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APPENDIX A

A1) EXPERIMENTAL DATA

A 1.1 Jar test experiments

Name of substance : o-Xylenol (XLN)

Run No. 1-4

Initial Condition

Co 78.05 mg-C/l

Table A1.1-1: Adsorption Equilibrium & Isotherm Data for o-Xylenol Solution

Sample No.	ACF (mg-C/l)	Ce (mg-C/l)	Q (mg-C/g ACF)	1/Ce	1/Q	log Ce	log Q
1	306	18.09	195.94	0.0553	0.0051	1.257	2.292
2	245	25.95	212.66	0.0385	0.0047	1.414	2.328
3	205	31.74	225.92	0.0315	0.0044	1.502	2.354
4	168	40.01	226.45	0.0250	0.0044	1.602	2.355
5	120	48.38	247.24	0.0207	0.0040	1.685	2.393
6	80	57.12	261.67	0.0175	0.0038	1.757	2.418
7	45	65.49	279.12	0.0153	0.0036	1.816	2.446
8	27	70.35	285.25	0.0142	0.0035	1.847	2.455

Adsorption Isotherm Empirical Equation

Freundlich eqn. : $\log Q = 0.2736 \log Ce + 1.9396$; $R^2 = 0.9629$

Langmuir eqn. : $1/Q = 0.0385\ (1/Ce) + 0.0031$; $R^2 = 0.9545$

Name of substance : **p-Chlorophenol (PCN)**

Run No. **5-8**

Initial Condition

Co 61.21 mg-C/l (sample No.1-7)

59.87 mg-C/l (sample No.8-13)

Table A1.1-2: Adsorption Equilibrium & Isotherm Data for p-Chlorophenol Solution

Sample No.	ACF (mg/l)	Ce (mg-C/l)	Q (mg-C/g ACF)	1/Ce	1/Q	Log Ce	Log Q
1	95	1.370	62.993	0.7298	0.0159	0.137	1.799
2	88.8	1.923	66.769	0.5201	0.0150	0.284	1.825
3	58.8	6.442	93.148	0.1552	0.0107	0.809	1.969
4	50.2	8.300	105.405	0.1205	0.0095	0.919	2.023
5	44.7	12.318	109.386	0.0812	0.0091	1.091	2.039
6	26.9	20.604	150.966	0.0485	0.0066	1.314	2.179
7	20.3	29.794	154.778	0.0336	0.0065	1.474	2.190
8	24.3	26.698	136.508	0.0375	0.0073	1.426	2.135
9	17.8	31.990	156.623	0.0313	0.0064	1.505	2.195
10	13.3	38.731	158.933	0.0258	0.0063	1.588	2.201
11	9.5	43.974	167.319	0.0227	0.0060	1.643	2.224
12	4.3	52.812	164.128	0.0189	0.0061	1.723	2.215
13	3.1	54.709	166.456	0.0183	0.0060	1.738	2.221

Adsorption Isotherm Empirical Equation

Freundlich eqn. : $\log Q = 0.2807 \log Ce + 1.7555$; $R^2 = 0.9773$

Langmuir eqn. : $1/Q = 0.0355 (1/Ce) + 0.0054$; $R^2 = 0.9462$

Name of substance : **Benzoic acid (BA)**

Run No. **9-12**

Initial Condition

Co 70.80 mg-C/l

Table A1.1-3: Adsorption Equilibrium & Isotherm Data for Benzoic acid

Sample No.	ACF (mg/l)	Ce (mg-C/l)	Q (mg-C/g ACF)	1/Ce	1/Q	log Ce	log Q
1	46	61.42	203.91	0.0163	0.0049	1.788	2.309
2	103	50.04	201.55	0.0200	0.0050	1.699	2.304
3	204	38.1	160.29	0.0262	0.0062	1.581	2.205
4	410	22.11	118.76	0.0452	0.0084	1.345	2.075
5	523	16.39	104.03	0.0610	0.0096	1.215	2.017
6	610	17.41	87.52	0.0574	0.0114	1.241	1.942
7	816	8.45	76.41	0.1183	0.0131	0.927	1.883
8	1038	5.46	62.95	0.1832	0.0159	0.737	1.799

Adsorption Isotherm Empirical Equation

Freundlich eqn. : $\log Q = 0.5124 \log Ce + 1.3923$; $R^2 = 0.9603$

Langmuir eqn. : $1/Q = 0.1313 (1/Ce) + 0.0026$; $R^2 = 0.9215$

Name of substance : **Cyclohexanol (CHN)**

Run No. **13-16**

Initial Condition

Co 82.05 mg-C/l

Table A1.1-4: Adsorption Equilibrium & Isotherm Data for Cyclohexanol

Sample No.	ACF (mg/l)	Ce (mg-C/l)	Q (mg-C/g ACF)	1/Ce	1/Q	log Ce	Log Q
1	122	74.25	63.93	0.0135	0.0156	1.871	1.806
2	205	69.87	59.41	0.0143	0.0168	1.844	1.774
3	300	65.44	55.37	0.0153	0.0181	1.816	1.743
4	425	59.33	53.46	0.0169	0.0187	1.773	1.728
5	547	52.49	54.04	0.0191	0.0185	1.720	1.733
6	630	49.02	52.43	0.0204	0.0191	1.690	1.720
7	879	42.3	45.22	0.0236	0.0221	1.626	1.655
8	1066	36.71	42.53	0.0272	0.0235	1.565	1.629

Adsorption Isotherm Empirical Equation

Freundlich eqn. : $\log Q = 0.5170 \log Ce + 0.8248$; $R^2 = 0.9266$

Langmuir eqn. : $1/Q = 0.5225 (1/Ce) + 0.0092$; $R^2 = 0.9369$

A1.2 Comparison integral adsorptin equilbrium curve between Experimental and Calcualtion results

1) Single Component

Table A1.2-1: IAEC between Experimental and Calculation for XLN Solution

XLN (C_o = 11.11 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	11.11	11.11
62	5.35	4.28
128	3.47	2.47
210	2.41	2.23
338	1.64	1.82
435	1.32	1.71
591	1.00	1.68

Table A1.2-2: IAEC between Experimental and Calculation for PCN Solution

PCN (C_o = 11.06 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	11.06	11.06
42	6.88	7.13
117	4.28	3.17
232	2.77	2.89
327	2.16	2.10
446	1.70	1.79
584	1.36	1.42

Table A1.2-3: IAEC between Experimental and Calculation for BA Solution

BA (C_o = 10.95 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	10.95	10.95
67	6.87	6.71
121	5.34	4.22
203	4.01	3.48
321	2.97	2.78
422	2.43	2.54
558	1.96	2.03

Table A1.2-4: IAEC between Experimental and Calculation for CHN Solution

CHN (C_o = 11.06 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	11.06	11.06
65	9.86	10.25
113	9.13	9.27
213	7.91	8.09
330	6.85	7.00
425	6.18	5.95
518	5.65	5.05

2) Binary System

Table A1.2-5: IAEC between Experimental and Calculation for XLN+PCN Solution

XLN + PCN (C_o = 11.09 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	11.09	11.09
60	5.58	5.64
90	4.55	3.35
212	2.66	2.31
324	1.96	1.86
439	1.55	1.68
547	1.30	1.49

Table A1.2-6: IAEC between Experimental and Calculation for PCN+CHN Solution

PCN + CHN (C_o = 11.02 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	11.02	11.02
51	9.20	8.50
135	7.34	6.88
278	5.56	5.50
352	4.97	4.53
427	4.50	4.40
614	3.66	3.43

3) Tertiary System

Table A1.2-7: IAEC between Experimental and Calculation for XLN+PCN+BA Solution

XLN + PCN +BA (C_o = 10.50 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	10.50	10.50
68	5.22	4.46
127	3.74	3.08
217	2.64	2.41
317	2.01	2.14
467	1.48	1.55
560	1.28	1.40

4) Unknown Component

Table A1.2-8: IAEC between Experimental and Calculation for NHS Solution

NHS (ACFs-15) (C_o = 5.84 mg-C/l)

ACF (mg/l)	$TOC_{cal.}$ (mg-C/l)	$TOC_{exp.}$ (mg-C/l)
0	5.84	5.84
59	5.74	5.66
164	5.58	5.48
215	5.51	5.40
313	5.37	5.27
409	5.24	5.20
581	5.02	4.98

5) Industrial wastewater

Table A1.2-9: IAEC between Experimental and Calculation for an Industrial Wastewater

Oil Refinery (C_o = 20.54 mg-C/l)

ACF (mg/l)	TOCcal. (mg-C/l)	TOCexp. (mg-C/l)
0	20.54	20.54
70	19.03	19.03
163	18.61	18.61
374	15.97	15.97
428	15.58	15.58
603	15.29	15.29
713	15.22	15.22
909	14.01	14.01
1002	13.83	13.83
1375	12.35	12.35

A1.3 Comparison between the predicted and experimental breakthrough curve (Column Test)

Table A1.3-1: Breakthrough curve for XLN solution Run no. 1-4

RUN NO.1

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.18E+01	8.19E-02	2.78	0
1.35E+01	1.69E-01	5.56	0
1.51E+01	2.61E-01	8.33	0
1.68E+01	3.60E-01	11.11	0.054
1.84E+01	4.62E-01	13.33	0.112
2.00E+01	5.67E-01	15.56	0.219
2.16E+01	6.75E-01	17.78	0.582
2.32E+01	7.85E-01	20	0.701
2.48E+01	8.95E-01	22.22	0.854
2.63E+01	1.00E+00	23.61	0.95
		26.94	0.996
		27.22	1.012

RUN NO.2

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
3.56E+01	8.19E-02	8.33	0
4.05E+01	1.69E-01	16.67	0
4.55E+01	2.61E-01	25	0.04
5.04E+01	3.60E-01	33.33	0.054
5.52E+01	4.62E-01	40	0.095
6.00E+01	5.67E-01	46.67	0.157
6.48E+01	6.75E-01	50	0.22
6.96E+01	7.85E-01	53.33	0.415
7.43E+01	8.95E-01	60	0.625
7.90E+01	1.00E+00	66.67	0.7
		70.83	0.826
		80.83	0.901

RUN NO.3

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.78E+01	8.19E-02	8.33	0.002
2.03E+01	1.69E-01	16.67	0.004
2.27E+01	2.61E-01	21.67	0.088
2.52E+01	3.60E-01	22.67	0.131
2.76E+01	4.62E-01	24.33	0.215
3.00E+01	5.67E-01	30	0.487
3.24E+01	6.75E-01	35	0.693
3.48E+01	7.85E-01	42.67	0.896
3.72E+01	8.95E-01	43.67	0.906
3.95E+01	1.00E+00	46.67	0.99
		50	0.998
		53.33	1.009

RUN NO.4

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.78E+01	8.19E-02	8.33	0.002
2.03E+01	1.69E-01	16.67	0.005
2.27E+01	2.61E-01	20	0.078
2.52E+01	3.60E-01	21.67	0.148
2.76E+01	4.62E-01	23.33	0.301
3.00E+01	5.67E-01	25	0.392
3.24E+01	6.75E-01	30	0.501
3.48E+01	7.85E-01	35	0.726
3.72E+01	8.95E-01	41.67	0.908
3.95E+01	1.00E+00	43.67	0.987
		46.67	0.996
		50	1.011
		53.33	1.009

Table A1.3-2: Breakthrough curve for PCN solution Run no. 5-8

RUN NO.5

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
7.01E+00	6.59E-02	0.56	0
8.63E+00	1.42E-01	2.22	0
1.03E+01	2.28E-01	5	0.055
1.19E+01	3.22E-01	7.22	0.088
1.35E+01	4.24E-01	7.78	0.149
1.51E+01	5.32E-01	11.11	0.205
1.67E+01	6.45E-01	13.33	0.571
1.83E+01	7.62E-01	14.44	0.686
1.98E+01	8.82E-01	15.56	0.864
2.14E+01	1.00E+00	16.67	0.916
		18.44	1.021

RUN NO.6

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
2.10E+01	6.59E-02	1.67	0
2.59E+01	1.42E-01	8.33	0
3.08E+01	2.28E-01	16.67	0
3.57E+01	3.22E-01	25	0.088
4.05E+01	4.24E-01	36.67	0.258
4.53E+01	5.32E-01	38.33	0.455
5.01E+01	6.45E-01	40	0.671
5.48E+01	7.62E-01	45	0.868
5.96E+01	8.82E-01	50	0.903
6.43E+01	1.00E+00	51.67	0.973
		56.67	0.997
		60	1.014

RUN NO.7

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.05E+01	6.59E-02	1.67	0
1.30E+01	1.42E-01	5	0
1.54E+01	2.28E-01	13.33	0.107
1.78E+01	3.22E-01	15	0.175
2.03E+01	4.24E-01	16.67	0.293
2.27E+01	5.32E-01	18.33	0.389
2.51E+01	6.45E-01	21.67	0.619
2.74E+01	7.62E-01	26.67	0.805
2.98E+01	8.82E-01	28.33	0.835
3.22E+01	1.00E+00	33.33	0.906
		38.33	0.989
		40	1.015

RUN NO.8

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.05E+01	6.59E-02	1.67	0
1.30E+01	1.42E-01	8.33	0
1.54E+01	2.28E-01	13.33	0.114
1.78E+01	3.22E-01	15	0.162
2.02E+01	4.24E-01	16.67	0.383
2.26E+01	5.32E-01	18.33	0.625
2.50E+01	6.45E-01	20	0.759
2.74E+01	7.62E-01	21.67	0.807
2.98E+01	8.82E-01	25	0.907
		30	0.942
		33.33	0.995

Table A1.3-3: Breakthrough curve for BA solution Run no. 9-12

RUN NO.9

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
3.80E+00	5.99E-02	0.28	0
5.09E+00	1.33E-01	0.56	0
6.38E+00	2.18E-01	1.11	0
7.67E+00	3.13E-01	3.33	0
8.95E+00	4.16E-01	5.78	0.086
1.02E+01	5.26E-01	9.44	0.21
1.15E+01	6.41E-01	10	0.42
1.28E+01	7.60E-01	11.11	0.676
1.41E+01	8.80E-01	13.33	0.96
1.53E+01	1.00E+00	14.44	1.019
		15.56	1.011

RUN NO.10

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.14E+01	5.99E-02	0.83	0
1.53E+01	1.33E-01	1.67	0
1.92E+01	2.18E-01	3.33	0
2.30E+01	3.13E-01	14	0.088
2.69E+01	4.16E-01	23.33	0.225
3.07E+01	5.26E-01	26.67	0.315
3.46E+01	6.41E-01	30	0.398
3.84E+01	7.60E-01	31.67	0.457
4.22E+01	8.80E-01	33.33	0.598
4.60E+01	1.00E+00	40	0.892
		43.33	0.951
		46.67	1.011
		50	1.024

RUN NO.11

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
5.71E+00	5.99E-02	1.67	0
7.65E+00	1.33E-01	3.33	0
9.59E+00	2.18E-01	6.67	0.077
1.15E+01	3.13E-01	10	0.184
1.34E+01	4.16E-01	13.33	0.258
1.54E+01	5.26E-01	16.67	0.553
1.73E+01	6.41E-01	18.33	0.686
1.92E+01	7.60E-01	20	0.802
2.11E+01	8.80E-01	21.67	0.94
2.30E+01	1.00E+00	23.33	1.015

RUN NO.12

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
5.70E+00	5.99E-02	1	0
7.64E+00	1.33E-01	1.67	0
9.58E+00	2.18E-01	3.33	0
1.15E+01	3.13E-01	6.67	0.085
1.34E+01	4.16E-01	8.33	0.16
1.54E+01	5.26E-01	10	0.165
1.73E+01	6.41E-01	13.33	0.295
1.92E+01	7.60E-01	16.67	0.61
2.11E+01	8.80E-01	18.33	0.768
2.30E+01	1.00E+00	20	0.989
		21.67	1.024
		23.33	1.019

Table A1.3-4: Breakthrough curve for CHN solution Run no. 13-16

RUN NO.13

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.39E+00	8.07E-02	0.11	0
1.53E+00	1.67E-01	0.22	0
1.68E+00	2.58E-01	0.56	0
1.83E+00	3.54E-01	1.11	0
1.98E+00	4.53E-01	1.67	0.136
2.13E+00	5.57E-01	2	0.404
2.28E+00	6.64E-01	2.22	0.698
2.43E+00	7.74E-01	2.78	0.99
2.58E+00	8.86E-01	3	1.004
2.73E+00	1.00E+00	3.33	1.051

RUN NO.14

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
4.16E+00	8.07E-02	0.33	0
4.61E+00	1.67E-01	0.67	0
5.06E+00	2.58E-01	1.67	0
5.50E+00	3.54E-01	3.33	0
5.95E+00	4.53E-01	4	0
6.40E+00	5.57E-01	4.8	0.125
6.85E+00	6.64E-01	6	0.358
7.29E+00	7.74E-01	6.67	0.62
7.74E+00	8.86E-01	8.33	0.854
8.19E+00	1.00E+00	9	0.901
		10	0.92
		11	0.998
		11.67	1.003

RUN NO.15

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
2.09E+00	8.07E-02	0.33	0
2.31E+00	1.67E-01	1	0
2.54E+00	2.58E-01	1.33	0
2.76E+00	3.54E-01	1.67	0.177
2.99E+00	4.53E-01	2	0.315
3.21E+00	5.57E-01	2.67	0.556
3.43E+00	6.64E-01	3.33	0.807
3.66E+00	7.74E-01	4	0.84
3.88E+00	8.86E-01	5	0.982
4.10E+00	1.00E+00	5.67	1.019

RUN NO.16

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
2.08E+00	8.07E-02	0.33	0
2.30E+00	1.67E-01	1	0
2.53E+00	2.58E-01	1.33	0
2.75E+00	3.54E-01	1.67	0
2.98E+00	4.53E-01	2	0
3.20E+00	5.57E-01	2.67	0.194
3.42E+00	6.64E-01	3.33	0.557
3.65E+00	7.74E-01	4	0.91
3.87E+00	8.86E-01	5	1.032
4.09E+00	1.00E+00	5.67	1.056

Table A1.3-5: Breakthrough curve for XLN+PCN solution Run no. 17-18

RUN NO.17

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
1.68E+00	2.67E-02	2.78	0
5.02E+00	7.47E-02	5.56	0
8.35E+00	1.42E-01	8.89	0
1.17E+01	2.28E-01	11.11	0.21
1.49E+01	3.31E-01	12.22	0.48
1.82E+01	4.47E-01	13.33	0.63
2.14E+01	5.76E-01	14.44	0.76
2.46E+01	7.14E-01	15.56	0.79
2.78E+01	8.57E-01	16.67	0.82
3.10E+01	1.00E+00	17.78	0.85
		18.89	0.93
		21.11	0.98
		23.33	0.99
		25.56	0.96
		26.67	1
		27.78	1.03

RUN NO.18

Prediction		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
8.44E-01	2.67E-02	0.56	0
2.52E+00	7.47E-02	1.67	0.01
4.18E+00	1.42E-01	3.33	0.1
5.83E+00	2.28E-01	5.67	0.26
7.48E+00	3.31E-01	6.22	0.51
9.10E+00	4.47E-01	7.89	0.78
1.07E+01	5.76E-01	9	0.82
1.23E+01	7.14E-01	12.89	0.92
1.39E+01	8.57E-01	14.56	0.93
1.55E+01	1.00E+00	16.22	0.94
		16.78	0.99
		17.89	1

Table A1.3-6: Breakthrough curve for PCN+CHN solution Run no. 19-20

RUN NO.19				RUN NO.20			
Prediction		**Experiment**		**Prediction**		**Experiment**	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
4.30E-01	4.82E-02	1.11	0.06	2.19E-01	4.82E-02	0.56	0.02
1.19E+00	1.09E-01	1.67	0.07	5.98E-01	1.09E-01	1	0.14
1.94E+00	1.82E-01	2.22	0.1	9.75E-01	1.82E-01	1.56	0.45
2.70E+00	2.68E-01	2.78	0.53	1.35E+00	2.68E-01	2.11	0.56
3.45E+00	3.65E-01	3.33	0.6	1.73E+00	3.65E-01	2.67	0.61
4.19E+00	4.73E-01	5	0.61	2.10E+00	4.73E-01	3.22	0.61
4.93E+00	5.92E-01	6.67	0.62	2.47E+00	5.92E-01	4.89	0.62
5.67E+00	7.21E-01	8.33	0.62	2.84E+00	7.21E-01	6.56	0.62
6.40E+00	8.58E-01	9.44	0.62	3.20E+00	8.58E-01	8.22	0.7
7.13E+00	1.00E+00	11.67	0.62	3.57E+00	1.00E+00	9.33	0.73
		13.33	0.62			11.56	0.95
		15	0.63			14.89	0.96
		16.67	0.69			16.56	0.96
		17.22	0.73			17.11	0.97
		18.33	0.81			18.22	0.97
		20	0.86			19.89	0.98
		21.67	0.9			21.56	0.99
		23.33	0.94			23.22	1.01
		25	1			24.89	1

Table A1.3-7: Breakthrough curve for XLN+PCN+BA solution Run no. 21-22

Run no.21				Run no.22			
Predict		**Experimental**		**Predict**		**Experimental**	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
2.05	0.03	3.33	0	1.02E+00	3.26E-02	1.11	0
6.11	0.09	5	0	3.04E+00	8.55E-02	3.33	0
10.16	0.16	6.67	0	5.05E+00	1.57E-01	4.44	0.13
14.19	0.25	8.33	0	7.06E+00	2.45E-01	5	0.27
18.19	0.35	10	0.16	9.05E+00	3.49E-01	6.11	0.69
22.17	0.46	11.67	0.51	1.10E+01	4.65E-01	6.67	0.75
26.12	0.59	13.33	0.78	1.30E+01	5.91E-01	8.33	0.89
30.04	0.72	15	0.89	1.49E+01	7.24E-01	10	0.95
33.93	0.86	16.67	0.94	1.69E+01	8.62E-01	11.67	1
37.79	1.00	21.11	0.98	1.88E+01	1.00E+00	13.33	1.01
		22.22	1.01			13.89	1.02
		23.33	1.02				

Table A1.3-8: Breakthrough curve for NHS solution ..Run no. 24-27

(on ACFs-15)

Run No.24

Predict		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.19	0.093	0.25	0.71
0.199	0.19	1.00	0.84
0.2	0.29	2.50	0.89
0.21	0.39	5.00	0.91
0.22	0.49	7.50	0.92
0.223	0.6	8.50	0.97
0.23	0.7	10.00	0.97
0.24	0.82	15.00	0.96
0.242	0.95	20.00	0.99
0.25	1	25.00	0.97
		30.00	0.99
		35.00	0.98
		40.00	1.00
		40.50	0.98
		41.00	0.99
		41.75	0.99

Run No.25

Predict		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.93	0.093	0.25	0.77
0.96	0.19	0.50	0.86
0.99	0.29	1.00	0.84
1.02	0.39	2.00	0.86
1.05	0.49	2.50	0.97
1.08	0.6	3.50	0.98
1.11	0.7		
1.14	0.82		
1.17	0.95		
1.2	1		

Run No.26

Predict		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.31	0.093	0.08	0.74
0.32	0.19	0.17	0.78
0.33	0.29	0.33	0.83
0.34	0.39	0.50	0.90
0.35	0.49	1.00	0.92
0.36	0.6	1.67	0.94
0.37	0.7	2.00	0.97
0.38	0.82	2.33	1.00
0.39	0.95	2.83	1.01
0.4	1		

Run No.27

Predict		Experiment	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.19	0.093	0.05	0.74
0.195	0.19	0.10	0.89
0.2	0.29	0.20	0.90
0.205	0.39	0.50	0.93
0.21	0.49	0.70	0.94
0.22	0.6	1.00	0.96
0.225	0.7	1.20	1.00
0.23	0.82	1.60	1.01
0.24	0.95	1.80	1.01
0.245	1	2.00	1.01

Table A1.3-9: Breakthrough curve for an industrial wastewater Run no. 30-33

Run No.30

Experiment		Predict	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.028	0.414	0.021	0.053
0.100	0.599	0.035	0.127
0.183	0.627	0.049	0.218
0.267	0.713	0.063	0.321
0.356	0.720	0.076	0.434
0.444	0.728	0.090	0.553
0.528	0.752	0.104	0.672
0.694	0.779	0.118	0.789
0.861	0.837	0.131	0.900
1.083	0.924	0.145	1.000
1.639	0.935		
2.194	0.944		

Run No.31

Experiment		Predict	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.028	0.440	0.041	0.053
0.083	0.463	0.067	0.127
0.139	0.486	0.092	0.218
0.194	0.501	0.118	0.321
0.306	0.518	0.144	0.434
0.528	0.575	0.170	0.553
0.694	0.584	0.196	0.672
0.861	0.626	0.221	0.789
1.389	0.657	0.247	0.900
1.556	0.789	0.273	1.000
1.889	0.880		
1.944	0.950		
2.167	0.991		
2.389	0.965		

Run No.32

Experiment		Predict	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.028	0.419	0.073	0.053
0.083	0.445	0.123	0.127
0.167	0.499	0.173	0.218
0.306	0.516	0.224	0.321
0.472	0.528	0.274	0.434
0.639	0.601	0.324	0.553
0.806	0.616	0.374	0.672
0.972	0.633	0.425	0.789
1.139	0.650	0.475	0.900
1.306	0.757	0.525	1.000
1.639	0.795		
2.194	0.960		
2.778	1.005		

Run No.33

Experiment		Predict	
Time (hr.)	C/Co (-)	Time (hr.)	C/Co (-)
0.028	0.451	0.082	0.053
0.083	0.458	0.134	0.127
0.139	0.483	0.185	0.218
0.194	0.483	0.237	0.321
0.306	0.518	0.289	0.434
0.528	0.569	0.341	0.553
0.694	0.577	0.393	0.672
0.861	0.654	0.444	0.789
1.483	0.665	0.496	0.900
1.567	0.674	0.548	1.000
1.863	0.778		
1.913	0.873		
2.167	0.942		
2.383	0.965		

Table 1.3-10 Breakthrough curve for NHS .. Run No.28-29

(on ACFs-20)

Run No. 28		Run No. 29	
Time (hr.)	C/Co	Time (hr.)	C/Co
0.25	0.804	0.25	0.85
0.5	0.815	0.5	0.88
1	0.891	1	0.89
2	0.902	2	0.91
4	0.905	4	1.01
6	0.909	6	1.02
8	0.953	8	1
12	1.004	12	1.01

Table 1.3-11 Breakthrough curve for Tapwater.. Run No. 23

Run No.23	
Time (hr.)	C/Co
0.25	0.835
0.5	0.856
1	0.892
2	0.901
4	0.952
6	1.002
8	1.001
12	1.003

A1.4 : Estimated breakthrough characteristics (mass transfer zone)

Case 1 : Bed density = 0.159 g/cc, Q = 3 ml/min.

ACF 0.2 gm., Column dia = 0.4 cm , Bed length = 10 cm.

	Nof	1/Kfav (min)	V (cm/min)	Za (cm.)	E-Time (min.)	T-eff (hr.)
XLN	2.732	0.042	0.009	**0.001**	0.114	18.14
PCN	2.759	0.042	0.014	**0.002**	0.116	12.07
CHN	4.494	0.042	0.067	**0.013**	0.188	2.47

Case 2 : Bed density = 0.159 g/cc, Q = 1 ml/min.

ACF 0.2 gm., Column dia = 0.4 cm , Bed length = 10 cm.

	Nof	1/Kfav (min)	V (cm/min)	Za (cm.)	E-Time (min.)	T-eff (hr.)
XLN	2.732	0.126	0.003	**0.001**	0.343	54.41
PCN	2.759	0.126	0.005	**0.002**	0.347	36.21
CHN	4.494	0.126	0.022	**0.013**	0.565	7.40

Case 3 : Bed density = 0.080 g/cc, Q = 1 ml/min.

ACF 0.1 gm., Column dia = 0.4 cm , Bed length = 10 cm.

	Nof	1/Kfav (min)	V (cm/min)	Za (cm.)	E-Time (min.)	T-eff (hr.)
XLN	2.732	0.269	0.006	**0.004**	0.736	27.37
PCN	2.759	0.269	0.009	**0.007**	0.743	18.21
CHN	4.494	0.269	0.044	**0.054**	1.211	3.72

Case 4 : Bed density = 0.159 g/cc, Q = 1 ml/min.

ACF 0.1 gm., Column dia = 0.4 cm , Bed length = 5 cm.

	Nof	1/Kfav (min)	V (cm/min)	Za (cm.)	E-Time (min.)	T-eff (hr.)
XLN	2.732	0.126	0.003	**0.001**	0.344	27.20
PCN	2.759	0.126	0.005	**0.002**	0.348	18.10
CHN	4.494	0.126	0.022	**0.013**	0.566	3.70

A2. Simulation Program

A2.1) Listing of Simulation Program of Parameter fitting method for Characteristic Distribution Curve Prediction

```
C SEKIBUN-FITTING <1-YAMA> NEW BY JUN
C NE : NUMBER OF DATA
C CT0 : INITIAL CONCENTRATION OF TOC
C AE(I) : AMOUNT OF ADSORBENT
C TOCE(I) : CONCENTRATION OF TOC
C P(I,1) : PARAMETER
C ************************************
  COMMON X(10), TOCC(50),A,Y
  COMMON NE, CT0 , EPS1, AE(50), TOCE(50)
  DIMENSION CRI(50) , P(10,14), PP(10)
  CALL DATAON
  READ(5,100) NE,CT0
  READ(5,110) (AE(I), TOCE(I), I=1,NE)
  READ(5,110) (CRI(I),P(I,1), I=1,5)
  READ(5,120) EPS1
120 FORMAT(F12.0)
100 FORMAT(I5,2F12.0)
110 FORMAT(2F12.0)
  IIN=0
  CALL SMPX(5,IIN,P,CRI,FUNCV,+1,AA,KK)
  DO 10 I=1,5
 10 PP(I) = P(I,14)
  SH1=(PP(5)**3-PP(4)**3)/3.0
  SH2=(PP(1)+PP(2)*(PP(5)**2-PP(4)**2)/2.0
  SH3=PP(1)*PP(2)*(PP(5)-PP(4))
  A=CT0/(SH1-SH2+SH3)
  WRITE(6,699)
699 FORMAT(1H1,44H* * * * * SEKIBUN-FITTING (1-YAMA) * * * * * *//)
  WRITE(6,660)A, (P(I,14) , I=1,5)
600 FORMAT(1H1,2HA=,E=15.7,3X,2HB=,E15.7,3X,2HC=,E15.7,
 C3X,2HK=,E15.7,3X,5HYMIN=,E15.7,3X,5HYMAN=,15.7/)
  ERR=0.0
  DO 20 I=1,NE
 20 ERR=ERR+ABS((1.0-TOCC(I)/TOCE(I)))
  ERR=ERR/FLOAT(NE)
  WRITE(6,610)(AE(I),TOCC(I),TOCE(I),I=1,NE)
610 FORMAT(1H0,3E15.7/)
  WRITE(6,620)ERR
620 FORMAT(1H0,5X,4HERR=,E15.7//)
  DO 40 I=1,5
 40 X(I)= P(I,14)
  W1 =1.1
  W2=0.9
  X(1) = X(1)*W1
  CALL JUN(X)
  X(1) = P(1,14)*W2
  CALL JUN(X)
  X(1) = P(1,14)
  X(2)= X(2)*W1
  CALL JUN(X)
```

```
   X(2) = P(2,14)*W2
   IF(X(2).LT.X(5)) GO TO 21
   CALL JUN(X)
   X(2) = P(2,14)
   X(3) = X(3)*W1
   CALL JUN(X)
   X(3) = P(3,14)*W2
   CALL JUN(X)
   X(3) = P(3,14)
   X(4) = X(4)*W1
   CALL JUN(X)
   X(4)= P(4,14)*W2
   CALL JUN(X)
   X(4)= P(4,14)
   X(5)= X(5)*W1
   IF(X(5).GT.X(2)) GO TO 21
   CALL JUN(X)
   X(5) = P(5,14)*W2
   CALL JUN(X)
21 STOP
   END

   SUBROUINE PERIN(N,PI,P,J,IIN)
   DIMENSION PI(14)
   DIMENSION P(10,14)
   COMMON X(10), TOCC(50),A,Y
   COMMON NE,CT0,EPS1, AE(50),TOCE(50)
   COMMON IK
   IIN = IIN+1
   X(1) = P(1,J)
   X(2) = P(2,J)
   X(3) = P(3,J)
   X(4) = P(4,J)
   X(5) = P(5,J)
   DO 12 I =2,5
12 IF(X(I).LT.O.O) GO TO 70
   IF(X(5).LT.X(4)) GO TO 70
   DO 54 I=4,5
   IF(X(I)-X(1))51,52,52
51 GO TO 70
52 IF(X(2)-X(I))53,54,54
53 GO TO 70
54 CONTINUE
   SH1 = (X(5)**3-X(4)**3)/3.0
   SH2 = (X(1)+X(2))*(X(5)**2-X(4)**2)/2.0
   SH3 = X(1)*X(2)*(X(5)-X(4))
   A= CT0/(SH1-SH2+SH3)
   IF(A.GE.0.0) GO TO 70
   SS = 0.0
   DO 20 IK=1,NE
   IX=1
   FA1=FF(TOCE(IK))
   CT2=-TOCE(IK)
   IF(FA1-1.0)5,90,3
 5 CT2=CT2-1.0
   IF(CT2.LE.0.0) GO TO 8
13 FA2 = FF(CT2)
   IF(FA2.GE.1.0)GO TO 4
```

```
      IF(FA2.GT.0.0)GO TO 5
      U1=CT2
      U2= CT2+1.0
   11 U3= (U1+U2)/2.0
      FU = FF(U3)
      IF(FU.LE.0.0)GO TO 9
      IF(FU.LT.1.0)GO TO 10
      CT2 = U3
      GO TO 4
    8 CT2 = 1.0E-5
      GO TO 13
    9 U1=U3
      GO TO 11
   10 U2 = U3
      GO TO 11
    3 CT2 = TOCE(IK)+1.0
    7 CT2 = CT2 +1.0
      FA3 = FF(CT2)
      IF(FA3.LE.1.0)GO TO 4
      GO TO 7
    4 W1 = TOCE(IK)
      W2=CT2
    1 X3=(W1+W2)/2.0
      IF(IX.GT.100)GO TO 25
      IF(ABS(W2-W1).LE.EPS1) GO TO 30
      FF1=FF(W1)-1.0
      FF2=FF(W2)-1.0
      FF3=FF(X3)-1.0
      IX=IX+1
      XA=FF1*FF3
      IF(XA.LE.0.0)GO TO 2
      W1=X3
      GO TO 1
    2 W2=X3
      GO TO 1
   25 WRUTE(6,601)
  601 FORMAT(1H0,5X,3HAHO)
   90 X3=TOCE(IK)
      GO TO 30
   30 SS =SS+(1.0-X3/TOCE(IK))**2
      TOCC(IK)=X3
   20 CONTINUE
      PI(J)=SQRT(SS/FLOAT(NE))
      ER=0.0
      DO 22 IK=1,NE
   22 ER = ER+ABS((1.0-TOCC(IK)/TOCE(IK)))
      ER=ER/FLOAT(NE)
      GO TO 71
   70 PI(J) = 1.0E+5
   71 RETURN
      END

      FUNCTION FF(W)
      COMMON X(10),TOCC(50),A,Y
      COMMON NE,CT0,ESP1,AE(50),TOCE(50)
      COMMON IK
      Y = W
      AA=AE(IK)*X(3)*Y/(1.0+X(3)*Y)
```

```
  S1=A*(X(5)**2-X(4)**2)/(2.0*AA)
  S2=A*Y*(X(5)-X(4))/(AA*2)
  S3=A*Y*Y*ALOG((AA*X(5)+Y)/(AA*X(4)+Y))/(AA**3)
  S4=-A*(X(1)+X(2))*(X(5)-X(4))/AA
  S5=A*(X(1)+X(2))*Y*ALOG((AA*X(5)+Y)/(AA*X(4)+Y))/(AA**2)
  S6=A*X(1)*X(2)*ALOG((AA*X(5)+Y)/(AA*X(4)+Y))/AA
  FF=S1-S2+S3+S4+S5+S6
  RETURN
  END

  SUBROUTINE JUN(N)
  DIMENSION PI(14)
  DIMENSION P(10,14)
  COMMON X(10),TOCC(50),A,Y
  COMMON NE,CT0,EPS1,AE(50),TOCE(50)
  COMMON IK
  SH1 =(X(5)**3-X(4)**3)/3.0
  SH2 =(X(1)+X(2))*(X(5)**2-X(4)**2)/2.0
  SH3 =X(1)*X(2)*(X(5)-X(4))
  A=CT0/(SH1-SH2+SH3)
  SS = 0.0
  DO 20 IK=1,NE
  IX=1
  FA1=FF(TOCE(IK))
  CT2=TOCE(IK)
  IF(FA1-1.0)5,90,3
5 CT2 = CT2-1.0
  IF(CT2.LE.0.0)GO TO 8
13 FA2=FF(CT2)
  IF(FA2.GE.1.0)GO TO 4
  IF(FA2.GT.0.0)GO TO 5
  U1=CT2
  U2=CT2+1.0
11 U3=(U1+U2)/2.0
  FU=FF(U3)
  IF(FU.LE.0.0)GO TO 9
  IF(FU.LT.1.0)GO TO 10
  CT2=U3
  GO TO 4
8 CT2=1.0E-5
  GO TO 13
9 U1=U3
  GO TO 11
10 U2 = U3
  GO TO 11
3 CT2=TOCE(IK)+1.0
7 CT2=CT2+1.0
  FA3=FF(CT2)
  IF(FA3.LE.1.0)GO TO 4
  GO TO 7
4 W1=TOCE(IK)
  W2=CT2
1 X3=(W1+W2)/2.0
  IF(IX.GT.100)GO TO 25
  IF(ABS(W2-W1).LE.EPS1)GO TO 30
  FF1=FF(W1)-1.0
  FF2=FF(W2)-1.0
  FF3=FF(X3)-1.0
```

```
      IX=IX+1
      XA=FF1*FF3
      IF(XA.LE.0.0)GO TO 2
      W1=X3
      GO TO 1
    2 W2=X3
      GO TO 1
   25 WRITE(6,601)
  601 FORMAT(1H0,5X,3HAHO)
   90 X3 = TOCE(IK)
      GO TO 30
   30 SS =SS+(1.0-X3/TOCE(IK))**2
      TOCC(IK)=X3
   20 CONTINUE
      ER=0.0
      DO 22 IK=1,NE
   22 ER= ER+ABS((1.0-TOCC(IK)/TOCE(IK)))
      ER=ER/FLOAT(NE)
      WRITE(6,699)
  699 FORMAT(1H1,52H* * * * SEKIBUN-FITTING <1-YAMA> 'KANDO' * * * *
     C/)
      WRITE(6,600)A,(X(I),I=1,5)
  600 FORMAT(1H1,2HA=,E15.7,3X,2HB=,E15.7,3X,2HC=,E15.7,
     C3X,2HK=,E15.7,3X,5HYMIN=,E15.7,3X,5HYMAX=,E15.7/)
      WRITE(6,610)(AE(I),TOCC(I),TOCE(I), I=1,NE)
  610 FORMAT(1H0,3E15.7)
      WRITE(6,620)ER
  620 FORMAT(1H0,5X,4HERR=,E15.7/)
   71 RETURN
      END

      SUBROUTINE SMPX(N,IIN,P,CRI,FUNCV,IND,AA,KK)
    C SIMPLEX METHOD BY J.A.NELDER AND R.MEAD
      DIMENSION P(10,14)PG(10),PI(14),CRI(10),PIS(10)
      ALPHA = 1.0
      BETA =0.5
      GAMMA = 2.0
      M=N+1
      MM = M+1
      DO 201 I=1,N
      DO 202 J=2,M
      P(I,J) = P(I,1)
  202 CONTINUE
  201 CONTINUE
      COEF = 200.0
      DO 200 I =1,N
      P(I,I+1) = P(I,1)+COEF*CRI(I)
      IF(I.EQ.3) GO TO 200
      COEF=-COEF
  200 CONTINUE
      MIND =0
      IIN=0
   10 DO 11 J=1,M
      CALL PERIN(N,PI,P,J,IIN)
   11 CONTINUE
      FM=M
   12 DO 72 I=1,N
      PG(I)=0.0
```

```
      DO 73 J=1,M
      PG(I) = PG(I)+P(I,J)
   73 CONTINUE
      PG(I) = PG(I)/FM
   72 CONTINUE
      DO 50 I=1,N
      PIS(I) = 0.0
      DO 51 J=1,M
   51 PIS(I) = PIS(I)+(P(I,J)-PG(I))**2
   50 PIS(I) = SQRT(PIS(I)/FM)
      AMAX = PI(1)
      AMIN=PI(1)
      MAX=1
      MIN=1
      DO 17 I=2,M
      IF(AMAX-PI(I))18,18,19
   18 AMAX =PI(I)
      MAX=I
   19 IF(AMIN-PI(I))17,21,21
   21 AMIN = PI(I)
      MIN = I
   17 CONTINUE
      IF(MIND-MIN)95,91,95
   95 MIND=DMIN
      IF(IND)91,90,90
   90 WRITE(6,101)
      WRITE(6,102)(P(I,MIN),I=1,N)
      WRITE(6,103)AMIN,IIN
  101 FORMAT(1H,11HTOCHU KEIKA)
  102 FORMAT(1H, 5E15.7)
  103 FORMAT(1H+,E15.7,I5)
   91 DO 53 J=1,N
      IF(PIS(J)-CRI(J))53,53,16
   53 CONTINUE
      GO TO 15
   16 DO 22 I=1,N
      PG(I)=0.0
      DO 23 J=1,M
      IF(J-MAX)24,23,24
   24 PG(I)=PG(I)+P(I,J)
   23 CONTINUE
      PG(I)=PG(I)/(FM-1.0)
   22 CONTINUE
      DO 25 I=1,N

   C REFLEXION
      P(I,MM)=(1.0+ALPHA)*PG(I)-ALPHA*P(I,MAX)
   25 CONTINUE
      CALL PERIN(N,PI,P,MM,IIN)
      IF(PI(MM)-PI(MIN))26,26,27
   27 DO 29 J=1,M
      IF(J-MAX)28,29,28
   28 IF(PI(MM)-PI(J))30,30,29
   29 CONTINUE
      IF(PI(MM)-PI(MAX))31,32,32

   C CONTRACTION
   32 DO 33 I=1,N
```

```
      P(I,MM+1)=BETA*P(I,MAX)+(1.0-BETA)*PG(I)
   33 CONTINUE
      CALL PERIN(N,PI,P,MM+1,IIN)
      IF(PI(MM+1)-PI(MAX))34,34,35

    C ADOPTION
   34 DO 36 I=1,N
      P(I,MAX) = PI(MM+1)
      GO TO 12

    C DRASTIC CHANGE OF POINTS
   35 DO 37 J=1,M
      DO 38 I=1,N
      P(I,J) = (P(I,J)+P(I,MIN))/2.0
   38 CONTINUE
   37 CONTINUE
      GO TO 10

    C EXPANSION
   26 DO 39 I=1,N
      P(I,MM+1) = GAMMA*P(I,MM)+(1.0-GAMMA)*PG(I)
   39 CONTINUE
      CALL PERIN(N,PI,P,MM+1,IIN)
      IF(PI(MM+1)-PP(MM))40,40,30

    C ADOPTION OF EXPANSION
   40 DO 42 I=1,N
      P(I,MAX)=PI(MM+1)
   42 CONTINUE
      PI(MAX) =PI(MM+1)
      GO TO 12

    C POSITIVE ADOPTION
   30 DO 43 I=1,N
      P(I,MAX) = P(I,MM)
   43 CONTINUE
      PI(MAX) = PI(MM)
      GO TO 12

    C NEGATIVE ADOPTION
   31 DO 41 I=1,N
      P(I,MAX) = P(I,MM)
   41 CONTINUE
      PI(MAX)=PI(MM)
      GO TO 32
   15 DO 99 I=1,N
      P(I,14) =P(I,MIN)
   99 CONTINUE
      FUNCV = AMIN
      RETURN
      END
```

A2.2) Listing of Breakthrough curve Prediction Program

```
C ***** HAKA-KYOKUSEN BY <1-YAMA> ******
C **** YMIN : MINIMUM OF X
C **** N    : BUNKATSU SU
C **** YMAX : MAXIMUM OF X
C **** Q0   : LANGMUIR CONSTANT K
C **** VV   : SUPERFICIAL VELOCITY OF WASTEWATER IN PACKED BED
C **** EPS  : VOIDAGE OF PACKED BED OF ADSORBENT
C **** RO   : DENSITY OF ADSORBENT
C **** TOC1 : INTITAIL CONCENTRATION OF TOC(COLUMN TEST)
C **** CT0  : INTIAL CONCENTRATION OF TOC (ADSORPTION EQUILIBRIUM)
C **** AAA,BBB,CCC : PARAMETERS
C **** NT   : NUMBER OF LENGTH OF PACKED BEDS
C **** AL(II) : LENGTH OF PACKED BED OF ADSORBENT
C ************************************************

   COMMON N,J,A(501),B(501),TOC1,AAA,BBB,CCC,Q0
   COMMON BETA(501),C(501,2),Q(501,2)
   DIMENSION C0(501), TOC(501),TTT(501),V(501),TT(501),AL(50),TP(100)
   CALL DATAON
   READ(5,199) YMIN
119 FORMAT(1F10.0)
   READ(5,100)N, YMAX,Q0,EPS,VV,EPS1
100 FORMAT(I10,5F10.0)
   READ(5,101)RO,TOC1,CT0,AAA,BBB,CCC
101 FORMAT(6F10.0)
   J=1
   CALL JUN2(YMIN,YMAX,C0,CT0,RO)
   WRITE(6,121)
121 FORMAT(1H0,35H*** INTIAL VALUE ** A,B, AND C0 ***/1H,
  C7X,1HI,11X,4HA(I),14X,4HB(I),13X,5HC0(I))
   WRITE(6,131)(IIA,A(IIA),B(IIA),C0(IIA),IIA=1,N)
131 FORMAT(1H,5X,I5,1X,1H*,1X,E15.7,3X,E15.7,3X,E15.7)
   TOCI=0.0
   DO 20 I=1,N
 20 TOCI = TOCI+C0(I)
   WRITE(6,603)TOCI
603 FORMAT(1H0,5X,4HTOC=,E15.7)
   ABC=0.0
   DO 50 I=1,N
   C(I,1) = C0(I)
 50 ABC = ABC+C(I,1)*Q0
 60 Q(I,1) = A(I)*C(I,1)/(1.0+ABC)
   BETA(J) = Q(N-J+1,J)/C(N-J+1,J)
   DO 10 J=1,N-1
   CALL JUN3(EPS,EPS1,TOC,V,VV,TTT,TOCI)
 10 CONTINUE
   TOC(N) = C(1,2)
   V(N) = VV*C(1,2)/(EPS*C(1,2)+(1.0-EPS)*Q(1,2))
   TTT(N) = TOC(N)/TOCI
   WRITE(6,201)
201 FORMAT(1H0,5X,32H ***EQUILIBRIUM CONCENTRATON ***)
   DO 30 J=1,N
   WRITE(6,613)J,TOC(J),J,TTT(J),J,V(J)
613 FORMAT(1H,5X,4HTOC(,I3,2H)=,E15.7,5X,4HTOC(,I3,6H)/TOC=,E15.7,
```

```
   C 5X,2HV(,I3,2H)=,E15.7)
 30 CONTINUE
951 READ(5,141)NT
141 FORMAT(I,10)
    IF(NT.LT.0)GO TO 950
    READ(5,142)(AL(II),II=1,NT)
142 FORMAT(7F10.0)
    II=1
961 WRITE(6,301)AL(II)
301 FORMAT(1H,5X,2HL=,E15.7)
    IJ=1
980 IF(IJ.GT.N)GO TO 960
    IF(TTT(IJ).GT.0.98)GO TO 970
    TT(IJ)= AL(II)/V(IJ)/3600.0
    TP(IJ)=12.0*TOC(IJ)
    WRITE(6,303)IJ,TTT(IJ),TT(IJ),TP(IJ)
303 FORMAT(1H,5X,4HTOC(,I3,6H)/TOC=,E15.7,5X,2HT=,E15.7,5X,4HPPM=,E1
   C5.7
970 IJ=IJ+1
    GO TO 980
960 IF(II.GE.NT)GO TO 951
    II = II+1
    GO TO 961
950 STOP
    END

    SUBROUTINE JUN2(YMIN,YMAX,C0,CT0,RO)
    DIMENSION C0(501)
    COMMON N,J,A(501),B(501),TOC1,AAA,BBB,CCC,Q0
    H=(YMAX-YMIN)/FLOAT(N)
    DO 10 IA=1,N
    X=IA
    Y=(X-0.5)*H+YMIN
    A(IA) = Q0*Y*RO
    B(IA) = Y
    C0(IA) = F(Y)*H*TO1/CT0
10 CONTINUE
    RETURN
    END

    SUBROUTINE JUN3(EPS,EPS1,TOC,V,VV,TTT,TOCI)
    DIMENSION TTT(501),TOC(501),V(501)
    COMMON N,J,A(501),B(501),TOC1,AAA,BBB,CCC,Q0
    COMMON BETA(501),C(501,2),Q(501,2)
    IX=1
    AB = 0.0
    DO 10 I=1,N-J+1
10 AB = AB+Q0*C(I,1)
    AB = AB+1.0
80 CD=AB
    FA1=FF(AB)
    AB =AB-0.01
    FA2=FF(AB)
    FFF=FA1*FZ2
    IF(FFF.LT.0.0)GO TO 90
    GO TO 80
90 W1=AB
    W2=CD
```

```
  1 X3 =(W1+W2)/2.0
    IF(IX.GT.500)GO TO 20
    IF(ABS(W2-W1).LE.EPS1)GO TO30
    FF1 = FF(W1)
    FF2 = FF(W2)
    FF3= FF(X3)
    IX = IX+1
    XA = FF1*FF3
    IF(XA.LE.0.0)GO TO 2
    W1=X3
    GO TO 1
  2 W2=X3
    GO TO 1
 20 WRITE(6,601)IX,X3
601 FORMAT(1H0,5X,3HIX=,I5,18HDE KAI MOTOMARAZU., 2X, 2HX=, E15.7,
   C19HTO SHITE TSUZUKERU.)
 30 TOC(J) =0.0
    DO 6 I=1,N-J
    AA = A(I)-X3*BETA(J)
    C(I,2) = X3*(Q(I,1)-BETA(J)*C(I,1))/AA
    Q(I,2) = BETA(J)*(C(I,2)-C(I,1))+Q(I,1)
  6 CONTINUE
    ABB = EPS*C(N-J+1,1)+(1.0-EPS)*(N-J+1,1)
    V(J) = VV*C(N-J+1,1)/ABB
    DO 40 I=1,N-J+1
 40 TOC(J) = TOC(J)+C(I,1)
    TTT(J) = TOC(J)/TOCI
    BETA(J+1) = Q(N-J,2)/C(N-J,2)
    DO 60 I=1,N-J
    C(I,1) = C(I,2)
 60 Q(I,1) = Q(I,2)
    DO 70 I=N-J+1,N
    C(I,1) = 0.0
 70 Q(I,1) = 0.0
    RETURN
    END

    FUNCTION FF(XX)
    COMMON N,J,A(501), B(501) , TOC1, AAA, BBB,CCC,Q0
    COMMON BETA(501),C(501,2),Q(501,2)
    DO 10 I=1,N-J
    AA = A(I)-XX*BETA(J)
 10 C(I,2) = XX*(Q(I,1)-BETA(J)*C(I,1))/AA
    BB=0.0
    DO 20 IY=1,N-J
 20 BB =BB+Q0*C(IY,2)
    BB = BB+1.0
    FF = XX-BB
    RETURN
    END

    FUNCTION F(Y)
    COMMON N,J,A(501),B(501),TOC1,AAA,BBB,CCC,AK
    F = AAA*(Y-BBB)*(Y-CCC)
  2 RETURN
    END
```

VITA

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