SUPPLEMENTAL MATERIAL

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A comprehensive bulk chlorine decay model for simulating residuals in water distribution systems

11 pages, 1 table, 8 figures

Table S1. Initial (ICC) and rechlorination (RIC) experimental data used for model calibration and validation

Location/ Model	Temp. °C	ICC mg/L	Rechlor time h	RIC mg/L	Min ID data-set
1. Armidale [#] ,	10	1.8			*
Australia	20	1.6	25	2.3	
	20	4.8			*
	20	1.2, 2.0			
	25	1.9			*
2. Greenvale [#] ,	15	1.5			*
Australia	15	2.0			
	20	1.5	25	1.1	
	20	1.5	47	1.2	
	20	4.0			*
	20	1.0, 1.5, 2.0, 3.0			
	25	1.5	24	1.3	*
	25	1.5			
	25	2.0			
3. Harbin ⁺ ,	3.5	1.1	2	0.7	*
China	3.5	1.3	5	1.9	
	3.5	2.5			*
	15.5	1.3, 2.4, 2.9			
	28	1.8	5	1.1	*
	28	2.3	8	2.0	
	28	2.9	18	1.5	*
4. Harsha Lake 1 ⁺	20	5.2	48	2.5	*

USA			48	3.9	
5. Harsha Lake 2%	20	3.1	24	3.0	*
USA			48	3.2	
			411	3.1	

[#]Fisher et al. (2012 and unpublished rechlorination data)

^{*}Decay-test data comprising “minimal ID dataset” for calibrations of specified water

⁺Jonkergouw et al. (2009)

[%]Boccelli et al. (2003)

Figure S1. Chlorine concentrations from augmented two-reactant (2RA) model, calibrated against (A) the Armidale data set comprising decay tests from three IDs and three temperatures plus one rechlorination test and (B) the minimal Armidale data set comprising decay tests from two IDs (three temperatures). Note (for all figures). Colours: rechlorination – green, ID temperature – red to blue; markers: data points – same marker for ID

and any associated rechlorination data; black curves – model fitted to calibration data; coloured curves – model predictions of reserved data; dash length – ICC magnitude. Legend – water, ICC, temperature and rechlorination time (hours after ID).

Figure S2. Chlorine concentrations from 2RA model, calibrated against the minimal Greenvale data set comprising decay tests from (A) one ID at 20°C and (B) one ID at 15°C and 25°C. Note: markers, curves and legend defined in Figure S1.

Figure S3. Chlorine concentrations from 2RA model, calibrated against the Harbin data set comprising decay tests from (A) three IDs and two rechlorinations at 3.5°C, (B) three IDs and three rechlorinations at 28°C and (C) three IDs at 15.5°C (shown in Figure S3) – data from Jonkergouw et al. (2009). Markers, curves and legend are as defined in Figure S1.

Figure S4. Chlorine concentrations at 15.5°C from 2RA model, calibrated against the Harbin data set described in Figure 3. Note: markers, curves and legend defined in Figure S1. Experimental data from Jonkergouw et al. (2009).

Figure S5. Chlorine concentrations from 2RA model, calibrated against the minimal Harbin data set comprising decay tests from (A) two IDs and lower rechlorination at 3.5°C, and (B) two IDs and highest rechlorination at 28°C (experimental data from Jonkergouw et al. 2009). Note: markers, curves and legend defined in Figure S1.

Figure S6. Chlorine concentrations from 2R model, calibrated against data set comprising single ID plus two rechlorination decay tests from Harsha Lake 1. Markers, curves and legend are as defined in Figure S1.

Figure S7. Chlorine concentrations from 2R model, calibrated against data set comprising the single ID plus higher rechlorination decay test from Harsha Lake 1 (data from Jonkergouw et al. 2009). Markers, curves and legend are as defined in Figure S1.

Figure S8. Chlorine concentrations from 2R model of Harsha Lake 2 water calibrated against the minimal data set comprising a single ID and latest rechlorination to 3 mg/L at 411h (data from Boccelli et al. 2003). Markers, curves and legend are as defined in Figure S1.

Accuracy of modelling post-rechlorination initial conditions. As described in the Methodology section, each model was forced to match closely the post-rechlorination initial concentration of chlorine (RIC) during the parameter optimization process in AQUASIM. The squared difference between modelled and measured RIC (SSD_{ric}) was given 100 times the weighting of any other squared difference in the calculation of SSD_c . This resulted in very small model deviations from the measured RICs (<0.03 mg/L). The only exception was for the successive rechlorinations of Harsha Lake 2 water, for which deviations (<0.05 to <0.08 mg/L) were still comparable with the experimental error associated with the higher chlorine levels dosed.

The additional contribution of the optimized weighted deviations to the SSD_c for each model calibration, as a percentage of total SSD, was <0.1 to 0.4% , which would affect only the third significant digit in these values. (The SSD_t values given in Table 2 include only the contributions from the data, not those from the deviations from the RICs). The only exception was the calibration involving all available data for Harsha Lake 2 water. The contribution of 1.9% was largely due to the uncharacteristically faster decay occurring immediately after the first rechlorination, so that forcing the model to replicate the RIC closely results in over-prediction of almost all data points until the second rechlorination. The two later RICs were just as accurately represented as RICs in other waters. It was therefore considered that this model's representation of the successive rechlorinations was also satisfactory.