26th International Congress on Modelling and Simulation, Adelaide, SA, Australia, 30 Nov–4 Dec 2025
mssanz.org.au/modsim2025

Industry application of multispecies modelling to track chloramine decay in a water network

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Keywords: *Monochloramine, Ammonia, Modelling, Water quality*

1. INTRODUCTION

Monochloramine is increasingly being selected as a primary disinfectant for treating drinking water by SA Water. To deliver safe drinking water to customers, the disinfectant residual should be monitored. Hydraulic modelling in conjunction with multi-species analysis can provide the concentrations of the disinfectant and its by-product at any point in a water network. This technology has the potential to improve water quality by highlighting locations in the network where the disinfectant concentration is inadequate. This technology has had limited application in the industry.

The decay mechanisms of monochloramine in water include auto-decomposition and biological decomposition. The Bentley software package, WaterCAD, has an inbuilt multi-species analysis option which can be used to model the concentration of disinfectants and by-products through the network. The inputs of the existing kinetics model are readily available measured data, including measured concentrations of monochloramine, free chlorine and ammonia. The suitability of this type of modelling outside of academia has been assessed by comparing it with measured data and assessing its limitations.

2. METHOD

To investigate the applicability of the multi-species reaction kinetics for monochloramine decay in an existing extensive water network, a calibrated hydraulic model of the Tailem Bend-Keith water network in South Australia was developed. Established monochloramine decay kinetics were applied which are the default kinetics for monochloramine decay in the model, see Equations 1-16, where I is the intermedial product, S1 is the fast reactive fraction of TOC, S2 is the slow reactive fraction of TOC. The model was run for average day and winter day demands.

The initial conditions for the multispecies analysis included specifying pH across the network, alkalinity and monochloramine concentration at the disinfectant injection points. The model was run with and without the dissolved organic carbon (DOC) component to represent the biological decay reactions. Measured data was used to determine the applicability of the multi-species model to the existing network.

Processing the results included extracting the concentrations for each component at the calibration point for the last 24 hours of the model run where the concentrations were at a steady state. The average, minimum and maximum concentration in this time frame were used for comparisons.

$HOCL + NH_3 \rightarrow NH_2Cl + H_2O$	(1)	$I + NH_2\,Cl \rightarrow products$	(9)
$NH_2Cl + H_2O \rightarrow HOCL + NH_3$	(2)	$NH_2\,Cl + NHCl_2 \rightarrow products$	(10)
$HOCL + NH_2Cl \rightarrow NHCl_2 + H_2O$	(3)	$NH_2\,Cl + S_1 \times TOC \rightarrow products$	(11)
$NHCl_2 + H_2O \rightarrow HOCL + NH_2\,Cl$	(4)	$HOCL + S_2 \times TOC \rightarrow products$	(12)
$NH_2\,Cl + NH_2Cl \rightarrow NHCl_2 + NH_3$	(5)	$HOCL \leftrightarrow H^+ + OCL^-$	(13)
$NHCl_2 + NH_3 \rightarrow NH_2\,Cl + NH_2Cl$	(6)	$NH_4^+ \leftrightarrow NH_3 + H^+$	(14)
$NHCl_2 + H_2O \rightarrow I$	(7)	$H_2CO_3 \leftrightarrow HCO_3^- + H^+$	(15)
$I + NHCl_2 \rightarrow HOCL + products$	(8)	$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$	(16)

3. RESULTS

The monochloramine concentrations were better predicted with the addition of DOC as a component in the network. Of the 11 calibration points for monochloramine concentration, 3 of the measured results were out of the

range of the modelled results. The kinetic calculations at the location of Tailem Bend tank outlet and Meningie tank outlet show significant error.

The ammonia concentration varied by a maximum of 0.3 mg/L for measured and modelled results for the chemical only decomposition model. When the biological decomposition was added, the modelled results were more than 10 times greater than the measured results. The kinetic calculations again showed significant variation between measured and modelled results at the Meningie tank outlet. This is because of the significant oscillations seen for concentration calculations at these points in the model. These oscillations are the result of the flow fluctuating by 40 L/s over short time intervals. Hence, the average concentration of the last 24 hours of the model run used to calculate concentration underestimates the monochloramine and ammonia results at these locations. Free chlorine (HOCL) concentration was <1mg/L through all measured data. The same was seen in the modelled results.

Increased hydraulic retention times (HRTs) result in reduced accuracy in the concentrations modelled. This is evidenced by the greater deviation between measured and modelled results generally seen for the longer retention times, see Figure 1.

Up to 76 hours of processing time were required for the model to be run to reach steady state. Oscillating concentrations require further analysis of results at some calibration points. In the case where flow fluctuates significantly multiple times over a 24 hour period, the kinetics need to be resolved with greater accuracy. One possible method to reduce error caused by these oscillations includes reducing the time step for the model run. This will extend the already long processing times. These factors prevent the multi-species model from being efficiently used in industry at this time.

4. CONCLUSIONS

The multi-species extension in Bentley is currently limited by extended run times, longer HRTs resulting in greater deviations in results and oscillating concentration values calculated as a result of large flow fluctuations when run with the default kinetics for monochloramine decay. Ammonia concentration is also not accurately predicted with the addition of DOC in the model. The complexity of the kinetic equations in the existing model limits its practical use in industry. To validate the reaction kinetics and use of the multi-species extension, it should also be applied on other existing water networks and calibrated against additional measured data.

Table 1: Monochloramine modelled verse measured results for average day

	Average Day Model Auto-decomposition Only			Average Day Model with DOC		
Location	**Average**	**% Error - Average**	**In range?**	**Average**	**% Error - Average**	**In range?**
Jervois Tank (EL 26) 0.5ML	3.3	18%	FALSE	3.5	11%	TRUE
Karoonda Tank (EL 100) 0.273ML	2.3	31%	FALSE	2.7	19%	FALSE
Meningie Tank Outlet (EL 67) 0.273ML	0.4	88%	FALSE	0.5	85%	FALSE
Seymour Tank (EL 96) 0.136ML	2.7	23%	FALSE	3.1	12%	TRUE
Sugarloaf Tank Inlet	1.9	41%	FALSE	2.3	28%	TRUE
Sugarloaf Tank Outlet	3.5	-7%	TRUE	3.5	-7%	TRUE
Trility Tailem Bend WTP Treated Water	3.9	5%	TRUE	4.1	2%	TRUE
Wingamin Tank (EL 118) 0.22ML - AC (temporary)	2.8	15%	TRUE	3.2	5%	TRUE
Wynarka Tank (EL 119) 0.14ML	2.9	15%	TRUE	3.2	7%	TRUE
Wynarka Tank (EL 119) 0.23ML	3.1	9%	TRUE	3.4	1%	TRUE
Tailem Bend Tank Outlet (EL 54) 0.455ML	1.9	54%	FALSE	2.3	44%	FALSE

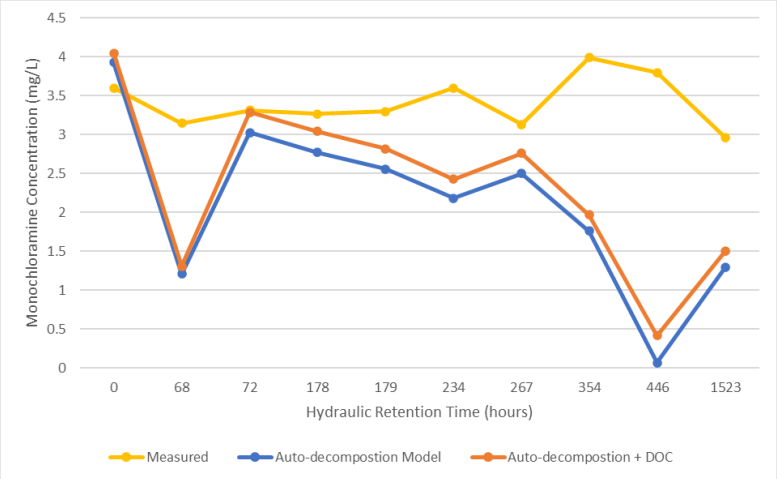

Figure 1: Monochloramine concentration versus HRT for winter day

