Supplementary Material

Modeling the Formation and Propagation of 2,4,6-trichloroanisole, a Dominant Taste and Odor Compound, in Water Distribution Systems

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Nomenclature

A = concentration of 2,4,6-trichloroanisole as a function of time and axial dimension (ng/L)

C = concentration of free chlorine as a function of time and axial dimension (mg/L)

H = concentration of trihalomethanes as a function of time and axial dimension (µg/L)

K_s = half-saturation constant (mg/L)

E_{K_d} = temperature coefficient corresponding to 2,4,46-TCP degradation

E_{Y_f} = temperature coefficient corresponding to 2,4,6-TCA formation

N = concentration of total organic carbon as a function of time and axial dimension (mg/L)

P = concentration of 2,4,6-trichlorophenol as a function of time and axial dimension (mg/L)

R_h = hydraulic mean radius (m)

S = concentration of biodegradable dissolved organic carbon as a function of time and axial dimension (mg/L)

T_i = temperature-dependent shape parameter (°C)

T_{opt} = optimal temperature for microbial activity (°C)

X_a = concentration of biofilm as a function of time (CFU/cm^2)

X_b = concentration of planktonic microorganisms as a function of time and axial dimension (CFU/mL)

Y = growth yield of microorganisms (CFU/mg)

Y_{H1} = reaction yield coefficient corresponding to THMs formation from chlorination of NOM (µg/mg)

Y_{H2} = reaction yield coefficient corresponding to THMs formation from chlorination of microorganisms (µg/mg)

Y_N = reaction yield coefficient for NOM (mg/mg)

Y_{pf} = pipe material-dependent yield coefficient (ng/mg)

Y_X = reaction yield coefficient for microorganisms (CFU/mg)

a = fraction of dead microorganisms contributing to BDOC

a_1 = 2,4,6-TCP degradation constant (1/s)

a_2 = yield coefficient corresponding to 2,4,6-TCA formation (ng. mL/mg. CFU)

b = microbial activation constant (mL/CFU)

k_{CN} = second-order kinetic constant corresponding to reactions between chlorine and NOM (L/mg. s)

k_{CX} = second-order kinetic constant corresponding to reactions between chlorine and microorganisms (L/CFU.s)

k_{dep} = deposition/ attachment constant (1/s)

k_{det} = microbial detachment coefficient (m.s/g)

k_f = mass-transfer coefficient of chlorine (m/s)

k_{inact} = bacterial growth inactivation constant (L/mg)

k_{mort} = microbial mortality constant (1/s)

k_r = resistance factor of biofilm to chlorine-induced mortality

k_w = wall decay coefficient (m/s)

μ_{max} = maximum specific growth rate of microorganisms (1/s)

τ_w = shear stress at pipe wall (g/m. s^2)

t = time (s)

u = flow velocity (m/s)

x = distance along the axial direction (m)

S1. Taste and odor in water distribution systems

The taste and odor (T&O) problems in drinking water always get massive complaints from water consumers based on their direct sensory judgment [1]. The terms 'taste' and 'odor' are used combinedly in the vernacular concerning drinking water. As a definite sensory process, out of the two, taste is seldom a problem in water distribution systems (WDSs) and most 'tastes' are concerned almost wholly with odors [2,3]. According to a water survey, the taste problems characterized by the consumers of the water utilities include sour, sweet, salty, bitter, metallic, chlorine, medicinal, and musty [4]. Out of them, sour was the taste problem most often identified, and metallic was the second most common problem. Interestingly, psychologists claim that there are only four taste sensations: sour, sweet, salty, and bitter [2]. Thus, it may be inferred that all the other taste sensations are odors, although the sensation remains unnoticed until the material gets actually into the mouth.

The human olfactory system can recognize various odors and distinguish the elusive differences between different chemicals in the water [5]. The odors recognized by the water consumers are commonly described as earthy, musty, chlorinous, grassy, swampy, septic, sulfide, hay-like, manure, geranium, fishy, moldy, paint-like, woody, marshy, iodoform-like, medicinal, phenol, aromatic, and petroleum [2,4]. The earthy-musty T&O is the one that is most frequently detected in WDSs [4]. These are caused predominantly by the presence of geosmin (GSM, earthy) [6], 2-methylisoborneol (2-MIB, musty) [7], and 2,4,6-trichloroanisole (2,4,6-TCA, musty) [8] in water. Algae and decaying vegetation are the principal substances related to natural sources of T&O [6,9], and the man-made sources include domestic and industrial wastes and agricultural activities [2]. The T&O problems in drinking water may mask the graver concerns related to microbiological and chemical quality failures [10]. Consequently, many countries have executed non-mandatory (secondary) standards to guide the drinking water's organoleptic quality [11].

Numerous analytical procedures have been proposed for measuring T&O in water. Even though the human olfactory sensory analytic measures are not totally acceptable, there is no alternative. Apparently, no devices instrumented for measuring T&O have been able to replace the human nose. However, some modifications to improve the sensory tests for T&O have been proposed. Nevertheless, none has been universally accepted.

One of the most common and most routinely used tests in water treatment plants is the threshold odor number (TON) test. Threshold odor number is defined as the ratio by which the odor-bearing sample has to be diluted with odor-free water for the odor to be just detectable [2]. The total volume of sample and odor-free water used in each test is 200 mL.

A second odor threshold test, ASTM-D-1292, is generally applied for industrial water and wastewater. The summary of the method as explained by [2] is given as follows:

"The sample of water is diluted with odor-free water until a dilution is obtained that has the least definite perceptible odor. The test is made by two or more testers. One makes dilutions, and the others determine odor intensity. Samples are tested in increasing concentration until the odor is perceived. The persons making the test select the odorous sample from three, two of which contain odor-free water. Cognizance is made of the fact that there is no absolute odor value and that the test is to be used for comparison only. The test is carried out at 40°C. The odor intensity index (OII), a related value of TON, can be determined. The OII is the number of times, *n*, the concentration of the original sample is halved by the addition of odor-free water to obtain the barely perceptible odor. The TON should be 2^n."

S2. Basic multi-species interactions considered in the model formulation

The physicochemical and biological interactions between the seven model species: chlorine, total organic carbon (TOC), biodegradable dissolved organic carbon (BDOC), microorganisms (planktonic and biofilm), trihalomethanes (THMs), 2,4,6-trichlorophenol (TCP), and 2,4,6-trichloroanisole (2,4,6-TCA) considered in the multi-species reactive-transport (MSRT) model are as follows:

(i) *Chlorine decay inside the distribution pipes*

The chlorine reactions with the natural organic matter (NOM) and the planktonic microbiota, causing its decay in the bulk phase, are denoted using second-order kinetics based on the hypothesis of competing reactions in water [12]. The mass transfer of chlorine from the bulk to the wall phase is assumed to occur through a boundary layer and is presumed to be limited by the bulk phase's chlorine concentration [13]. The chlorine reactions with the biofilm layers at the pipe wall are described by first-order kinetics concerning bulk chlorine concentration [14].

(ii) *Microbial regrowth dynamics*

The Monod equation denoted the regrowth and substrate utilization of the planktonic microbial regrowth [15], while a first-order model defined the biofilm regrowth against the inhibitory effects of chlorine and temperature. A resistance factor was used to indicate the greater resistance of the biofilm microorganisms against the chlorine-induced inactivity [16]. The microbial senescence was modeled with first-order kinetics, and the chlorine-induced mortality of planktonic microbiota was modeled with second-order kinetics. 30 percent of the dead bacteria were assumed to be enriching the BDOC by discharging intracellular matter during cell lysis after senescence as well as due to the effects of chlorine [17]. The microbial deposition on the biofilm was assumed to have first-order dependence concerning the planktonic microbial density [18] and zero-order dependence on the biofilm density. The microbial detachment from the biofilm layers was presumed to have first-order dependence on the shear stress induced by the flow velocity [19] and the biofilm density [20].

(iii) *Disinfection by-products formation dynamics*

The trihalomethanes (THMs) formation was assumed to be caused by the chlorination of NOM and microbial-derived disinfection by-product (DBP) precursors. Their formation rate was

assumed to be the same as that of chlorine decay, and their kinetics was modeled using the reaction yield coefficients [21].

(iv) *2,4,6-TCP degradation and 2,4,6-TCA formation dynamics*

A first-order model was applied to model the 2,4,6-TCP degradation based on the assumption that the 2,4,6-TCP concentration in the bulk phase limits the reaction rate, and the planktonic microbial density governs the reaction kinetics. The 2,4,6-TCA formation rate was presumed to be the same as that of 2,4,6-TCP degradation rate and was modeled using a reaction yield coefficient. The planktonic microbial density was expected to be regulating the 2,4,6-TCP degradation kinetics logarithmically, while a linear relationship was presumed between planktonic microbial cell count and the 2,4,6-TCA formation yield.

S3. Governing equations of the MSRT model

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{CN} \times N \times C - k_{CX} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S1)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_N \times k_{CN} \times N \times C + a(Y_X \times k_{CX} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S2)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_N \times k_{CN} \times S \times C + a(Y_X \times k_{CX} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S3)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_X \times k_{CX} \times X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S4)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times R_h - k_{det} \times \tau_w \times X_a \quad \text{(S5)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_{H1} \times k_{CN} \times N \times C + Y_{H2} \times k_{CX} \times X_b \times C \quad \text{(S6)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times P \quad \text{(S7)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T+273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times P \quad \text{(S8)}$$

Table S1. Values and literature sources of the model parameters used

Parameter	Value/ Formula	Unit	Reference	Value used
k_{CN}	$3 \times 10^{4} \times \exp\left(-\frac{6050}{T+273}\right)$	L/mg. s	[22]	-
k_{CX}	$3 \times 10^{-4} \times \exp\left(-\frac{6050}{T+273}\right)$	L/CFU. s	[23]	-
k_w	1.04 x 10^{-7}- 1.43 x 10^{-5}	m/s	[24]	1.04 x 10^{-7} m/s
	0.0072	mg/m^2. s	[25]	
$\mu_{max,b}$	1.39 x 10^{-5} - 4.2 x 10^{-4}	1/s	[13,26]	4.2 x 10^{-4} 1/s
$\mu_{max,a}$	7.2 x 10^{-16} – 6.1 x 10^{-10}	mg/CFU.s	[18]	8.6 x 10^{-7} 1/s
K_S	0.05 – 1.20	mgC/L	[27,28]	0.195 mg/L
Y	0.007 – 1.50	mg/mg	[18]	0.007 x 10^{6} CFU/mg
k_{inact}	0.05 – 5.0	L/mg	[13,18,23]	0.35 L/mg
T_{opt}	37	°C	[25]	37 °C
T_i	7	°C	[25]	7 °C
Y_X	0.59 ± 0.15	mg/mg	[16]	0.34 x 10^{6} CFU/mL
Y_N	0.4 – 4.88	mg/mg	[29]	0.98 mg/mg
a	0.3	-	[17]	0.3
k_{mort}	9 x 10^{-7} - 1.8 x 10^{-5}	1/s	[13,18]	6.3 x 10^{-5} 1/s
k_{dep}	5.5 x 10^{-6} - 4.2 x 10^{-4}	1/s	[18]	5.5 x 10^{-6} 1/s
k_{det}	4 x 10^{-4}	1/s	[13]	6.618 x 10^{-7} m.s/g
	6.618 x 10^{-7}	m.s/g	[20]	
τ_w	Blasius equation	g. m/s^2	[19]	-
k_r	3 – 3,000	-	[18]	100
Y_{H1}	5.68 – 188.20	µg /mg	[21,29]	118.435 µg/mg
Y_{H2}	4.487	µg/mg	[23]	4.487 µg/mg

Table S2. Results of KLmod network simulations

C_o (mg-/L)	Average 2,4,6-TCA concentration (ng/L)		α_1		Average biofilm density (CFU/cm^2)	Average planktonic microbial cell count (CFU/mL)	α_2	Average residual chlorine concentration (mg/L)	Average THMs concentration (µg/L)	α_2
	P_o = 0.2 mg/L	P_o = 0.01 mg/L	P_o = 0.2 mg/L	P_o = 0.01 mg/L						
T = 10 °C										
NIL	2.67	0.13	0.446	0.967	6.95 x 10^5	0.029	1	-	-	1
0.5	2.63	0.13	0.450	0.967	6.64 x 10^5	0.023	1	0.365	14.54	1
1.0	2.60	0.13	0.454	0.968	6.33 x 10^5	0.018	1	0.749	26.79	1
T = 25 °C										
NIL	7.51	0.38	0.142	0.906	7.61 x 10^5	0.034	1	-	-	1
0.5	7.32	0.37	0.146	0.908	6.93 x 10^5	0.021	1	0.250	27.67	1
1.0	7.15	0.36	0.150	0.911	6.21 x 10^5	0.014	1	0.553	49.17	0.913

Table S3. Average 2,4,6-TCA concentrations at the nodes and α_1 values for the Balerma network under T = 10 °C

S_o (mg/L)	C_o (mg-/L)	Average 2,4,6-TCA concentration (ng/L)				α_1			
		P_o = 0.2 mg/L	P_o = 0.1 mg/L	P_o = 0.05 mg/L	P_o = 0.01 mg/L	P_o = 0.2 mg/L	P_o = 0.1 mg/L	P_o = 0.05 mg/L	P_o = 0.01 mg/L
Scenario I									
	NIL	0.48	0.24	0.12	0.02	0.881	0.940	0.970	0.994
0.01	0.5	0.48	0.24	0.12	0.02	0.881	0.940	0.970	0.994
	1.0	0.47	0.24	0.12	0.02	0.882	0.940	0.970	0.994
	NIL	0.48	0.24	0.12	0.02	0.880	0.940	0.970	0.994
0.1	0.5	0.48	0.24	0.12	0.02	0.880	0.940	0.970	0.994
	1.0	0.48	0.24	0.12	0.02	0.881	0.940	0.970	0.994
	NIL	0.48	0.24	0.12	0.02	0.879	0.939	0.970	0.994
0.3	0.5	0.48	0.24	0.12	0.02	0.880	0.940	0.970	0.994
	1.0	0.48	0.24	0.12	0.02	0.880	0.940	0.970	0.994
Scenario II									
	NIL	1.35	0.67	0.34	0.07	0.663	0.831	0.916	0.983
0.01	0.5	1.33	0.67	0.33	0.07	0.666	0.833	0.917	0.983
	1.0	1.32	0.66	0.33	0.07	0.670	0.835	0.918	0.984
	NIL	1.38	0.69	0.35	0.07	0.655	0.827	0.914	0.983
0.1	0.5	1.36	0.68	0.34	0.07	0.660	0.830	0.915	0.983
	1.0	1.34	0.67	0.34	0.07	0.665	0.832	0.916	0.983
	NIL	1.41	0.71	0.35	0.07	0.647	0.823	0.912	0.982
0.3	0.5	1.39	0.69	0.35	0.07	0.653	0.827	0.913	0.983
	1.0	1.36	0.68	0.34	0.07	0.659	0.830	0.915	0.983

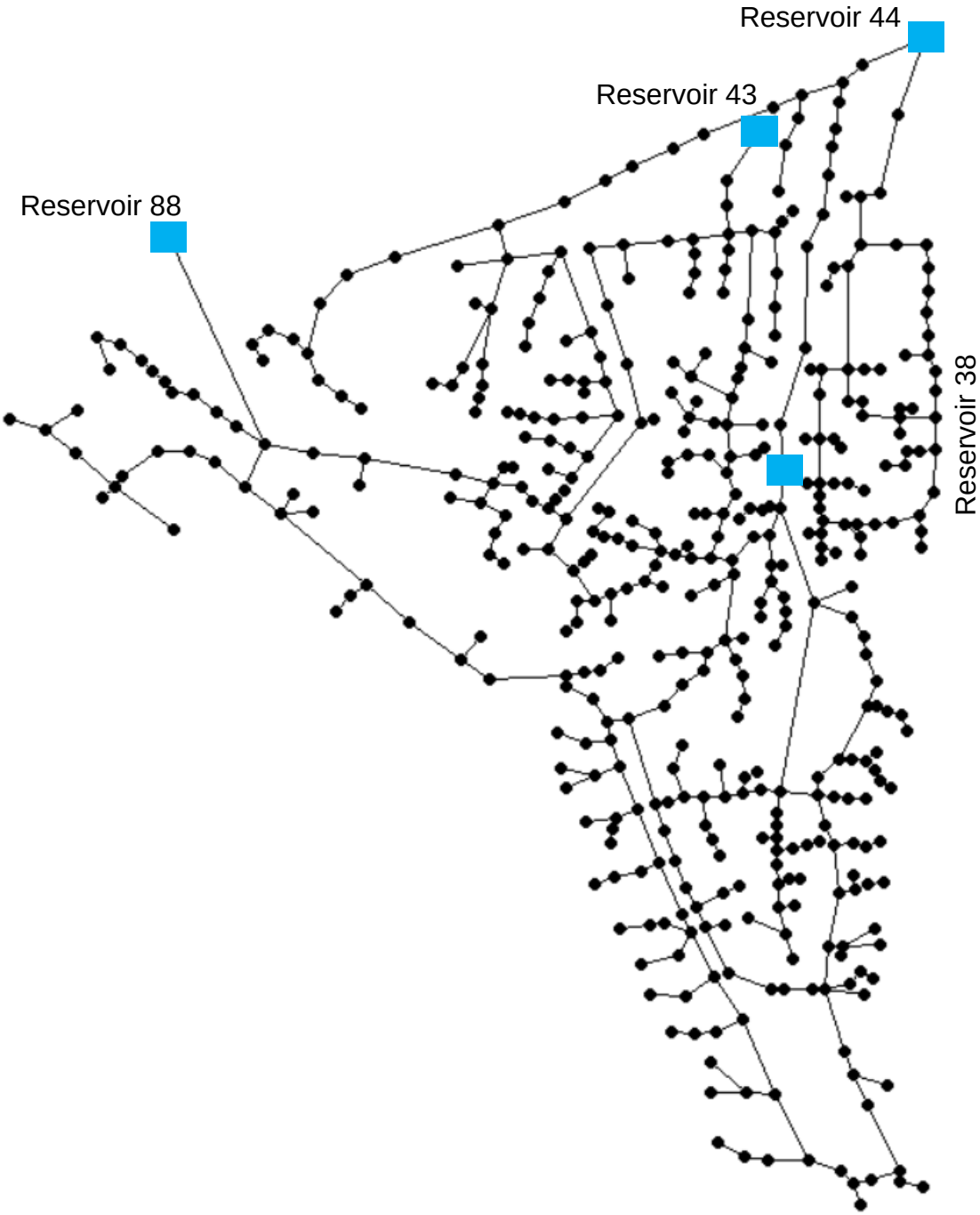


Figure S1. Schematic of Balerma network

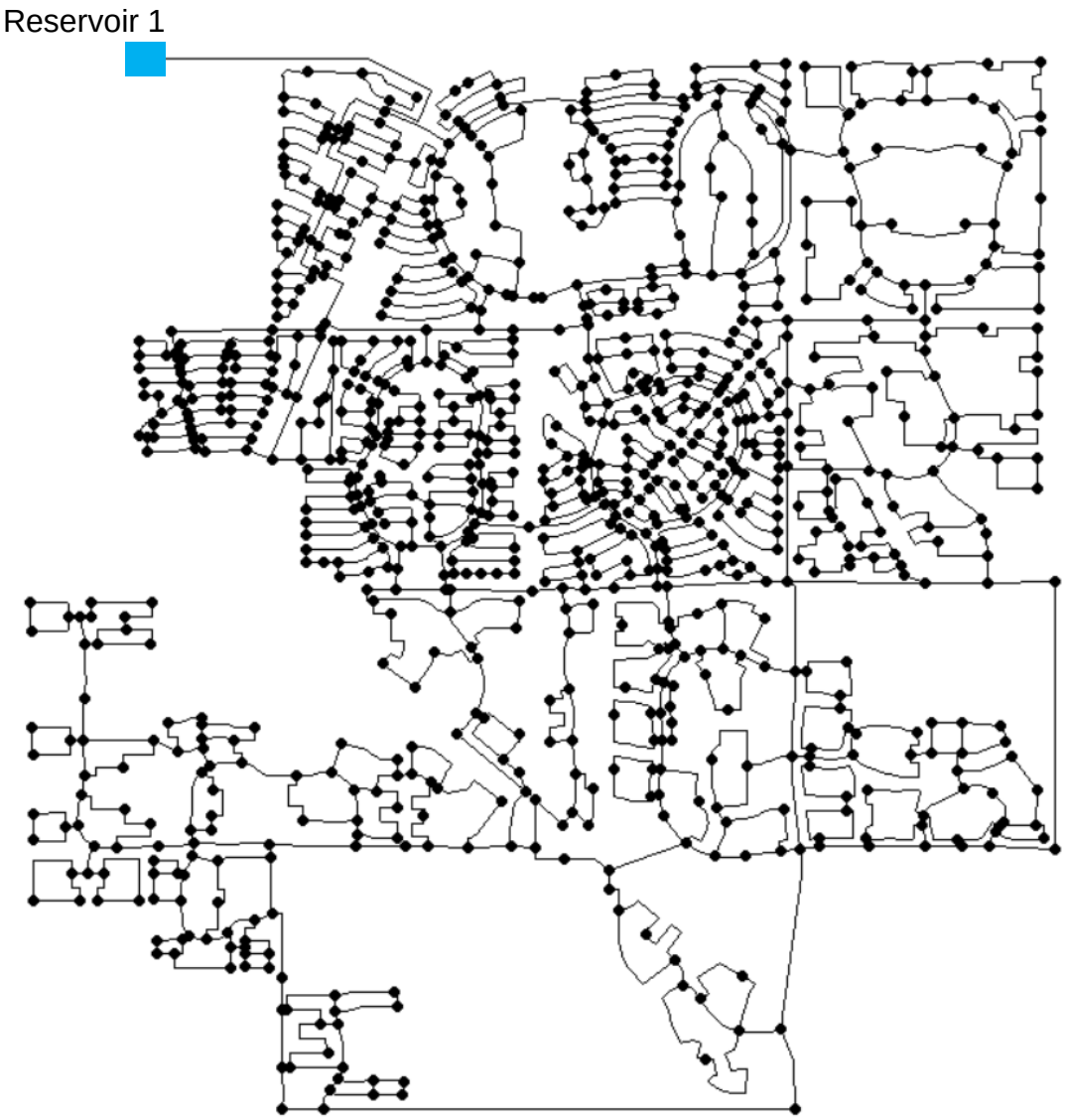


Figure S2. Schematic of KLmod network

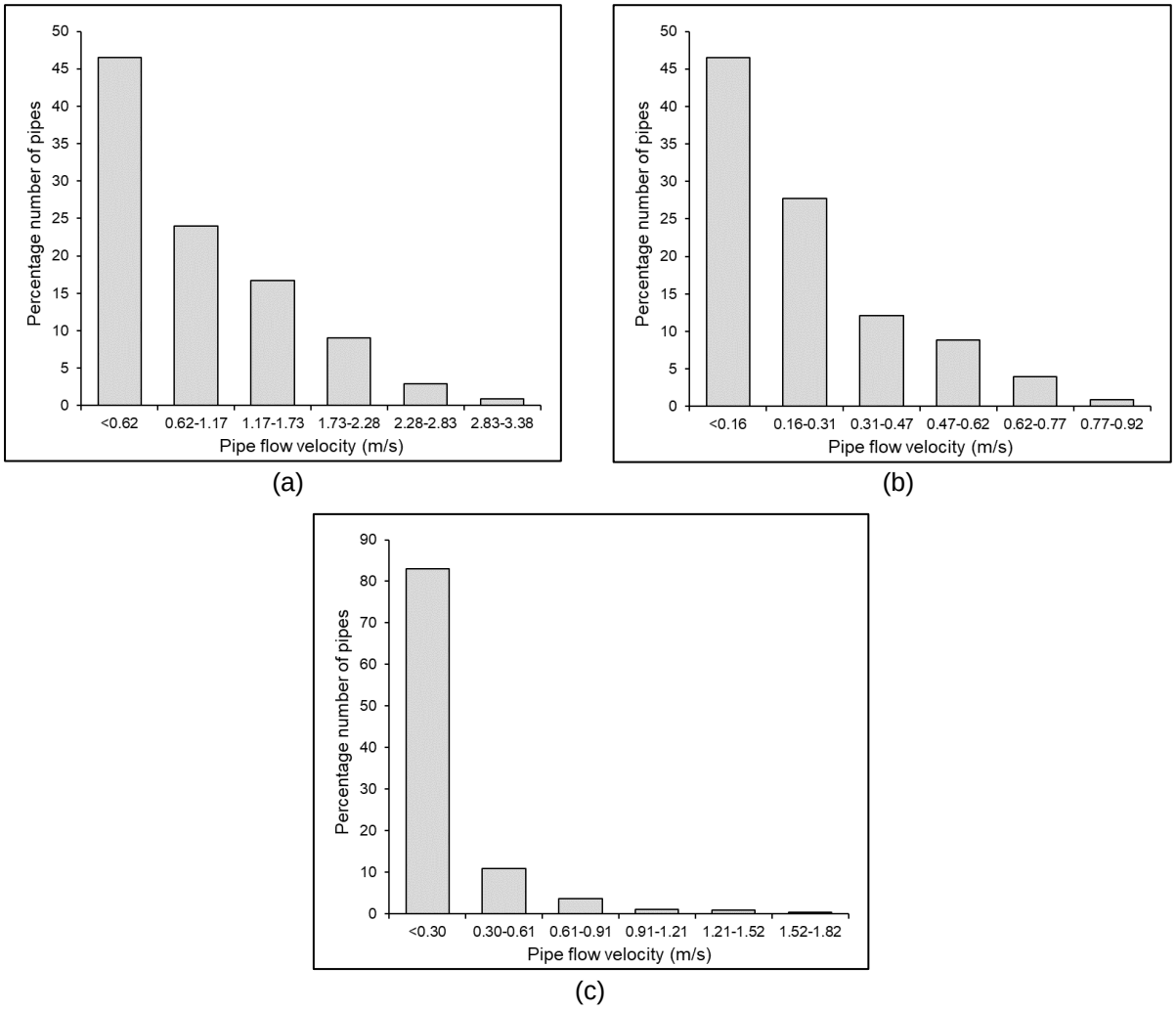


Figure S3. Distribution of pipe flow velocity in the Balerma network ((a) Scenario I and (b) Scenario II) and KLmod network

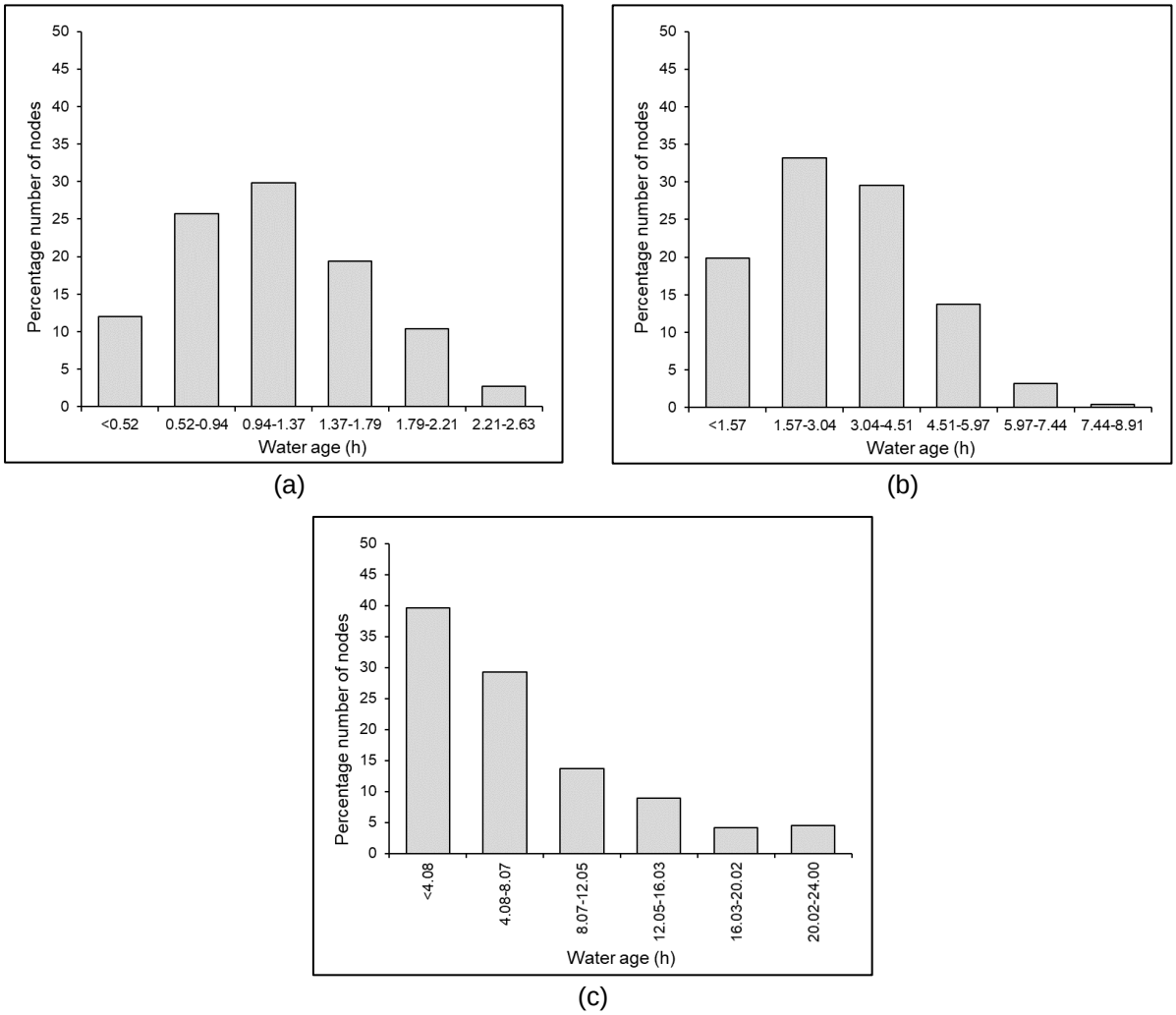


Figure S4. Distribution of water age in the nodes of Balerma network ((a) Scenario I and (b) Scenario II) and KLmod network

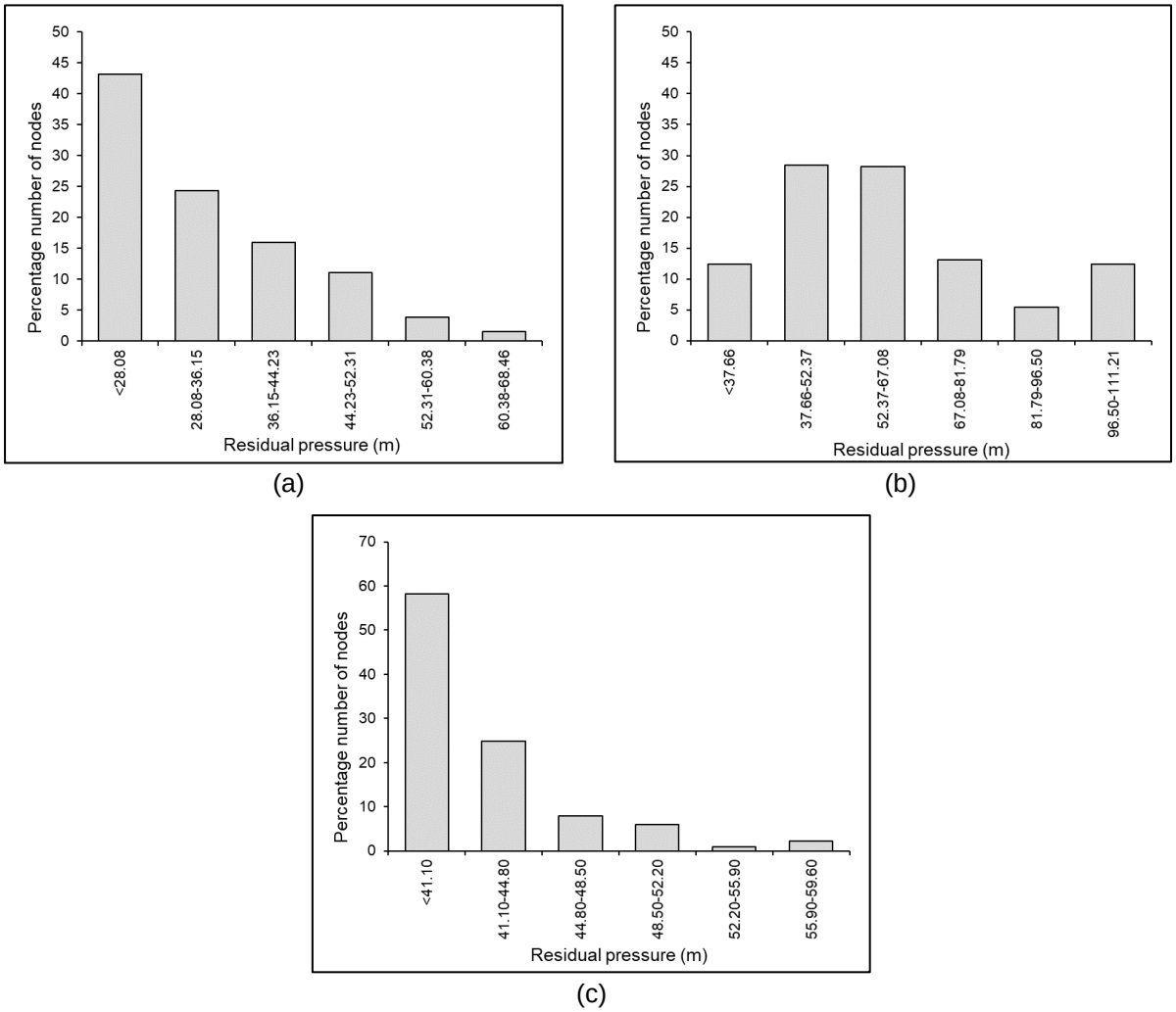


Figure S5. Distribution of residual pressure in the nodes of the Balerma network ((a) Scenario I and (b) Scenario II) and KLmod network

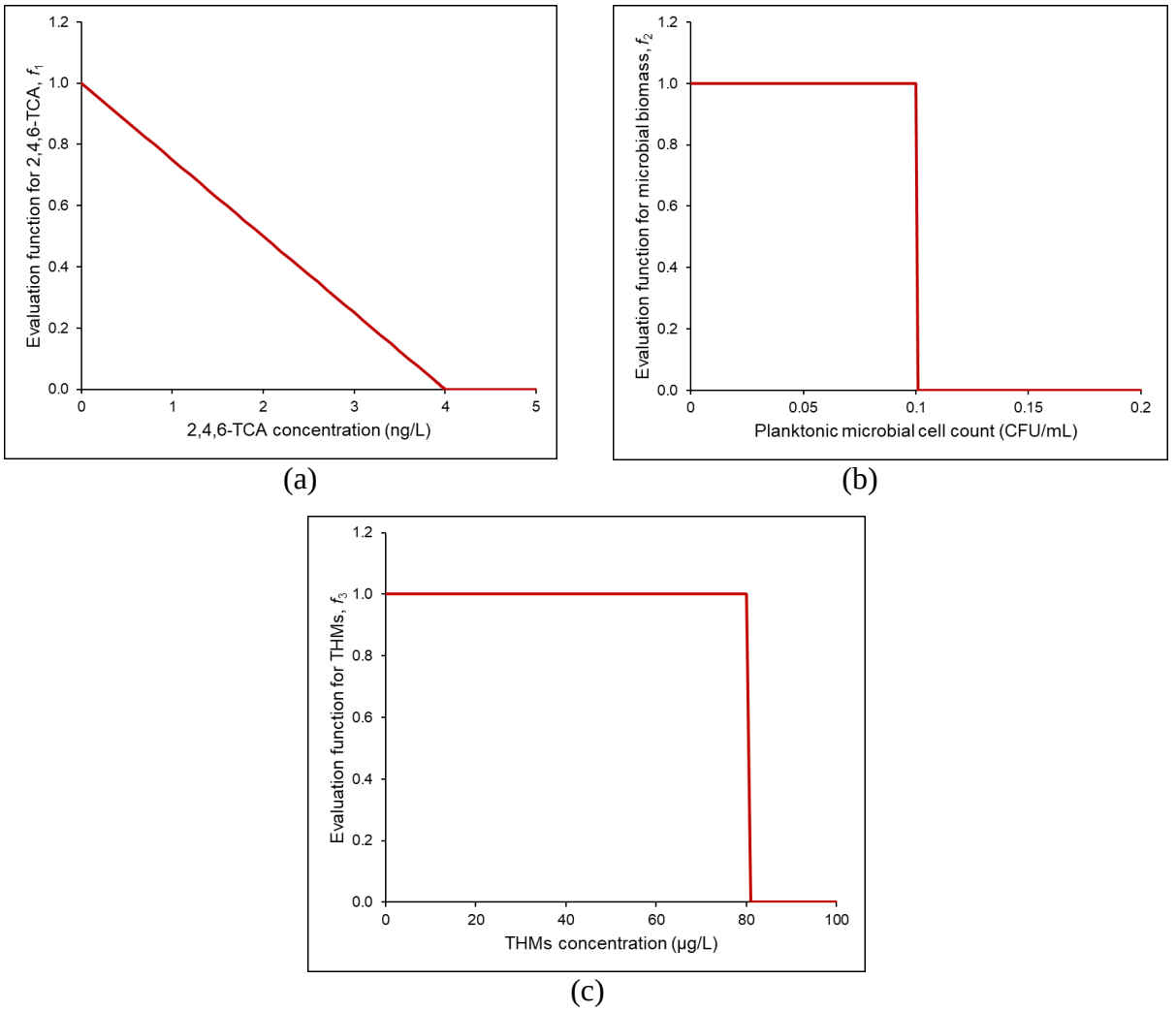
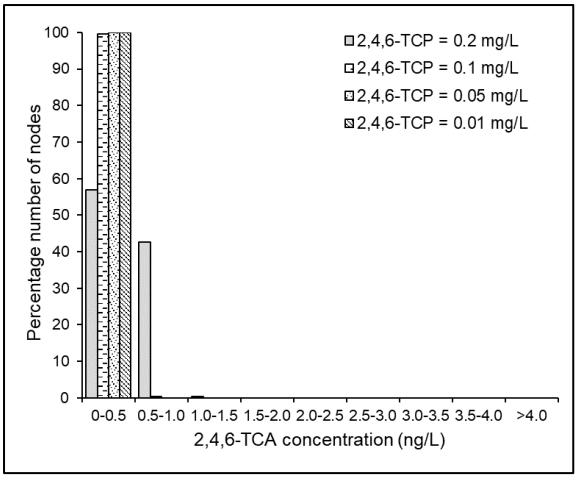
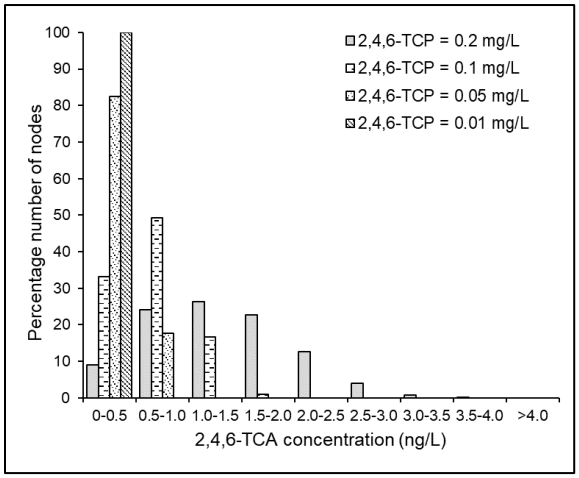


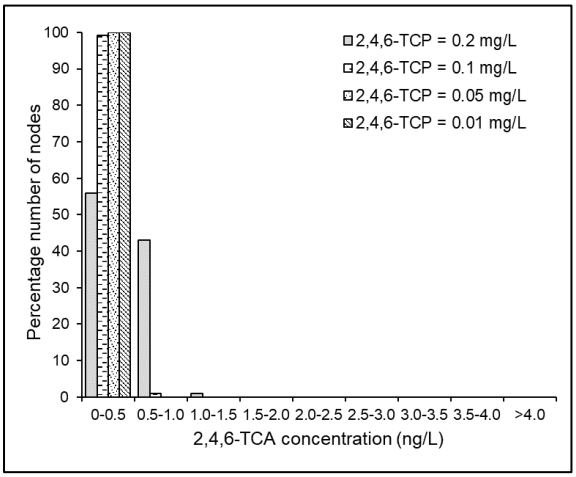
Figure S6. Dedicated evaluation functions for the determination of reliability in terms of (a) 2,4,6-TCA, (b) microbial biomass, and (c) THMs



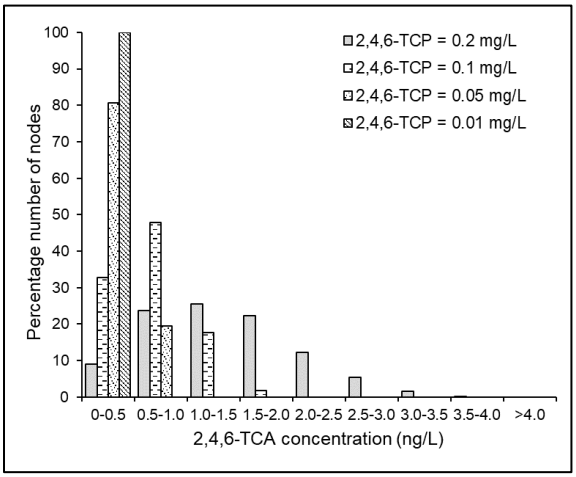
(a)



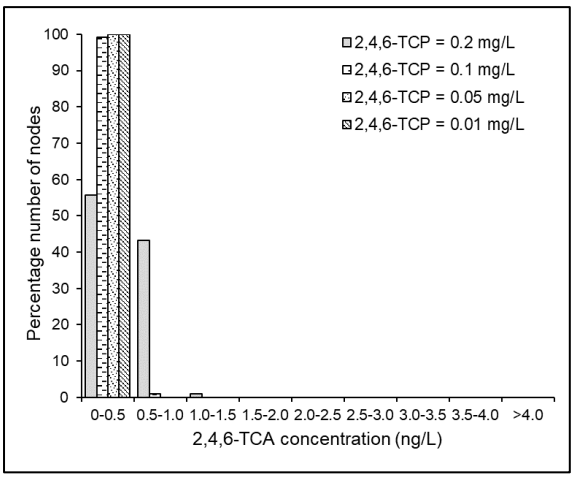
(b)



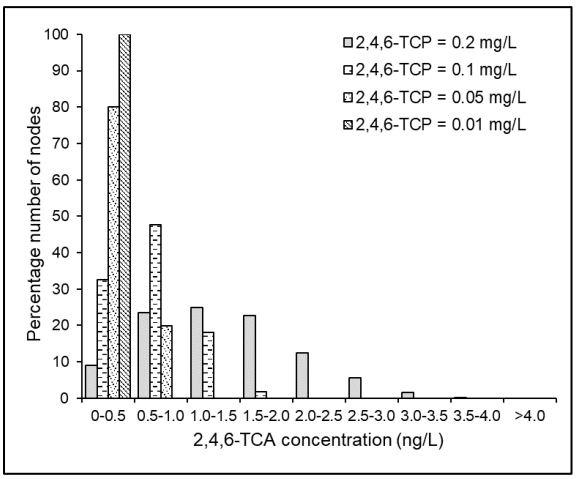
(c)



(d)



(e)



(f)

Figure S7. Predicted distribution of 2,4,6-TCA in the Balerma network under T = 10 °C, S_o = (a)(b) 0.01, (c)(d) 0.1, and (e)(f) 0.3 mg-C/L, Scenario (a)(c)(e) I and (b)(d)(f) II, and under non-chlorinated condition

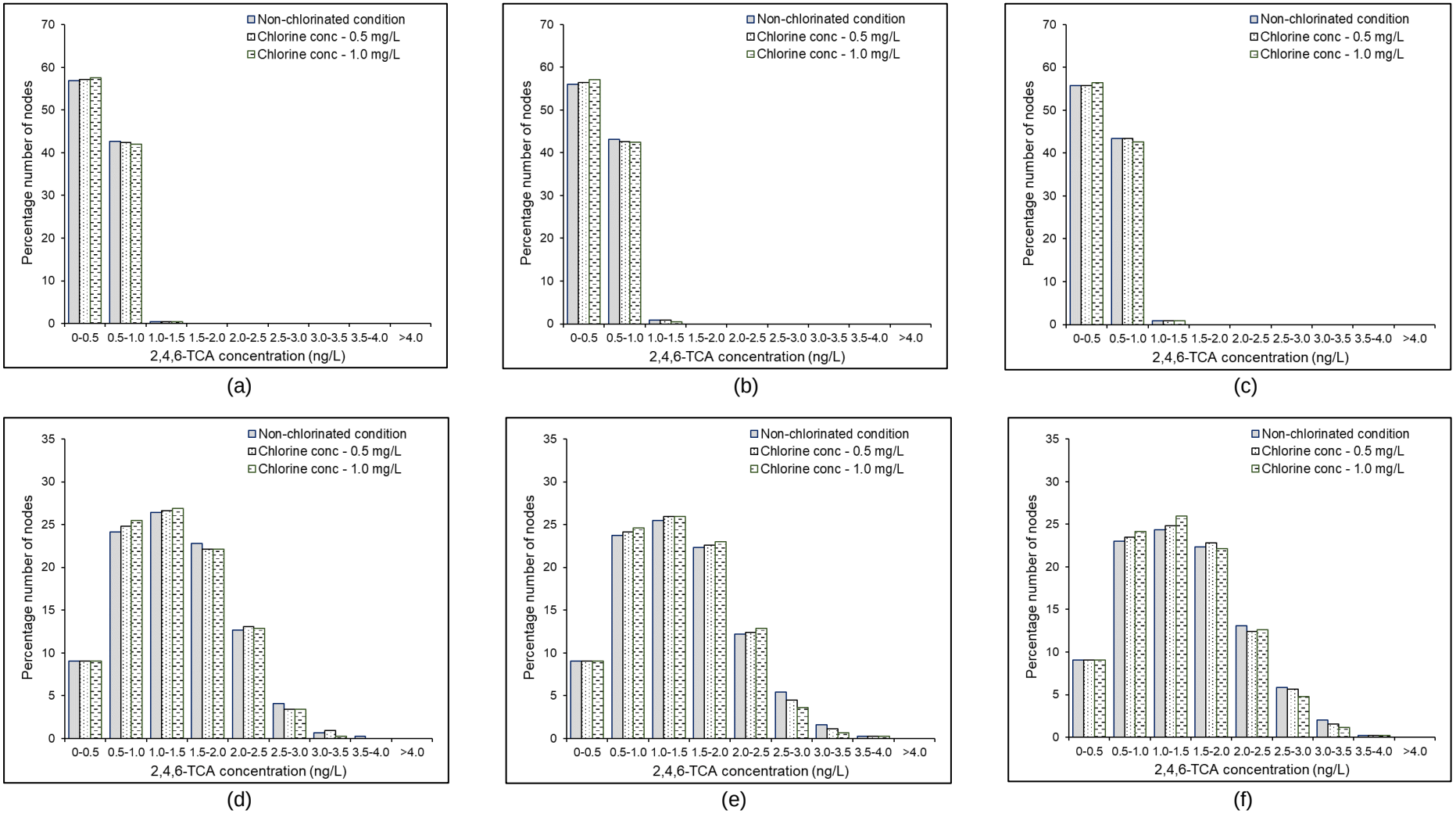


Figure S8. Predicted distribution of 2,4,6-TCA in the Balerma network under T = 10 °C, P_o = 0.2 mg/L, S_o = (a)(d) 0.01, (b)(e) 0.1, and (c)(f) 0.3 mg-C/L, and Scenarios (a)(b)(c) I and (d)(e)(f) II

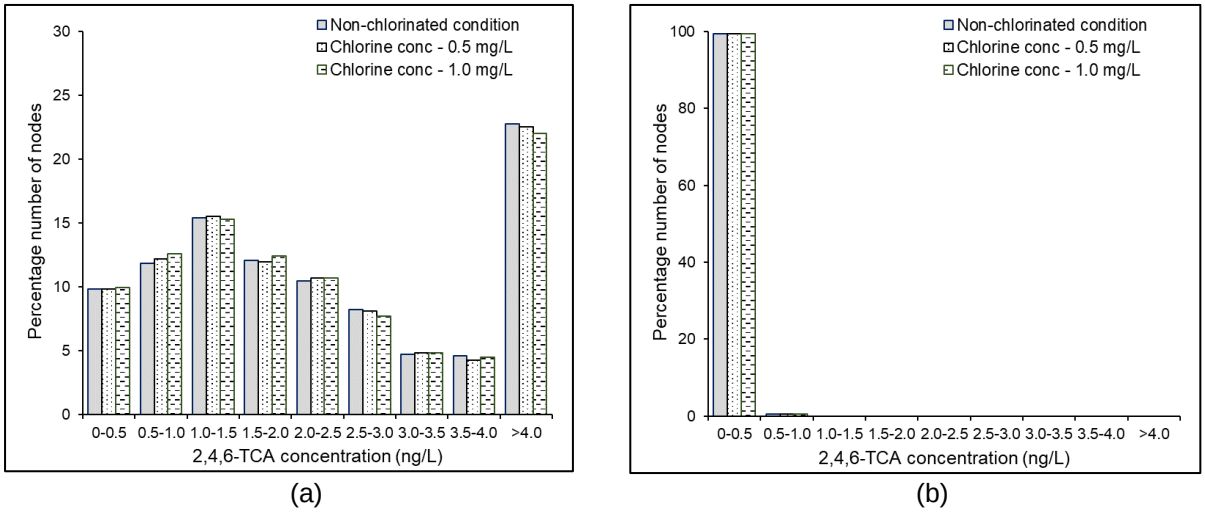


Figure S9. Predicted distribution of 2,4,6-TCA in the KLmod network under T = 10 °C, and P_o = (a) 0.2 and (b) 0.01 mg/L

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