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Modeling approaches to predict removal of trace organic compounds by ozone oxidation in potable reuse applications

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Supplementary information

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1. Latin hypercube-One-factor-At-a-Time (LH-OAT) method

LH-OAT method is a sensitivity analysis successively applying LH sampling and OAT sampling[1, 2]. As a procedure of LH sampling, N sample points for N intervals were taken. Then, each of the N points is changed P times by changing each of the P paramters one at a time as OAT sampling. Partial effect $S_{i,j}$ for each paramter e_i can be calculated using the following equation:

$$S_{i,j} = \left| \frac{100 * \left(\frac{M\left(e_1,...,e_i*(1+f_i),...,e_p\right) - M\left(e_1,...,e_i,...,e_p\right)}{\left[M\left(e_1,...,e_i*(1+f_i),...,e_p\right) + M\left(e_1,...,e_i,...,e_p\right)/2 \right]} \right)}{f_i} \right|$$

where $M(\cdot)$ is the model function, f_i is the fraction by which the parameter e_i is changed and j refers to an LH point. The final effect S was determined by averaging the partial effects ($S_{i,j}$) after 1000 loops for all the LH points.

2. Tables

Table S1 Modeling result of four- and three parameter MLR models.

Four-parameter MLR model				
	Estimate	SE	t statistics	*p*-value
Intercept	-32.77	9.715	-3.373	0.001120
O_3	10.22	0.6813	15.00	7.490×10^{-24}
TOC	1.130	1.185	0.9532	0.3437
k_{O3}	6.912×10^{-5}	6.166×10^{-6}	11.21	1.900×10^{-17}
$k_{\bullet OH}$	6.023×10^{-9}	9.450×10^{-10}	6.373	1.546×10^{-8}
Three-parameter MLR model				
	Estimate	SE	t statistics	*p*-value
Intercept	-25.92	6.541	-3.963	1.7042×10^{-4}
O_3	10.27	0.6787	15.13	3.288×10^{-24}
k_{O3}	6.900×10^{-9}	6.161×10^{-6}	11.20	1.639×10^{-17}
$k_{\bullet OH}$	6.052×10^{-9}	9.439×10^{-10}	6.412	1.546×10^{-8}

3. Figures

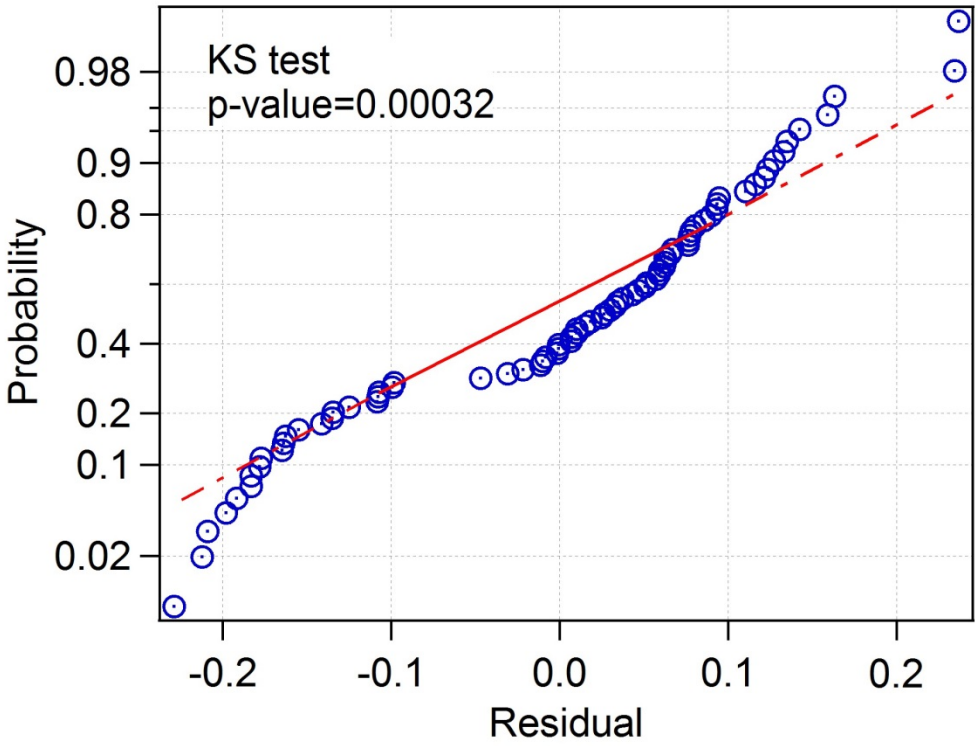

Fig. S1. A normal probability plot of the residuals from the four-parameter MLR model.

References

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2. K. H. Cho, S. Sthiannopkao, Y. A. Pachepsky, K.-W. Kim and J. H. Kim, *Water Research*, 2011, **45**, 5535-5544.