

Supplementary Information for:

Physical Consistency of Axial-Dispersion Boundary Conditions and Tanks-in-Series Models for Multi-Compartment Wastewater Treatment Reactors

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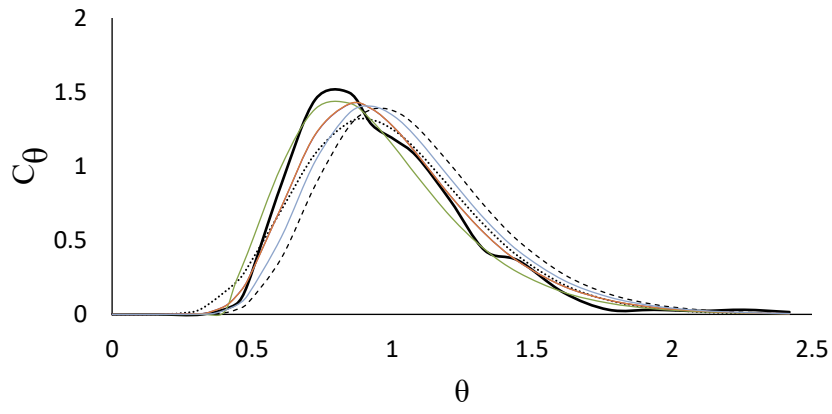
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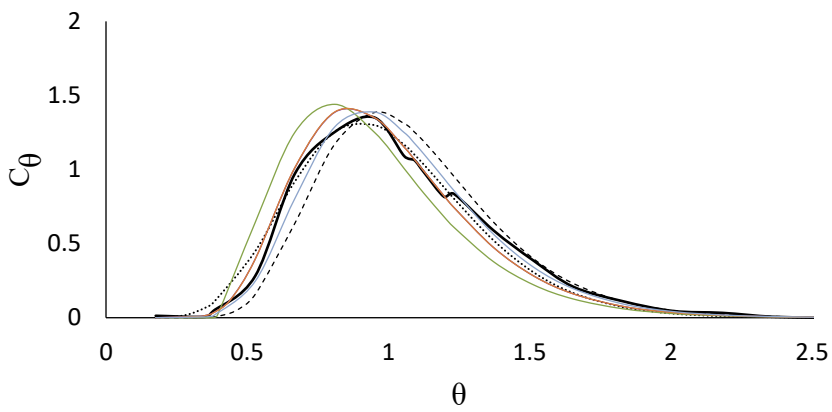
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Online Resource 1

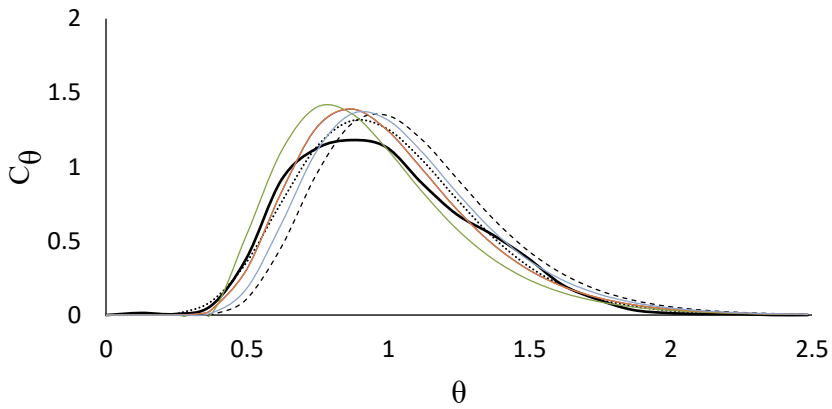
Additional RTD curves and detailed hydrodynamic parameters



(a)



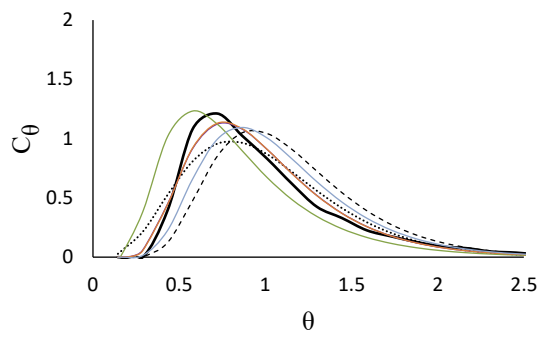
(b)



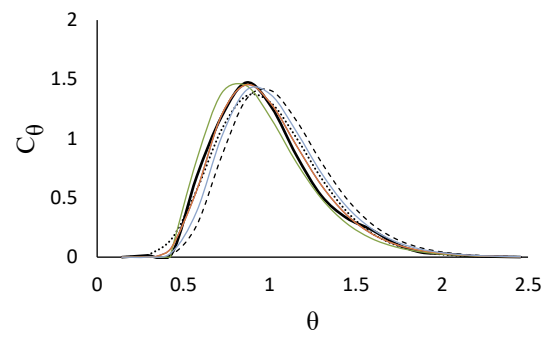
(c)

— Experimental TIS - - - Open BC — BC I — BC II — BC III — BC IV

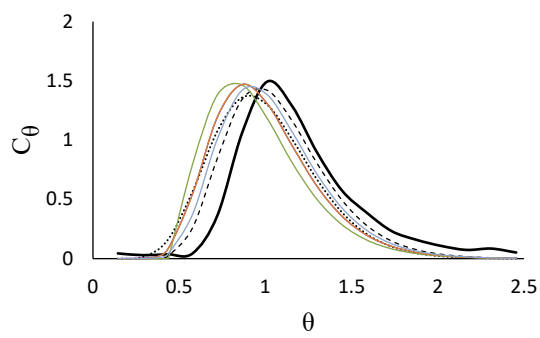
Fig. A.1 Residence time distribution (RTD) curves at (a) HRT = 248 min, (b) HRT = 284 min, and (c) HRT = 332 min (additional cases not shown in Fig. 2)



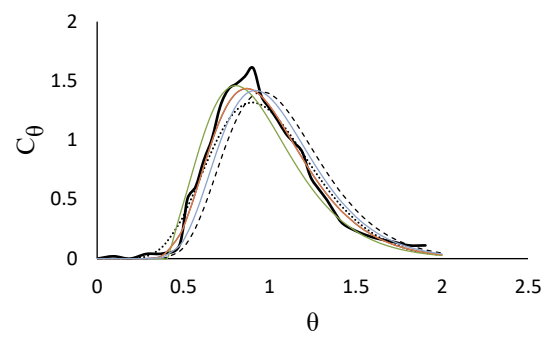
(a) Temperature (30 °C)



(b) Dissolved Solids (1000 mg/L)



(c) Suspended Solids (5000 mg/L)



(d) Scale-up

— Experimental TIS - - - Open BC — BC I — BC II — BC III — BC IV

Fig. A.2 Experimental and modelled RTD curves for all evaluated formulations under varying environmental, operational, and geometric conditions

Table A.1 Hydrodynamic parameters and corresponding prediction errors for different formulations at multiple HRTs.

HRT (min)	RTD	flow regime indicator		breakthrough time		mean time		peak time		peak concentration		goodness of fit	
		N	Pe	value	error (%)	value	error (%)	value	error (%)	value	error (%)	RMSE	NRMSE (%)
93	Experimental	-	-	0.46	0	0.90	0	0.83	0	1.83	0	-	-
	TIS	13	-	0.32	30	1.00	11	0.93	12	1.49	19	0.25	36
	Open BC	-	29.30	0.43	7	1.07	19	0.97	17	1.54	16	0.35	50
	BC I	-	24.74	0.39	15	1.00	11	0.89	7	1.57	14	0.22	31
	BC II	-	22.98	0.52	13	0.98	9	0.84	1	1.59	13	0.14	20
	BC III	-	25.78	0.39	15	1.00	11	0.89	7	1.57	14	0.22	31
	BC IV	-	27.21	0.42	9	1.04	16	0.95	14	1.55	15	0.29	41
Lowest Error		Open BC		BC II		BC II		BC II		BC II		BC II	
180	Experimental	-	-	0.46	0	0.99	0	0.89	0	1.60	0	-	-
	TIS	11	-	0.28	39	0.99	0	0.91	2	1.38	14	0.14	17
	Open BC	-	26.00	0.40	13	1.06	7	0.98	10	1.45	9	0.23	27
	BC I	-	21.48	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	BC II	-	19.67	0.45	2	0.96	3	0.81	9	1.50	6	0.11	13
	BC III	-	22.53	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	BC IV	-	23.94	0.39	15	1.03	4	0.91	2	1.47	8	0.17	20
Lowest Error		BC II		TIS, BC I, III		BC I, III		BC II		BC I, II, III		BC I, II, III	
248	Experimental	-	-	0.32	0	0.97	0	0.81	0	1.51	0	-	-
	TIS	10	-	0.25	22	0.99	2	0.90	11	1.32	13	0.12	17
	Open BC	-	23.84	0.40	25	1.07	10	0.96	19	1.40	7	0.22	31
	BC I	-	19.36	0.34	6	1.00	3	0.87	7	1.44	5	0.08	11
	BC II	-	17.50	0.40	25	0.95	2	0.80	1	1.44	5	0.08	11
	BC III	-	20.41	0.34	6	1.00	3	0.87	7	1.44	5	0.08	11
	BC IV	-	21.82	0.37	16	1.04	7	0.92	14	1.39	8	0.15	21
Lowest Error		BC I, III		TIS, BC II		BC II		BC I, II, III		BC I, II, III		BC I, II, III	
284	Experimental	-	-	0.35	0	1.03	0	0.93	0	1.36	0	-	-
	TIS	10	-	0.25	29	1.00	3	0.90	3	1.30	4	0.06	9
	Open BC	-	23.60	0.39	11	1.08	5	0.97	4	1.39	2	0.13	19
	BC I	-	19.12	0.33	6	1.00	3	0.85	9	1.40	3	0.06	9
	BC II	-	17.26	0.39	11	0.95	8	0.81	13	1.44	6	0.15	22
	BC III	-	20.18	0.33	6	1.00	3	0.85	9	1.40	3	0.06	9
	BC IV	-	21.58	0.37	6	1.04	1	0.95	2	1.39	2	0.07	10
Lowest Error		BC I, III, IV		BC IV		BC IV		Open BC, BC IV		TIS, BC I, III		TIS, BC I, III	
332	Experimental	-	-	0.35	0	0.98	0	0.90	0	1.18	0	-	-
	TIS	10	-	0.25	29	1.00	2	0.90	0	1.33	13	0.07	12
	Open BC	-	22.71	0.39	11	1.09	11	0.96	7	1.35	14	0.16	28
	BC I	-	18.25	0.31	11	1.00	2	0.87	3	1.39	18	0.07	12
	BC II	-	16.35	0.37	6	0.94	4	0.78	13	1.42	20	0.11	20
	BC III	-	19.31	0.31	11	1.00	2	0.87	3	1.39	18	0.07	12
	BC IV	-	20.70	0.37	6	1.05	7	0.91	1	1.38	17	0.11	20
Lowest Error		BC II, IV		TIS, BC I, III		TIS		TIS		TIS, BC I, III		TIS, BC I, III	
366	Experimental	-	-	0.33	0	0.95	0	0.90	0	1.44	0	-	-
	TIS	11	-	0.28	15	1.00	5	0.91	1	1.38	4	0.06	9
	Open BC	-	25.60	0.37	12	1.08	14	0.96	7	1.43	1	0.16	23
	BC I	-	21.09	0.36	9	1.00	5	0.87	3	1.47	2	0.05	7
	BC II	-	19.27	0.44	33	0.96	1	0.81	10	1.49	3	0.10	15
	BC III	-	22.14	0.36	9	1.00	5	0.87	3	1.47	2	0.05	7
	BC IV	-	23.55	0.39	18	1.04	9	0.92	2	1.46	1	0.10	15
Lowest Error		BC I, III		BC II		TIS		Open BC, BC IV		BC I, III		BC I, III	

Table A.2 Hydrodynamic parameters and corresponding prediction errors grouped by formulation across varying HRTs.

Model	HRT (min)	flow-regime indicator		breakthrough time		mean time		peak time		peak concentration		goodness of fit	
		N	Pe	value	error (%)	value	error (%)	value	error (%)	value	error (%)	RMSE	NRMSE (%)
Experimental	93	-	-	0.46	-	0.90	-	0.83	-	1.83	-	-	-
	180	-	-	0.46	-	0.99	-	0.89	-	1.60	-	-	-
	248	-	-	0.32	-	0.97	-	0.81	-	1.51	-	-	-
	284	-	-	0.35	-	1.03	-	0.93	-	1.36	-	-	-
	332	-	-	0.35	-	0.98	-	0.90	-	1.18	-	-	-
	366	-	-	0.33	-	0.95	-	0.90	-	1.44	-	-	-
	Average			0.38	-	0.97	-	0.88	-	1.49	-	-	-
TIS	93	13	-	0.32	30	1.00	11	0.93	12	1.49	19	0.25	36
	180	11	-	0.28	39	0.99	0	0.91	2	1.38	14	0.14	17
	248	10	-	0.25	22	0.99	2	0.90	11	1.32	13	0.12	17
	284	10	-	0.25	29	1.00	3	0.90	3	1.30	4	0.06	9
	332	10	-	0.25	29	1.00	2	0.90	0	1.33	13	0.07	12
	366	11	-	0.28	15	1.00	5	0.91	1	1.38	4	0.06	9
	Average			0.27	27	1.00	4	0.91	5	1.37	11	0.12	17
Open BC	93	-	29.3	0.43	7	1.07	19	0.97	17	1.54	16	0.35	50
	180	-	26	0.40	13	1.06	7	0.98	10	1.45	9	0.23	27
	248	-	23.84	0.40	25	1.07	10	0.96	19	1.40	7	0.22	31
	284	-	23.6	0.39	11	1.08	5	0.97	4	1.39	2	0.13	19
	332	-	22.71	0.39	11	1.09	11	0.96	7	1.35	14	0.16	28
	366	-	25.60	0.37	12	1.08	14	0.96	7	1.43	1	0.16	23
	Average			0.40	13	1.08	11	0.97	11	1.43	8	0.21	30
BC I	93	-	24.74	0.39	15	1.00	11	0.89	7	1.56	14	0.22	31
	180	-	21.48	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	248	-	19.36	0.34	6	1.00	3	0.87	7	1.44	5	0.08	11
	284	-	19.12	0.33	6	1.00	3	0.85	9	1.40	3	0.06	9
	332	-	18.25	0.31	11	1.00	2	0.87	3	1.39	18	0.07	12
	366	-	21.09	0.36	9	1.00	5	0.87	3	1.47	2	0.05	7
	Average			0.35	12	1.00	4	0.88	5	1.46	8	0.10	14
BC II	93	-	22.98	0.52	13	0.98	9	0.84	1	1.59	13	0.14	20
	180	-	19.67	0.45	2	0.96	3	0.81	9	1.50	6	0.11	13
	248	-	17.5	0.40	25	0.95	2	0.80	1	1.44	5	0.08	11
	284	-	17.26	0.39	11	0.95	8	0.81	13	1.44	6	0.15	22
	332	-	16.35	0.37	6	0.94	4	0.78	13	1.42	20	0.11	20
	366	-	19.27	0.44	33	0.96	1	0.81	10	1.49	3	0.10	15
	Average			0.43	15	0.96	5	0.81	8	1.48	9	0.12	17
BC III	93	-	25.78	0.39	15	1.00	11	0.89	7	1.56	14	0.22	31
	180	-	22.53	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	248	-	20.41	0.34	6	1.00	3	0.87	7	1.44	5	0.08	11
	284	-	20.18	0.33	6	1.00	3	0.85	9	1.40	3	0.06	9
	332	-	19.31	0.31	11	1.00	2	0.87	3	1.39	18	0.07	12
	366	-	22.14	0.36	9	1.00	5	0.87	3	1.47	2	0.05	7
	Average			0.35	12	1.00	4	0.88	5	1.46	8	0.10	14
BC IV	93	-	27.21	0.42	9	1.04	16	0.95	14	1.55	15	0.29	41
	180	-	23.94	0.39	15	1.03	4	0.91	2	1.47	8	0.17	20
	248	-	21.82	0.37	16	1.04	7	0.92	14	1.39	8	0.15	21
	284	-	21.58	0.37	6	1.04	1	0.95	2	1.39	2	0.07	10
	332	-	20.7	0.37	6	1.05	7	0.91	1	1.38	17	0.11	20
	366	-	23.55	0.39	18	1.04	9	0.92	2	1.46	1	0.10	15
	Average			0.39	12	1.04	7	0.93	6	1.44	9	0.15	21

Table A.3 Detailed hydrodynamic parameters and corresponding prediction errors for different formulations under varying environmental, operational, and geometric conditions.

Specification	RTD	flow-regime indicator		breakthrough time		mean time		peak time		peak concentration		goodness of fit	
		N	Pe	value	error (%)	value	error (%)	value	error (%)	value	error (%)	RMSE	NRMSE (%)
Baseline	Experimental	-	-	0.46	0	0.99	0	0.89	0	1.60	0	-	-
	TIS	11	-	0.28	39	0.99	0	0.91	2	1.38	14	0.14	17
	Open BC	-	26.00	0.40	13	1.06	7	0.98	10	1.45	9	0.23	27
	BC I	-	21.48	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	BC II	-	19.67	0.45	2	0.96	3	0.81	9	1.50	6	0.11	13
	BC III	-	22.53	0.35	24	0.99	0	0.90	1	1.48	8	0.11	13
	BC IV	-	23.94	0.39	15	1.03	4	0.91	2	1.47	8	0.17	20
Lowest Error		BC II		TIS, BC I, III		BC I, III		BC II		BC I, II, III			
T = 30 °C	Experimental	-	-	0.29	0	0.99	0	0.72	0	1.21	0	-	-
	TIS	5	-	0.11	62	1.00	1	0.80	11	0.98	19	0.11	22
	Open BC	-	13.81	0.30	3	1.14	15	0.93	29	1.07	12	0.20	40
	BC I	-	9.60	0.23	21	1.00	1	0.76	6	1.14	6	0.06	12
	BC II	-	6.74	0.16	45	0.86	13	0.59	18	1.23	2	0.18	36
	BC III	-	10.71	0.23	21	1.00	1	0.76	6	1.14	6	0.06	12
	BC IV	-	12.05	0.27	7	1.08	9	0.87	21	1.09	10	0.14	28
Lowest Error		Open BC		TIS, BC I, III		BC I, III		BC II		BC I, III			
DS = 1000 mg/L	Experimental	-	-	0.42	0	0.99	0	0.87	0	1.47	0	-	-
	TIS	11	-	0.28	34	1.00	1	0.90	4	1.38	6	0.07	12
	Open BC	-	25.07	0.40	5	1.08	9	0.97	12	1.42	4	0.16	28
	BC I	-	20.57	0.35	17	1.00	1	0.88	2	1.46	1	0.04	7
	BC II	-	18.73	0.43	2	0.96	3	0.83	4	1.47	0	0.07	11
	BC III	-	21.62	0.35	17	1.00	1	0.88	2	1.46	1	0.05	7
	BC IV	-	23.02	0.39	8	1.04	5	0.92	6	1.44	2	0.11	17
Lowest Error		BC II		TIS, BC I, III		BC I, III		BC II		BC I, III			
SS = 5000 mg/L	Experimental	-	-	0.54	0	1.20	0	1.03	0	1.50	0	-	-
	TIS	11	-	0.28	48	1.00	17	0.91	12	1.38	8	0.26	42
	Open BC	-	25.66	0.41	24	1.08	10	0.97	6	1.43	5	0.16	26
	BC I	-	21.15	0.35	35	1.00	17	0.88	15	1.47	2	0.29	47
	BC II	-	19.33	0.44	19	0.96	20	0.84	18	1.48	1	0.38	61
	BC III	-	22.20	0.35	35	1.00	17	0.88	15	1.47	2	0.29	47
	BC IV	-	23.61	0.39	28	1.04	13	0.92	11	1.45	3	0.22	35
Lowest Error		BC II		Open BC		Open BC		BC II		Open BC			
Scale-Up	Experimental	-	-	0.23	0	0.97	0	0.90	0	1.61	0	-	-
	TIS	10	-	0.25	9	0.99	2	0.90	0	1.32	18	0.12	14
	Open BC	-	24.32	0.40	74	1.07	10	0.95	6	1.41	12	0.23	27
	BC I	-	19.83	0.34	48	0.99	2	0.88	2	1.44	11	0.07	8
	BC II	-	17.98	0.41	78	0.94	3	0.81	10	1.46	9	0.12	14
	BC III	-	20.89	0.34	48	0.99	2	0.88	2	1.44	11	0.07	8
	BC IV	-	22.29	0.37	61	1.03	6	0.92	2	1.43	11	0.15	18
Lowest Error		TIS		TIS, BC I, III		TIS		BC II		BC I, III			