

Supporting information for

# Kinetic of PCDD/Fs Formation from Non-Wood Pulp Bleaching with Chlorine

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**Table S1** Average relative deviations of concentrations ( $\text{ng kg}^{-1}$ ) of seventeen 2,3,7,8-cholrine substituted PCDD/Fs in duplicate samples at 13 experimental points.

congeners	average relative deviation	congeners	average relative deviation
2,3,7,8-TCDF	11.1%	2,3,7,8-TCDD	14.1%
1,2,3,7,8-PeCDF	12.8%	1,2,3,7,8-PeCDD	13.7%
2,3,4,7,8-PeCDF	11.1%	1,2,3,4,7,8-HxCDD	13.4%
1,2,3,4,7,8-HxCDF	10.9%	1,2,3,6,7,8-HxCDD	9.5%
1,2,3,6,7,8-HxCDF	18.0%	1,2,3,7,8,9-HxCDD	15.2%
1,2,3,7,8,9-HxCDF	8.6%	1,2,3,4,6,7,8-HpCDD	9.5%
2,3,4,6,7,8-HxCDF	15.6%	OCDD	10.4%
1,2,3,4,6,7,8-HpCDF	7.7%		
1,2,3,4,7,8,9-HpCDF	14.3%		
OCDF	12.3%		

**Table S2** Concentrations ( $\text{ng kg}^{-1}$ ) of summed tetra- to octa-CDD/Fs in duplicate samples at 13 experimental points together with the relative deviations.

treatment	summed tetra- to octa-CDD/Fs		relative deviation
	sample 1	sample 2	
chlorination time (min)			
5	180.85	142.23	12.0%
20	330.42	306.70	3.7%
70	614.46	755.21	10.3%
180	907.80	850.01	3.3%
pH value			
0.5	843.70	755.21	2.8%
2	203.57	187.51	4.1%
4	123.06	88.97	16.1%
chlorination temperature ( $^{\circ}\text{C}$ )			
20	653.95	755.21	7.2%
40	254.10	273.22	3.6%
60	231.42	210.16	4.8%
available chlorine dosage			
8%	1752.07	1998.06	6.6%
12%	1908.25	2158.50	6.2%
16%	3645.09	3815.57	2.3%

**Table S3.** Concentrations ( $\text{ng kg}^{-1}$ ) of summed tetra- to octa-PCDFs (PCDFs) and summed tetra- to octa-PCDDs (PCDDs) together with their I-TEQ values and concentration ratios in pulps under different chlorination conditions.

	PCDDs ( $\text{ng Kg}^{-1}$ )	PCDFs ( $\text{ng Kg}^{-1}$ )	I-TEQ ( $\text{ng TEQ Kg}^{-1}$ )	PCDFs:PCDDs
chlorination time (min)				
0	100.22	21.55	1.40	0.22
5	97.72	83.12	6.46	0.85
10	109.80	95.77	7.75	0.87
20	79.27	251.15	19.84	3.17
40	96.20	227.60	17.90	2.37
70	193.98	420.48	28.06	2.17
120	210.93	588.53	35.87	2.79
180	270.11	637.68	43.48	2.36
pH value				
0.5	210.94	588.52	35.87	2.79
1	244.56	409.39	32.02	1.67
2	84.11	119.46	8.62	1.42
3	122.56	14.27	1.23	0.12
4	88.97	34.09	2.93	0.38
5	141.05	9.82	0.73	0.07
6	106.97	10.06	0.75	0.09
chlorination temperature ( $^{\circ}\text{C}$ )				
20	244.56	409.40	32.02	1.67
30	442.91	88.87	7.01	0.20
40	188.33	65.77	5.00	0.35
50	63.73	79.33	5.31	1.24
60	149.16	82.26	5.03	0.55
70	108.59	92.72	4.96	0.85
available chlorine dosage				
5%	244.56	409.40	32.02	1.67
8%	506.33	1245.74	88.32	2.46
10%	414.90	1997.19	135.92	4.81
12%	474.70	1433.55	106.46	3.02
14%	156.97	1684.67	126.62	10.73
16%	269.84	3375.25	237.46	12.51

**Table S4.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of homologue groups from di- to octa-CDD/Fs in pulps under different available chlorine dosages.

	blank	5%	8%	10%	12%	14%	16%
PCDD/Fs	146.28	1719.63	5328.21	5852.08	6752.52	8438.16	9271.04
PCDDs	101.01	258.95	535.47	446.24	512.53	191.71	306.16
PCDFs	45.27	1460.68	4792.73	5405.84	6239.98	8246.44	8964.88
$\sum \text{DiCDDs}$	0.65	1.14	0.55	1.34	0.53	1.77	2.01
$\sum \text{TriCDDs}$	0.14	13.25	28.60	30.01	37.30	32.97	34.31
$\sum \text{TeCDDs}$	23.19	47.37	12.95	16.52	13.99	13.32	17.50
$\sum \text{PeCDDs}$	3.66	20.06	21.23	11.40	13.26	4.50	5.68
$\sum \text{HxCDDs}$	2.33	51.23	22.22	17.05	23.34	8.15	11.18
$\sum \text{HpCDDs}$	6.49	44.46	34.81	21.77	58.79	8.40	17.05
OCDD	64.55	81.44	415.12	348.16	365.32	122.61	218.44
$\sum \text{DiCDFs}$	11.45	266.89	596.29	383.59	831.80	1804.63	753.76
$\sum \text{TriCDFs}$	12.28	784.39	2950.70	3025.06	3974.64	4757.14	4835.88
$\sum \text{TeCDFs}$	8.70	300.48	933.54	1753.50	1354.21	1600.32	3148.86
$\sum \text{PeCDFs}$	5.46	81.09	246.90	201.00	72.38	78.30	199.78
$\sum \text{HxCDFs}$	3.24	23.33	52.48	33.62	4.86	4.75	21.20
$\sum \text{HpCDFs}$	1.48	2.83	9.00	6.92	1.11	0.69	4.30
OCDF	2.67	1.66	3.82	2.15	0.99	0.60	1.11

**Table S5.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of 2,3,7,8-chlorine substituted dioxin congeners in pulps under different available chlorine dosage.

	5%	8%	10%	12%	14%	16%
2,3,7,8-TCDD	8.75	8.98	13.58	9.42	9.53	12.11
1,2,3,7,8-PeCDD	2.18	1.73	2.35	1.69	0.91	1.81
1,2,3,4,7,8-HxCDD	13.30	1.62	0.80	1.04	0.45	1.06
1,2,3,6,7,8-HxCDD	5.61	1.89	1.68	2.35	0.88	1.14
1,2,3,7,8,9-HxCDD	15.28	6.25	7.66	8.31	4.76	5.68
1,2,3,4,6,7,8-HpCDD	30.98	19.97	10.97	26.86	4.66	9.55
OCDD	81.44	415.12	348.16	365.32	122.61	218.44
2,3,7,8-TCDF	163.28	514.05	985.06	855.65	1044.62	1941.56
1,2,3,7,8-PeCDF	2.54	85.00	64.94	18.19	20.61	61.04
2,3,4,7,8-PeCDF	2.71	31.76	29.01	14.84	19.76	47.94
1,2,3,4,7,8-HxCDF	0.95	37.56	22.85	1.85	2.49	13.66
1,2,3,6,7,8-HxCDF	0.49	9.23	6.10	0.57	0.94	3.57
1,2,3,7,8,9-HxCDF	ND	5.69	4.67	1.60	1.32	3.97
2,3,4,6,7,8-HxCDF	3.84	ND	ND	0.84	ND	ND
1,2,3,4,6,7,8-HpCDF	2.68	4.94	4.42	1.11	0.69	3.20
1,2,3,4,7,8,9-HpCDF	0.15	4.06	2.50	ND	ND	1.10
OCDF	1.66	3.82	2.15	0.99	0.60	1.11

ND: not detected out.

**Table S6.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of homologue groups from di- to octa-CDD/Fs in pulps under different initial pH values.

	blank	pH = 0.5	pH = 1	pH = 2	pH = 3	pH = 4	pH = 5	pH = 6
PCDD/Fs	146.70	1650.15	1719.63	1402.47	2113.94	4335.07	193.11	142.57
PCDDs	101.01	225.29	258.95	120.10	178.68	176.58	147.71	112.44
PCDFs	45.27	1424.86	1460.68	1282.37	1935.26	4158.49	45.41	30.13
$\Sigma\text{DiCDDs}$	0.65	0.42	1.14	23.89	46.77	44.66	2.82	0.56
$\Sigma\text{TriCDDs}$	0.14	13.94	13.25	12.10	9.35	42.95	3.82	4.91
$\Sigma\text{TeCDDs}$	23.19	39.88	47.37	25.04	4.13	6.22	9.69	5.18
$\Sigma\text{PeCDDs}$	3.66	18.02	20.06	4.44	1.32	1.88	1.97	1.57
$\Sigma\text{HxCDDs}$	2.33	47.29	51.23	1.88	1.63	1.39	0.26	1.50
$\Sigma\text{HpCDDs}$	6.49	49.43	44.46	4.37	1.26	0.95	6.38	5.28
OCDD	64.55	56.32	81.44	48.38	114.22	78.53	122.75	93.44
$\Sigma\text{DiCDFs}$	11.45	23.22	266.89	669.05	1873.46	3836.70	21.05	8.97
$\Sigma\text{TriCDFs}$	12.28	813.11	784.39	493.86	47.53	287.70	14.54	11.11
$\Sigma\text{TeCDFs}$	8.70	389.69	300.48	104.09	9.51	27.75	6.57	6.49
$\Sigma\text{PeCDFs}$	5.46	164.78	81.09	8.74	3.71	4.94	2.69	2.85
$\Sigma\text{HxCDFs}$	3.24	27.57	23.33	3.33	0.44	0.69	0.26	0.39
$\Sigma\text{HpCDFs}$	1.48	4.07	2.83	1.34	0.36	0.32	0.30	0.33
OCDF	2.67	2.41	1.66	1.96	0.25	0.39	ND	ND

ND: not detected out.

**Table S7.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of 2,3,7,8-chlorine substituted dioxin congeners in pulps under different initial pH values.

	pH = 0.5	pH = 1	pH = 2	pH = 3	pH = 4	pH = 5	pH = 6
2,3,7,8-TCDD	8.27	8.75	2.03	0.49	1.09	0.27	0.28
1,2,3,7,8-PeCDD	2.97	2.18	0.26	0.02	0.11	ND	ND
1,2,3,4,7,8-HxCDD	16.06	13.30	0.12	0.86	0.42	0.19	0.27
1,2,3,6,7,8-HxCDD	5.09	5.61	0.26	ND	0.06	ND	ND
1,2,3,7,8,9-HxCDD	5.06	15.28	0.26	0.10	0.09	0.08	0.11
1,2,3,4,6,7,8-HpCDD	25.09	30.98	1.97	0.54	0.35	2.54	2.34
OCDD	56.32	81.44	48.38	114.22	78.53	122.75	93.44
2,3,7,8-TCDF	198.58	163.28	56.96	3.33	13.50	1.70	1.83
1,2,3,7,8-PeCDF	3.64	2.54	1.05	0.33	0.74	0.25	0.23
2,3,4,7,8-PeCDF	4.19	2.71	0.84	0.24	0.38	0.15	0.16
1,2,3,4,7,8-HxCDF	1.38	0.95	0.56	0.28	0.36	0.26	0.26
1,2,3,6,7,8-HxCDF	1.06	0.49	0.22	0.08	0.11	ND	0.06
1,2,3,7,8,9-HxCDF	ND	ND	0.10	0.08	0.08	ND	0.06
2,3,4,6,7,8-HxCDF	7.63	3.84	0.49	ND	0.14	ND	ND
1,2,3,4,6,7,8-HpCDF	3.96	2.68	1.20	0.33	0.32	0.30	0.33
1,2,3,4,7,8,9-HpCDF	0.11	0.15	0.14	0.04	ND	ND	ND
OCDF	2.41	1.66	1.96	0.25	0.39	ND	ND

ND: not detected out.

**Table S8.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of homologue groups from di- to octa-CDD/Fs in pulps under different temperatures.

	blank	20 °C	30 °C	40 °C	50 °C	60 °C	70 °C
PCDD/Fs	146.28	1719.63	3894.41	3750.54	4025.00	3250.33	2319.35
PCDDs	101.01	258.95	471.58	218.71	88.67	182.62	132.94
PCDFs	45.27	1460.68	3422.83	3531.83	3936.33	3067.71	2186.42
$\Sigma\text{DiCDDs}$	0.65	1.14	4.66	5.45	4.77	6.66	4.79
$\Sigma\text{TriCDDs}$	0.14	13.25	24.01	24.92	20.17	26.80	19.56
$\Sigma\text{TeCDDs}$	23.19	47.37	5.19	6.10	4.25	8.09	6.73
$\Sigma\text{PeCDDs}$	3.66	20.06	4.62	4.72	5.05	6.59	10.13
$\Sigma\text{HxCDDs}$	2.33	51.23	3.86	3.54	2.93	3.70	3.38
$\Sigma\text{HpCDDs}$	6.49	44.46	11.87	10.81	2.77	7.39	5.73
OCDD	64.55	81.44	417.36	163.15	48.74	123.40	82.61
$\Sigma\text{DiCDFs}$	11.45	266.89	2177.24	2465.76	2434.87	1638.44	961.07
$\Sigma\text{TriCDFs}$	12.28	784.39	1156.72	1000.30	1422.12	1347.01	1132.63
$\Sigma\text{TeCDFs}$	8.70	300.48	78.34	57.42	69.90	69.86	84.01
$\Sigma\text{PeCDFs}$	5.46	81.09	9.39	7.50	8.58	11.29	7.76
$\Sigma\text{HxCDFs}$	3.24	23.33	0.78	0.55	0.56	0.69	0.63
$\Sigma\text{HpCDFs}$	1.48	2.83	0.36	0.29	0.29	0.42	0.32
OCDF	2.67	1.66	ND	ND	ND	ND	ND

ND: not detected out.

**Table S9.** Concentrations (ng kg<sup>-1</sup> pulp) of 2,3,7,8-chlorine substituted dioxin congeners in pulps under different chlorination temperatures.

	20 °C	30 °C	40 °C	50 °C	60 °C	70 °C
2,3,7,8-TCDD	8.75	1.66	1.31	1.12	0.95	0.63
1,2,3,7,8-PeCDD	2.18	0.29	0.25	0.20	0.26	0.17
1,2,3,4,7,8-HxCDD	13.30	0.73	0.52	0.67	0.82	0.54
1,2,3,6,7,8-HxCDD	5.61	0.45	0.40	0.29	0.41	0.39
1,2,3,7,8,9-HxCDD	15.28	0.89	0.65	0.53	0.66	0.51
1,2,3,4,6,7,8-HpCDD	30.98	5.23	4.35	1.16	3.35	2.44
OCDD	81.44	417.36	163.15	48.74	123.40	82.61
2,3,7,8-TCDF	163.28	41.51	28.83	35.52	32.59	37.04
1,2,3,7,8-PeCDF	2.54	1.24	1.24	1.27	1.25	0.99
2,3,4,7,8-PeCDF	2.71	0.46	0.40	0.43	0.42	0.35
1,2,3,4,7,8-HxCDF	0.95	0.36	0.33	0.30	0.31	0.27
1,2,3,6,7,8-HxCDF	0.49	0.16	0.12	0.08	0.14	0.11
1,2,3,7,8,9-HxCDF	ND	0.14	0.10	0.18	0.24	0.25
2,3,4,6,7,8-HxCDF	3.84	0.12	ND	ND	ND	ND
1,2,3,4,6,7,8-HpCDF	2.68	0.36	0.29	0.29	0.42	0.32
1,2,3,4,7,8,9-HpCDF	0.15	ND	ND	ND	ND	ND
OCDF	1.66	ND	ND	ND	ND	ND

ND: not detected out.

**Table S10.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of homologue groups from di- to octa-CDD/Fs in pulps under different chlorination times.

	blank	5min	10min	20min	40min	70min	120min	180min
PCDD/Fs	146.28	1941.50	2849.56	4198.82	3899.68	1286.93	1292.99	2113.64
PCDDs	101.01	137.97	165.65	170.32	188.92	216.52	230.22	313.39
PCDFs	45.27	1803.53	2683.91	4028.50	3710.76	1070.40	1062.76	1800.25
$\Sigma\text{DiCDDs}$	0.65	5.35	12.88	11.42	11.39	0.93	1.94	0.33
$\Sigma\text{TriCDDs}$	0.14	34.91	42.97	79.62	81.32	21.62	17.35	42.95
$\Sigma\text{TeCDDs}$	23.19	8.17	7.55	13.55	10.65	40.72	39.88	55.55
$\Sigma\text{PeCDDs}$	3.66	8.95	8.33	16.16	8.53	29.59	18.02	23.23
$\Sigma\text{HxCDDs}$	2.33	5.17	5.31	11.86	5.95	61.75	47.29	52.58
$\Sigma\text{HpCDDs}$	6.49	1.82	4.93	2.52	2.25	45.65	49.43	47.66
OCDD	64.55	73.61	83.68	35.18	68.84	16.26	56.32	91.09
$\Sigma\text{DiCDFs}$	11.45	1336.84	1888.12	2151.65	1991.03	129.36	8.68	233.42
$\Sigma\text{TriCDFs}$	12.28	383.56	700.03	1625.70	1492.12	520.56	465.56	929.14
$\Sigma\text{TeCDFs}$	8.70	68.91	82.91	223.48	210.41	262.72	389.69	464.45
$\Sigma\text{PeCDFs}$	5.46	12.68	11.18	25.80	15.36	121.50	164.78	132.99
$\Sigma\text{HxCDFs}$	3.24	0.85	0.81	1.16	1.10	32.82	27.57	32.88
$\Sigma\text{HpCDFs}$	1.48	0.68	0.43	0.53	0.41	2.93	4.07	4.19
OCDF	2.67	ND	0.43	0.17	0.33	0.52	2.41	3.17

**Table S11.** Concentrations ( $\text{ng kg}^{-1}$  pulp) of 2,3,7,8-chlorine substituted dioxin congeners in pulps under different chlorination times.

	blank	5 min	10 min	20 min	40 min	70 min	120 min	180 min
2,3,7,8-TCDD	0.38	1.52	1.81	4.73	4.28	5.83	8.27	9.28
1,2,3,7,8-PeCDD	0.73	0.80	0.77	1.81	1.24	3.36	2.97	2.89
1,2,3,4,7,8-HxCDD	0.13	0.47	0.43	0.59	0.48	15.88	16.06	13.12
1,2,3,6,7,8-HxCDD	0.19	0.61	0.56	1.47	0.76	6.94	5.09	5.55
1,2,3,7,8,9-HxCDD	0.21	1.73	2.34	5.86	2.46	14.77	5.06	15.17
1,2,3,4,6,7,8-HpCDD	0.93	0.92	2.44	1.57	1.31	33.41	25.09	32.04
OCDD	3.89	73.61	83.68	35.18	68.84	16.26	56.32	91.09
2,3,7,8-TCDF	3.50	37.84	46.72	123.98	117.52	139.87	198.58	254.78
1,2,3,7,8-PeCDF	0.26	0.71	1.34	2.73	2.25	2.81	3.64	4.70
2,3,4,7,8-PeCDF	0.24	0.51	0.57	1.40	1.14	2.81	4.19	4.67
1,2,3,4,7,8-HxCDF	0.53	0.38	0.41	0.42	0.50	0.96	1.38	1.32
1,2,3,6,7,8-HxCDF	0.20	0.17	0.13	0.23	0.21	0.54	1.06	0.88
1,2,3,7,8,9-HxCDF	0.02	0.23	0.18	0.40	0.30	ND	ND	ND
2,3,4,6,7,8-HxCDF	0.20	0.07	0.10	0.11	0.10	7.29	7.63	6.40
1,2,3,4,6,7,8-HpCDF	0.70	0.56	0.37	0.49	0.41	2.84	3.96	4.00
1,2,3,4,7,8,9-HpCDF	0.05	0.12	0.05	0.04	ND	0.09	0.11	0.20
OCDF	0.66	ND	0.43	0.17	0.33	0.52	2.41	3.17

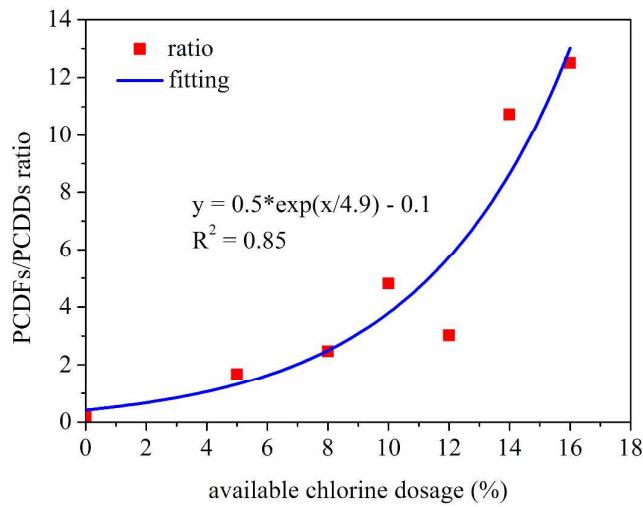
ND: not detected out.

**Table S12** Molar concentrations (nmol kg<sup>-1</sup>) of summed tetra- to octa-CDDs (PCDDs) and summed tetra- to octa-CDFs (PCDFs) in pulps under different chlorination conditions.

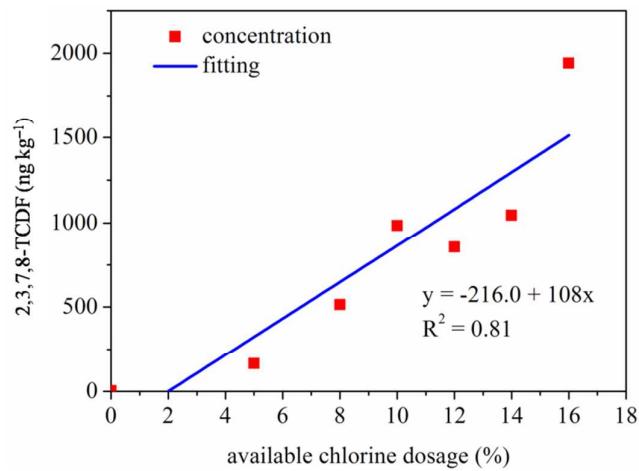
	PCDDs (nmol kg <sup>-1</sup> )	PCDFs (nmol kg <sup>-1</sup> )	PCDD/Fs (nmol kg <sup>-1</sup> )
chlorination time (min)			
0	0.25	0.06	0.31
5	0.23	0.27	0.5
10	0.26	0.31	0.57
20	0.2	0.82	1.02
40	0.23	0.74	0.97
70	0.51	1.32	1.83
120	0.54	1.86	2.4
180	0.69	2.03	2.72
pH value			
0.5	0.54	1.86	2.4
1	0.62	1.3	1.92
2	0.21	0.39	0.6
3	0.27	0.04	0.32
4	0.2	0.11	0.31
5	0.32	0.03	0.35
6	0.24	0.03	0.27
chlorination temperature (°C)			
20	0.62	1.3	1.92
30	0.98	0.29	1.27
40	0.43	0.21	0.64
50	0.15	0.26	0.41
60	0.34	0.27	0.61
70	0.25	0.3	0.56
available chlorine dosage			
5%	0.62	1.3	1.92
8%	1.15	3.97	5.13
10%	0.94	6.48	7.42
12%	1.08	4.69	5.77
14%	0.36	5.51	5.88
16%	0.62	11.02	11.64

**Table S13** One-way ANOVA results for fitting a first order kinetic model to the formation rate of summed tetra- to octa-CDFs under different chlorination conditions.

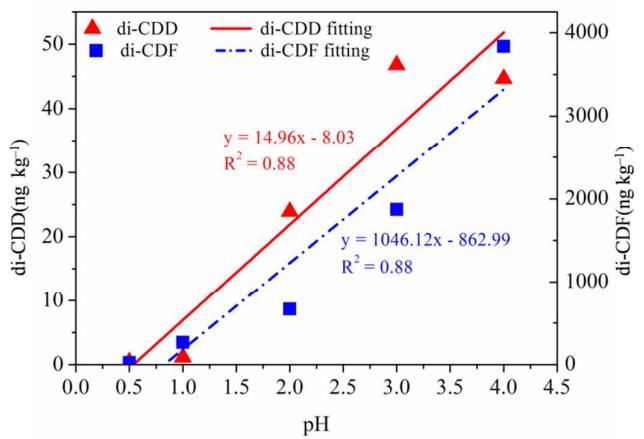
treatment	DF	Sum of Squares	Mean Square	F Value	Prob > F
<i>Chlorination time</i>					
Regression	2	15.86743	5.34512	28.1984	0.00439
Residual	5	0.92616	0.18955		
Uncorrected Total	7	16.79359			
Corrected Total	6	2.92675			
<i>available chlorine dosage</i>					
Regression	1	67.02039	67.02039	84.63607	0.03809
Residual	5	3.95933	0.79187		
Uncorrected Total	6	70.97972			
Corrected Total	5	12.69688			
<i>pH value</i>					
Regression	2	2.32213	1.16107	116.28358	1.18933E-4
Residual	5	0.04992	0.00998		
Uncorrected Total	7	2.37206			
Corrected Total	6	1.18882			
<i>Chlorination temperature</i>					
Regression	2	1.43713	0.71857	60.08114	0.00149
Residual	4	0.04784	0.01196		
Uncorrected Total	6	1.48497			
Corrected Total	5	0.4254			



**Figure S1.** The dependence of the ratio of summed tetra- to octa-PCDFs to summed tetra- to octa-CDDs on available chlorine dosages.



**Figure S2.** The dependence of 2,3,7,8-TCDF concentration on available chlorine dosage.



**Figure S3.** The dependence of di-CDD/F concentration on pH value.