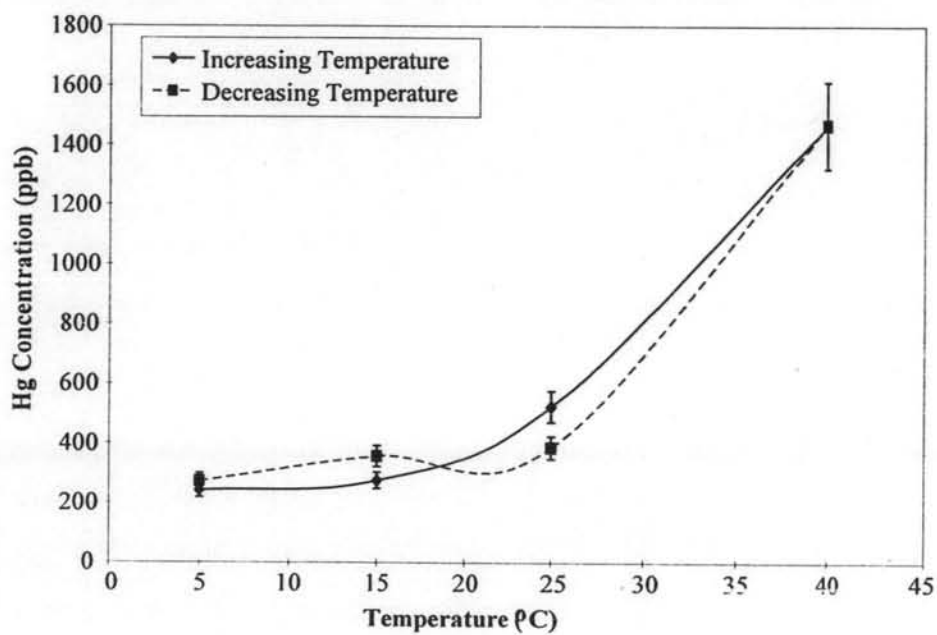


Figure D5 Hysteresis study in simulated crude oil at the temperature range of 5-40°C.

Appendix E Certificate of Analysis in Ethylbenzene



SIGMA-ALDRICH

Certificate of Analysis

Product Name	Ethylbenzene, purum $\geq 98.0\%$ (GC)
Product Number	03082
Product Brand	Fluka
CAS Number	100-41-4
Molecular Formula	C_8H_{10}
Molecular Weight	106.17

TEST

APPEARANCE (COLOUR)

APPEARANCE (FORM)

ASSAY (GC AREA %)

DENSITY D20/4

REFRACTIVE INDEX N20/D

NMR SPECTRUM 1H

DATE OF QC-RELEASE

LOT 454440/1 RESULTS

COLOURLESS

CLEAR LIQUID

99.9 % REL

0.867

1.496

CORRESPONDS

14/AUG/03

Fluka guarantees the 'Sales-Specification' values only, non-specified tests may be included as additional information. The current 'Sales-Specifications' sheet is available on request. For further inquiries, please contact our Technical Service. Fluka warrants, that its products conform to the information contained in this and other Fluka publications. Purchaser must determine the suitability of the product for its particular use. See reverse side of invoice for additional terms and conditions of sale. The values given on the 'Certificate of Analysis' are the results determined at the time of analysis.

Dr. Gert van Look, Manager
Quality Control
Buchs Switzerland

Figure E1 The certificate analysis on ethylbenzene.

Appendix F Calculation Note of Simulated Crude Oil at Increasing Temperature

According to equation 4.1: $[Hg]_{cal, sim\ crude\ oil} = \sum X_i [Hg]_{i, exp\ value}$

Where $[Hg]_{cal, sim\ crude\ oil}$ = the calculated mercury solubility in the simulated crude oil

X_i = mole fraction of mercury solubility in single solvent i

$[Hg]_{i, exp\ value}$ = mercury solubility of single solvent i (mole fraction)

Basis 100 g of simulated crude oil.

- Finding molecular weight of simulated crude oil.

Component	% wt	MW	Mole	Mole fraction (Xi)	MW*Xi
n-pentane	2.98	72.15	0.041	0.055	3.942
n-hexane	1.84	86.18	0.021	0.028	2.434
cyclohexane	1.39	84.16	0.017	0.022	1.839
n-heptane	1.90	100.2	0.019	0.025	2.514
methylcyclohexane	1.37	98.19	0.014	0.018	1.812
toluene	0.43	92.14	0.005	0.006	0.569
i-octane	1.87	114.2	0.016	0.022	2.474
n-octane	1.11	114.2	0.010	0.013	1.468
o-xylene	0.38	106.2	0.004	0.005	0.503
n-Decane	86.73	142.3	0.609	0.806	114.736
Total	100.00		0.756	1	132.29

Molecular weight of simulated crude = 132.29 g/gmole

- Calculation of equation 4.1

At temperature 5°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	5.22772E-08	0.055	2.85642E-09
n-hexane	1.43062E-07	0.028	4.04078E-09
cyclohexane	#VALUE!	0.022	#VALUE!
n-heptane	6.36863E-08	0.025	1.59757E-09
methylcyclohexane	8.87474E-08	0.018	1.63809E-09
toluene	1.01768E-07	0.006	6.2829E-10
i-octane	5.53905E-08	0.022	1.19989E-09
n-octane	1.6205E-07	0.013	2.0837E-09
o-xylene	1.31685E-07	0.005	6.23342E-10
n-Decane	1.33362E-07	0.806	1.07529E-07
Total			

Cannot found because there is no solubility data of cyclohexane at this temperature.

At temperature 15°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	7.70897E-08	0.055	4.21217E-09
n-hexane	1.53966E-07	0.028	4.34876E-09
cyclohexane	3.51954E-07	0.022	7.68997E-09
n-heptane	7.95246E-08	0.025	1.99488E-09
methylcyclohexane	1.70825E-07	0.018	3.15307E-09
toluene	1.49658E-07	0.006	9.2395E-10
i-octane	9.74686E-08	0.022	2.1114E-09
n-octane	1.81769E-07	0.013	2.33726E-09
o-xylene	1.79764E-07	0.005	8.50923E-10
n-Decane	1.73438E-07	0.806	1.39842E-07
Total			1.67464E-07

At temperature 25°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	1.3975E-07	0.055	7.63591E-09
n-hexane	2.19801E-07	0.028	6.20828E-09
cyclohexane	5.70733E-07	0.022	1.24702E-08
n-heptane	2.25937E-07	0.025	5.66766E-09
methylcyclohexane	3.73545E-07	0.018	6.89487E-09
toluene	3.81656E-07	0.006	2.35625E-09
i-octane	2.05396E-07	0.022	4.44936E-09
n-octane	2.96441E-07	0.013	3.81176E-09
o-xylene	4.88477E-07	0.005	2.31224E-09
n-Decane	3.80088E-07	0.806	3.06463E-07
Total			3.58269E-07

At temperature 40°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	3.69393E-07	0.055	2.01836E-08
n-hexane	5.97941E-07	0.028	1.68888E-08
cyclohexane	1.04873E-06	0.022	2.2914E-08
n-heptane	6.07639E-07	0.025	1.52427E-08
methylcyclohexane	8.59749E-07	0.018	1.58692E-08
toluene	8.52105E-07	0.006	5.26069E-09
i-octane	5.47044E-07	0.022	1.18502E-08
n-octane	8.21618E-07	0.013	1.05647E-08
o-xylene	1.19245E-06	0.005	5.64453E-09
n-Decane	7.5896E-07	0.806	6.11946E-07
Total			7.36364E-07

Appendix G Calculation Note of Simulated Crude Oil at Decreasing Temperature

According to equation 4.1: $[Hg]_{cal, \text{ sim crude oil}} = \sum X_i [Hg]_{i, \text{ exp value}}$

Molecular weight of simulated crude = 132.29 g/gmole

At temperature 15°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	5.06046E-08	0.055	2.76503E-09
n-hexane	2.15707E-07	0.028	6.09263E-09
cyclohexane	3.8887E-07	0.022	8.49655E-09
n-heptane	1.35964E-07	0.025	3.41068E-09
methylcyclohexane	1.77771E-07	0.018	3.28128E-09
toluene	1.55478E-07	0.006	9.59881E-10
i-octane	6.5453E-08	0.022	1.41786E-09
n-octane	1.79609E-07	0.013	2.30948E-09
o-xylene	2.55793E-07	0.005	1.21081E-09
n-Decane	1.86715E-07	0.806	1.50547E-07
Total			1.80491E-07

At temperature 15°C

Component	Solubility [Hg] _i	Mole fraction (X _i)	[Hg] _i *X _i
n-pentane	1.37696E-07	0.055	7.52369E-09
n-hexane	2.68639E-07	0.028	7.5877E-09
cyclohexane	5.41831E-07	0.022	1.18387E-08
n-heptane	2.25623E-07	0.025	5.65976E-09
methylcyclohexane	4.20331E-07	0.018	7.75843E-09
toluene	4.7968E-07	0.006	2.96143E-09
i-octane	2.06733E-07	0.022	4.47831E-09
n-octane	3.15598E-07	0.013	4.05808E-09
o-xylene	5.28175E-07	0.005	2.50015E-09
n-Decane	3.75898E-07	0.806	3.03085E-07
Total			3.57451E-07

CURRICULUM VITAE

Name: Mr. Piya Kittichaichana

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