SUPPLEMENTARY INFORMATION

Contaminant Fate and Transport Modeling in Distribution Systems: EPANET-C

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ABBREVIATIONS

BDOC	Biodegradable dissolved organic carbon
MSRT	Multi-species reactive-transport
PFOA	Perfluorooctanoic acid
PFOAAmS	Perfluorooctaneamido ammonium salt
PFOAB	Perfluorooctaneamido betaine
THMs	Trihalomethanes
TOC	Total organic carbon

NOMENCLATURE

K_s	Half-saturation constant (mg/L)
T_i	Temperature-dependent shape parameter (°C)
T	Temperature of delivered water (°C)
X_a	Biofilm density as a function of time (CFU/cm^2)
R_h	Hydraulic mean radius (m)
T_{opt}	Optimal temperature for microbial activity (°C)
X_a	Biofilm microbial density as a function of time (CFU/m^2)
X_b	Planktonic microbial colony count as a function of time and axial dimension (CFU/mL)
Y_1	Yield coefficient for chlorine corresponding to chlorine-PFOAB reactions (mg/ng)
Y_2	Yield coefficient for chlorine corresponding to chlorine-PFOAAmS reactions (mg/ng)
Y_h	Reaction yield coefficient corresponding to THMs formation from organic matter (µg/mg)
Y_{f1}	Yield-coefficient for PFOA formation from chlorine-PFOAB reactions (ng/ng)
Y_{f2}	Yield-coefficient for PFOA formation from chlorine-PFOAAmS reactions (ng/ng)
Y_n	Yield coefficient for TOC/BDOC corresponding to chlorine-TOC/BDOC reactions (mg/mg)
Y_x	Yield coefficient for microbes corresponding to chlorine-microbial biomass reactions (CFU/mg)

k_1	Second-order rate constant corresponding to chlorine-PFOAB reactions (L/mg/h)
k_2	Second-order rate constant corresponding to chlorine-PFOAAmS reactions (L/mg/h)
k_{cn}	Second-order rate constant corresponding to chlorine-TOC/BDOC reactions (L/mg/h)
k_{cx}	Second-order rate constant corresponding to chlorine-microbial biomass reactions (L/mg/h)
k_{dep}	Microbial deposition rate constant (1/h)
k_{det}	Microbial detachment rate coefficient (m.h/g)
k_f	Mass-transfer coefficient for chlorine (m/h)
k_r	Resistance factor signifying additional resistance of biofilm microorganisms to chlorine-induced mortality
k_{inact}	Microbial growth inactivation constant (L/mg)
k_{mort}	Microbial mortality rate constant (1/h)
k_w	Wall decay coefficient for chlorine (m/h)
$\mu_{max,a}$	Maximum specific growth rate of biofilm microbes (1/h)
$\mu_{max,b}$	Maximum specific growth rate of planktonic microbes (1/h)
τ_w	Shear stress caused by pipe flow velocity at wall (g/m.h^2)
C	Concentration of residual chlorine as a function of time and axial dimension (mg/L)
H	Concentration of THMs as a function of time and axial dimension (µg/L)
N	Concentration of TOC as a function of time and axial dimension (mg/L)
S	Concentration of BDOC as a function of time and axial dimension (mg/L)
F_1	Concentration of PFOAB as a function of time and axial dimension (ng/L)
F_2	Concentration of PFOAAmS as a function of time and axial dimension (ng/L)
Y	Microbial growth yield coefficient (CFU/mg)
a	Dead microbial fraction getting converted as BDOC after cell lysis (mg/CFU)

t	Time (h)
u	Flow velocity (m/h)
x	Distance along the axial direction (m)
2,4,6-TCA	2,4,6-trichloroanisole
2,4,6-TCP	2,4,6-trichlorophenol
E_{K_d}	Temperature coefficient corresponding to 2,4,6-TCP degradation
E_{Y_f}	Temperature coefficient corresponding to 2,4,6-TCA formation
Y_{pf}	Pipe material dependent constant concerning 2,4,6-TCP bioconversion (ng/mg)
a_2	Reaction yield coefficient concerning 2,4,6-TCP bioconversion (L/CFU)
T_p	Concentration of 2,4,6-TCP as a function of time and axial dimension (mg/L)
a_1	2,4,6-TCP degradation constant (1/h)
A	Concentration of 2,4,6-TCA as a function of time and axial dimension (ng/L)
b	Microbial activation rate constant concerning 2,4,6-TCP bioconversion (L/CFU)

S1. Governing Equations of EPANET-C MSRT Modules

Module '1'

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

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

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

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

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

Module '2'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S6)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -Y_n \times k_{cn} \times N \times C \quad \text{(S7)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S8)}$$

Module '3'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S9)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S10)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S11)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b \quad \text{(S12)}$$

Module '4'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - \frac{k_w \times k_f}{(k_w+k_f)\times R_h} \times C \quad \text{(S13)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -Y_n \times k_{cn} \times N \times C \quad \text{(S14)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S15)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S16)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S17)}$$

Module '12'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w+k_f)\times R_h} \times C \quad \text{(S18)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S19)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S20)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times$$

$$X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S21)}$$

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

$$R_h - k_{det} \times \tau_w \times X_a \quad \text{(S22)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S23)}$$

Module '13'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w+k_f)\times R_h} \times C \quad \text{(S24)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times$$

$$k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S25)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times$$

$$k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S26)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times$$

$$X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S27)}$$

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

$$R_h - k_{det} \times \tau_w \times X_a \quad \text{(S28)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S29)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T+273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S30)}$$

Module ‘14’

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S31)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S32)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S33)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b} \frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S34)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times R_h - k_{det} \times \tau_w \times X_a \quad \text{(S35)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S36)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S37)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S38)}$$

Module ‘23’

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S39)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S40)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S41)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b} \frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b \quad \text{(S42)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S43)}$$

Module '24'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w+k_f) \times R_h} \times C \quad \text{(S44)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -Y_n \times k_{cn} \times N \times C \quad \text{(S45)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S46)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S47)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S48)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S49)}$$

Module '34'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w+k_f) \times R_h} \times C \quad \text{(S50)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S51)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b} \frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S52)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b -$$
$$Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b \quad \text{(S53)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S54)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T+273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S55)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S56)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S57)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S58)}$$

Module '123'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w+k_f)\times R_h} \times C \quad \text{(S59)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times$$
$$k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S60)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times$$
$$k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S61)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times$$
$$X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S62)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times$$
$$R_h - k_{det} \times \tau_w \times X_a \quad \text{(S63)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S64)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S65)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T+273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S66)}$$

Module '124'

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S67)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S68)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S69)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S70)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times R_h - k_{det} \times \tau_w \times X_a \quad \text{(S71)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S72)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S73)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S74)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S75)}$$

Module ‘134’

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S76)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S77)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S78)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S79)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times R_h - k_{det} \times \tau_w \times X_a \quad \text{(S80)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T + 273}\right)\right] \times T_P \quad \text{(S81)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T + 273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T + 273}\right)\right] \times T_P \quad \text{(S82)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S83)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S84)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S85)}$$

Module ‘234’

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S86)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S87)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S88)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b \quad \text{(S89)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S90)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T + 273}\right)\right] \times T_P \quad \text{(S91)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = \left(a_2 \times X_b + Y_{pf}\right) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T + 273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T + 273}\right)\right] \times T_P \quad \text{(S92)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S93)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S94)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S95)}$$

Module ‘1234’

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -k_{cn} \times N \times C - Y_1 \times k_1 \times C \times F_1 - Y_2 \times k_2 \times C \times F_2 - k_{cx} \times X_b \times C - \frac{k_w \times k_f}{(k_w + k_f) \times R_h} \times C \quad \text{(S96)}$$

$$\frac{\partial N}{\partial t} + u\frac{\partial N}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s + S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt} - T)}{(T_{opt} - T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times N \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S97)}$$

$$\frac{\partial S}{\partial t} + u\frac{\partial S}{\partial x} = -\frac{1}{Y} \times \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_n \times k_{cn} \times S \times C + a(Y_x \times k_{cx} \times X_b \times C + k_{mort} \times X_b) \quad \text{(S98)}$$

$$\frac{\partial X_b}{\partial t} + u\frac{\partial X_b}{\partial x} = \mu_{max,b}\frac{S}{K_s+S} \times \exp(-k_{inact} \times C) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_b - Y_x \times k_{cx} \times X_b \times C - k_{mort} \times X_b - k_{dep} \times X_b + k_{det} \times \tau_w \times \frac{X_a}{R_h} \quad \text{(S99)}$$

$$\frac{dX_a}{dt} = \mu_{max,a} \times \exp\left(-\frac{k_{inact}}{k_r} \times C\right) \times \exp\left[\left(-\frac{(T_{opt}-T)}{(T_{opt}-T_i)}\right)^2\right] \times X_a - k_{mort} \times X_a + k_{dep} \times X_b \times R_h - k_{det} \times \tau_w \times X_a \quad \text{(S100)}$$

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} = Y_h \times k_{cn} \times N \times C \quad \text{(S101)}$$

$$\frac{\partial T_P}{\partial t} + u\frac{\partial T_P}{\partial x} = -a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S102)}$$

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = (a_2 \times X_b + Y_{pf}) \times \exp\left[E_{Y_f} \times \left(1 - \frac{293}{T+273}\right)\right] \times a_1 \times \log_e(b \times X_b) \times \exp\left[E_{K_d} \times \left(1 - \frac{293}{T+273}\right)\right] \times T_P \quad \text{(S103)}$$

$$\frac{\partial F_1}{\partial t} + u\frac{\partial F_1}{\partial x} = -k_1 \times C \times F_1 \quad \text{(S104)}$$

$$\frac{\partial F_2}{\partial t} + u\frac{\partial F_2}{\partial x} = -k_2 \times C \times F_2 \quad \text{(S105)}$$

$$\frac{\partial P}{\partial t} + u\frac{\partial P}{\partial x} = Y_{f1} \times k_1 \times C \times F_1 + Y_{f2} \times k_2 \times C \times F_2 \quad \text{(S106)}$$

Table S1. Values of the reaction rate coefficients reported in the literature and used in EPANET-C.

Model Parameter	Notation	Unit	Values Range Reported in the Literature	Reference	Value Used in EPANET-C
Second-order rate constant corresponding to chlorine-TOC/BDOC reactions	k_{cn}	L/mg/h	0.148–0.180	Kiene et al. [1]	0.164
Second-order rate constant corresponding to chlorine-microbial biomass reactions	k_{cx}	L/mg/h	0.015–0.018	Abokifa et al. [2]	0.016
Second-order rate constant corresponding to chlorine-PFOAB reactions	k_1	L/mg/h	0.003–0.050		0.02
Second-order rate constant corresponding to chlorine-PFOAAmS reactions	k_2	L/mg/h	0.003–0.080		0.03
Yield coefficient for chlorine corresponding to chlorine-PFOAB reactions	Y_1	mg/ng	7.5×10^{-6}–2.5×10^{-5}	Abhijith and Ostfeld [3]	8.5×10^{-6}
Yield coefficient for chlorine corresponding to chlorine-PFOAAmS reactions	Y_2	mg/ng	7.5×10^{-6}–3.0×10^{-5}		2.0×10^{-5}
Wall decay coefficient for chlorine	k_w	m/h	3.7×10^{-4}–0.052	Abhijith and Mohan [4]; Camper [5]; Munavalli and MohanKumar [6]	3.7×10^{-4}
Maximum specific growth rate of planktonic microbes	$\mu_{max,b}$	1/h	0.05–1.512		1.512
Maximum specific growth rate of biofilm microbes	$\mu_{max,a}$	1/h	0.003–0.029	Bois et al. [7]	0.003

Model Parameter	Notation	Unit	Values Range Reported in the Literature	Reference	Value Used in EPANET-C
Half-saturation constant	K_s	mg/L	0.05–1.20	Billen et al. [8]	0.195
Microbial growth yield coefficient	Y	CFU/mg	5.0×10^7–1.5×10^9	Bois et al. [7]	7.0×10^7
Microbial growth inactivation constant	k_{inact}	L/mg	0.05–5.0	Abokifa et al. [2]; Bois et al. [7]; Munavalli and MohanKumar [6]	0.35
Yield coefficient for microbes corresponding to chlorine-microbial biomass reactions	Y_x	CFU/mg	3.4×10^8–7.4×10^8	Bois et al. [7]	3.4×10^8
Dead microbial fraction getting converted as BDOC after cell lysis	a	mg/CFU	3.0×10^{-10}–3.0×10^{-11}	Dukan et al. [9]	3.0×10^{-10}
Microbial mortality rate constant	k_{mort}	1/h	0.003–0.065	Bois et al. [7]; Munavalli and MohanKumar [6]	0.023
Microbial deposition rate constant	k_{dep}	1/h	0.020–1.512	Bois et al. [7]	0.2
Microbial detachment rate coefficient	k_{det}	m.h/g	1.9×10^{-10}–1.9×10^{-11}	Schrottenbaum et al. [10]	1.9×10^{-10}
Yield coefficient for TOC/BDOC corresponding to chlorine-TOC/BDOC reactions	Y_n	mg/mg	0.4–4.88	Clark [11]	0.98
Reaction yield coefficient corresponding to THMs formation from organic matter	Y_h	µg/mg	5.68–188.20	Clark [11]; Clark and Sivaganesan [12]	112.435
2,4,6-TCP degradation constant	a_1	1/h	2.0×10^{-4}–0.002		0.002
Microbial activation rate constant concerning 2,4,6-TCP bioconversion	b	L/CFU	5500–5.5×10^4		5.5×10^4
Reaction yield coefficient concerning 2,4,6-TCP bioconversion	a_2	L/CFU	4.3×10^{-6}–4.3×10^{-7}	Abhijith and Ostfeld [13]	4.3×10^{-7}
Pipe material dependent constant concerning 2,4,6-TCP bioconversion	Y_{pf}	ng/ng	0.163–1.049		0.163
Yield-coefficient for PFOA formation from chlorine-PFOAB reactions	Y_{f1}	ng/ng	0.18–0.55	Abhijith and Ostfeld [3]	0.36

Model Parameter	Notation	Unit	Values Range Reported in the Literature	Reference	Value Used in EPANET-C
Yield-coefficient for PFOA formation from chlorine-PFOAAmS reactions	Y_{f1}	ng/ng	0.26–0.55		0.41

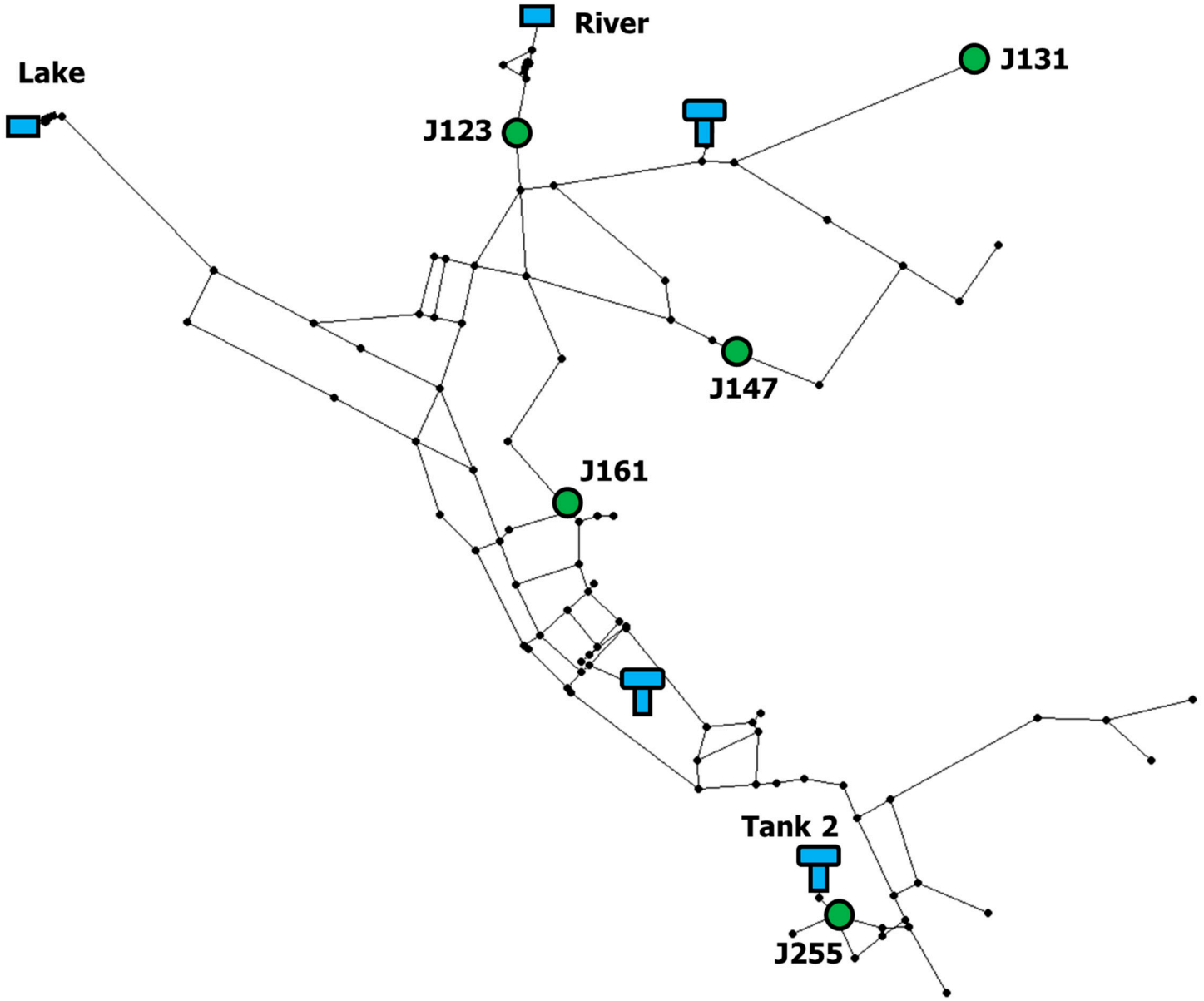

Figure S1. Schematic of North Marin Water District WDS or EPANET Example Network 3 (Test network 1).

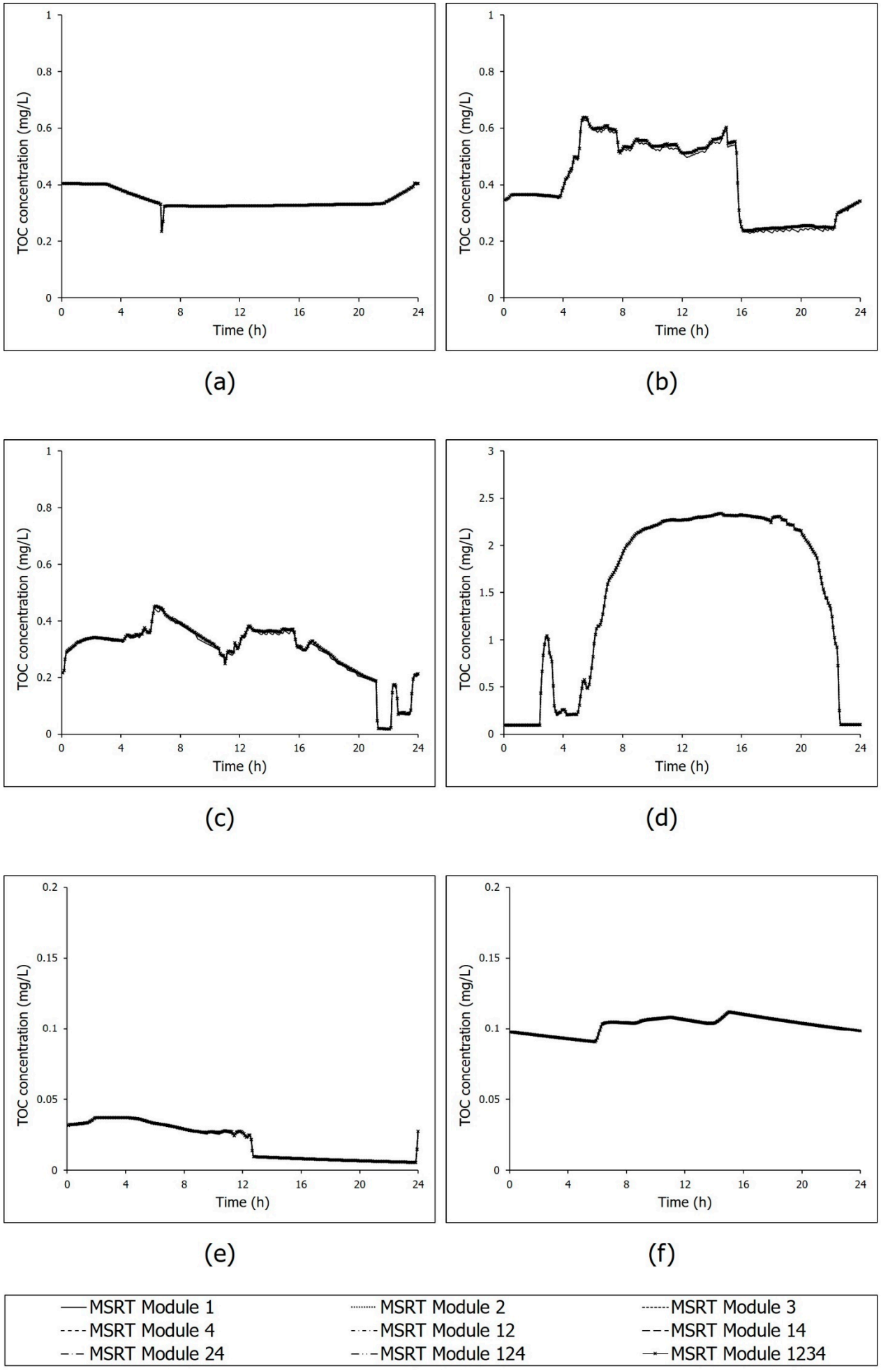

Figure S2. 24-h variations in TOC concentrations simulated with EPANET-C Modules 1, 2, 3, 4, 12, 14, 24, 124, and 1234 at network locations (**a**) J123, (**b**) J161, (**c**) J147, (**d**) J255, (**e**) J131, and (**f**) Tank 2 of Test network 1.

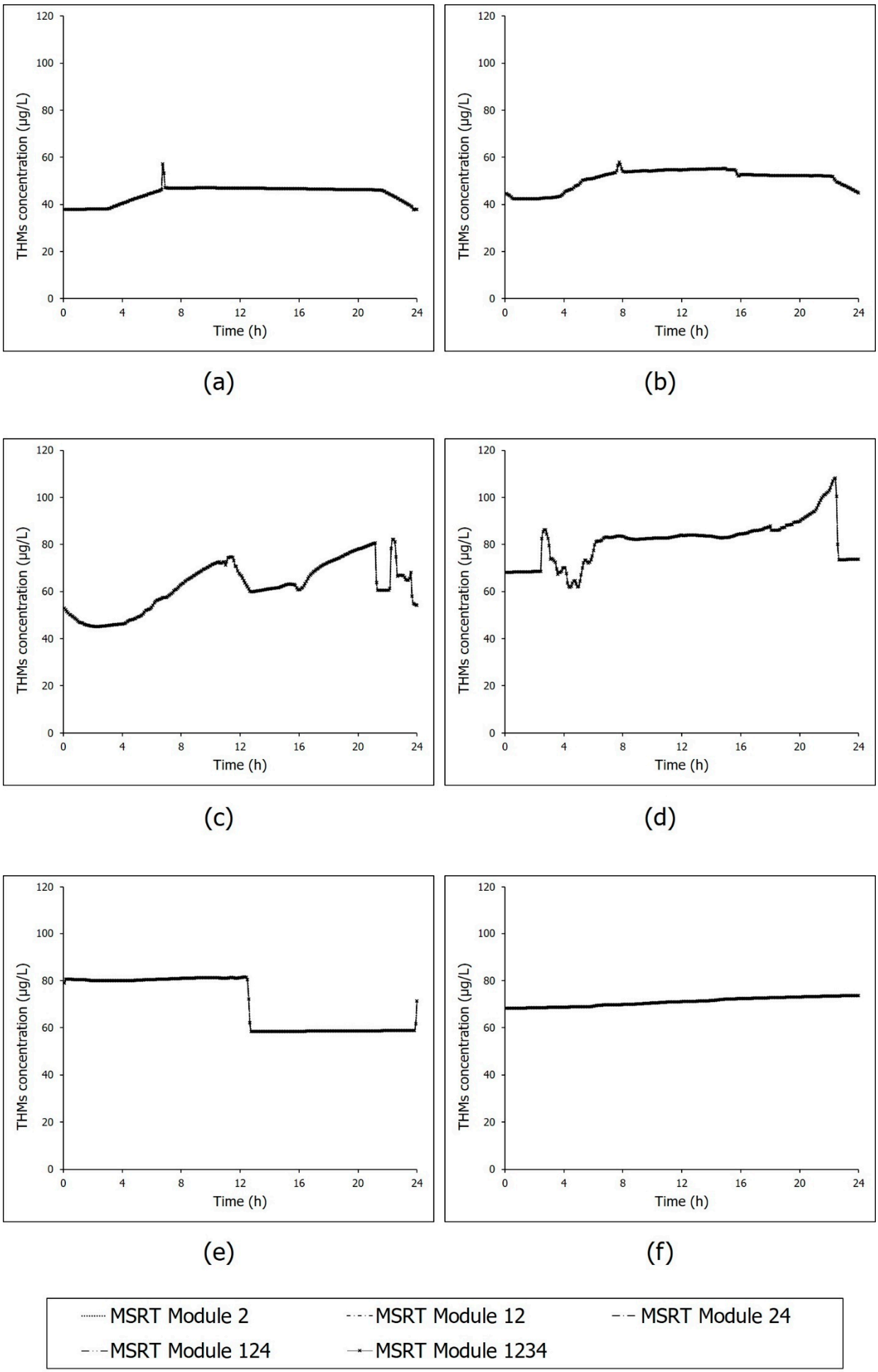

Figure S3. 24-h variations in THMs concentrations simulated with EPANET-C Modules 2, 12, 24, 124, and 1234 at network locations (**a**) J123, (**b**) J161, (**c**) J147, (**d**) J255, (**e**) J131, and (**f**) Tank 2 of Test network 1.

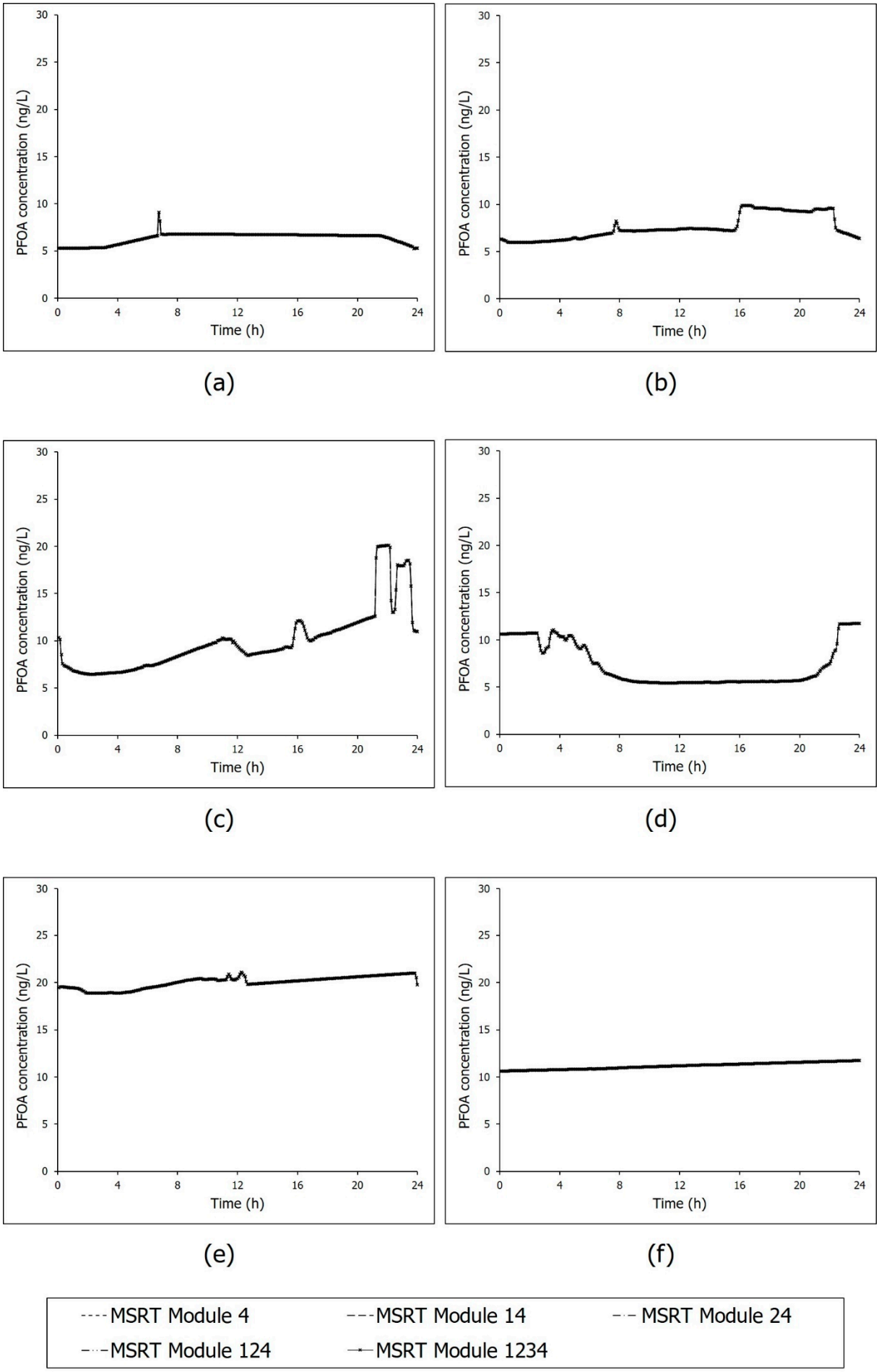

Figure S4. 24-h variations in PFOA concentrations simulated with EPANET-C Modules 4, 14, 24, 124, and 1234 at network locations (**a**) J123, (**b**) J161, (**c**) J147, (**d**) J255, (**e**) J131, and (**f**) Tank 2 of Test network 1.

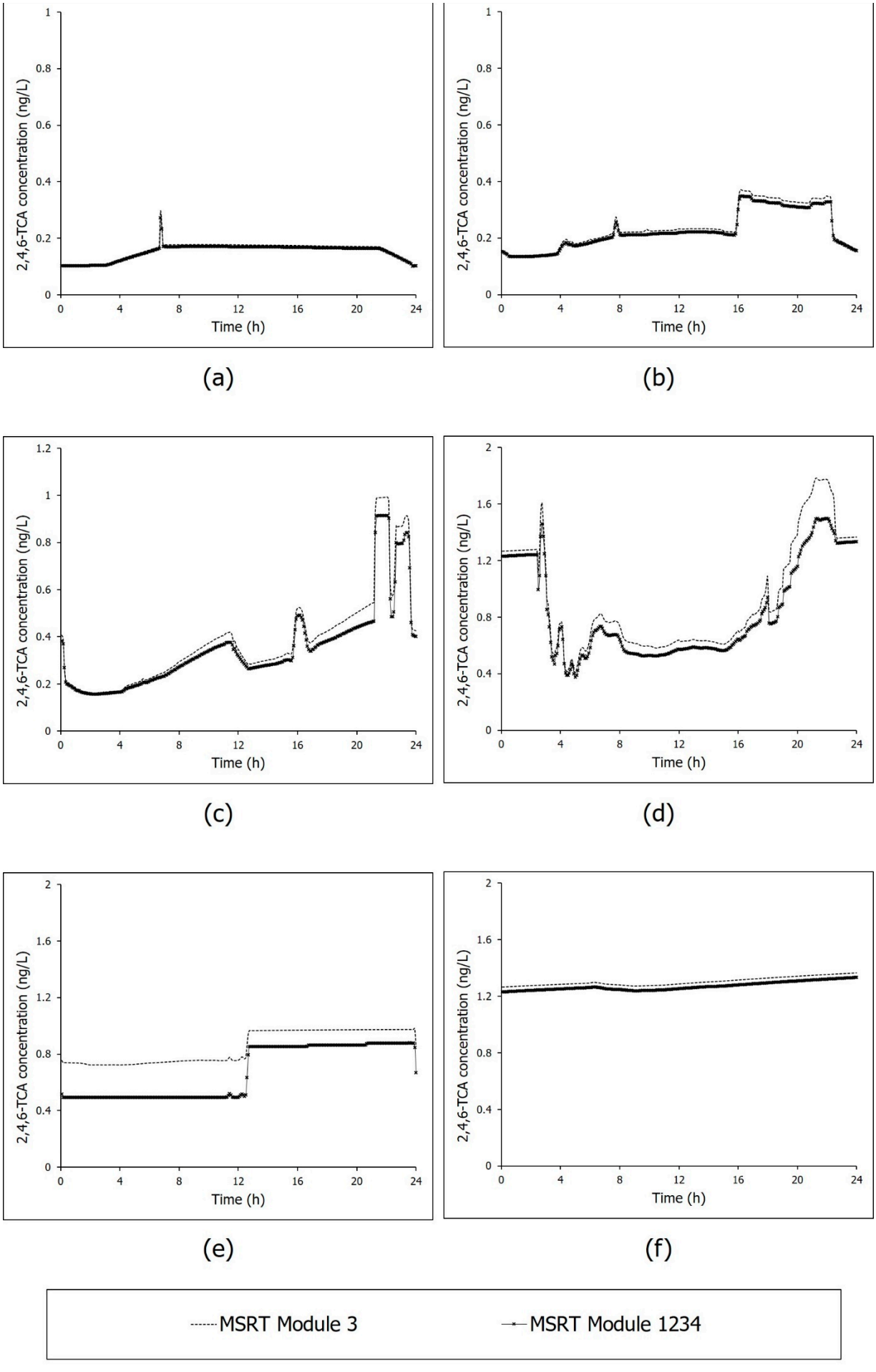

Figure S5. 24-h variations in 2,4,6-TCA concentrations simulated with EPANET-C Modules 3 and 1234 at network locations (**a**) J123, (**b**) J161, (**c**) J147, (**d**) J255, (**e**) J131, and (**f**) Tank 2 of Test network 1.

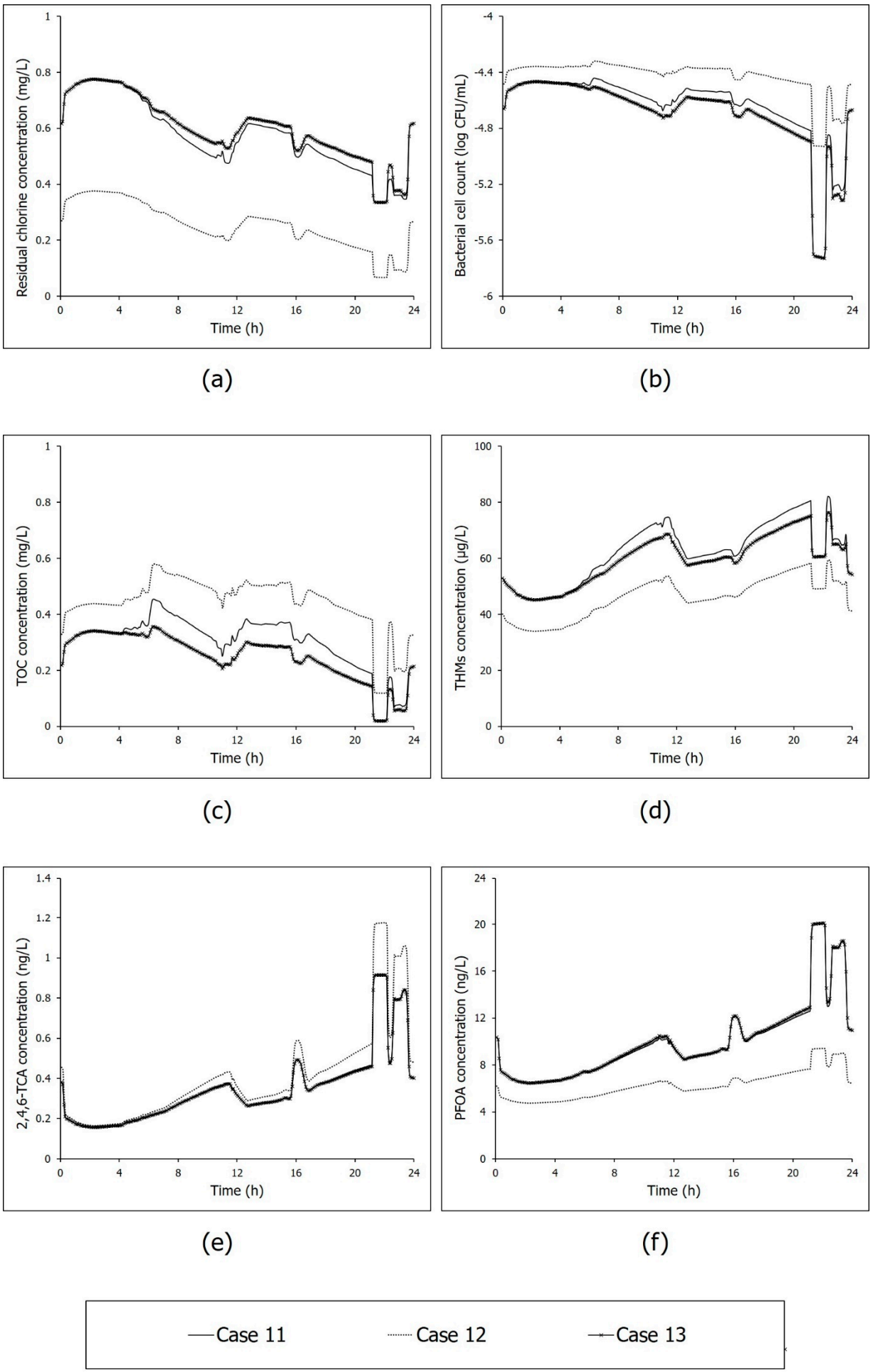

Figure S6. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 11, 12, and 13 at network location J147 of Test network 1.

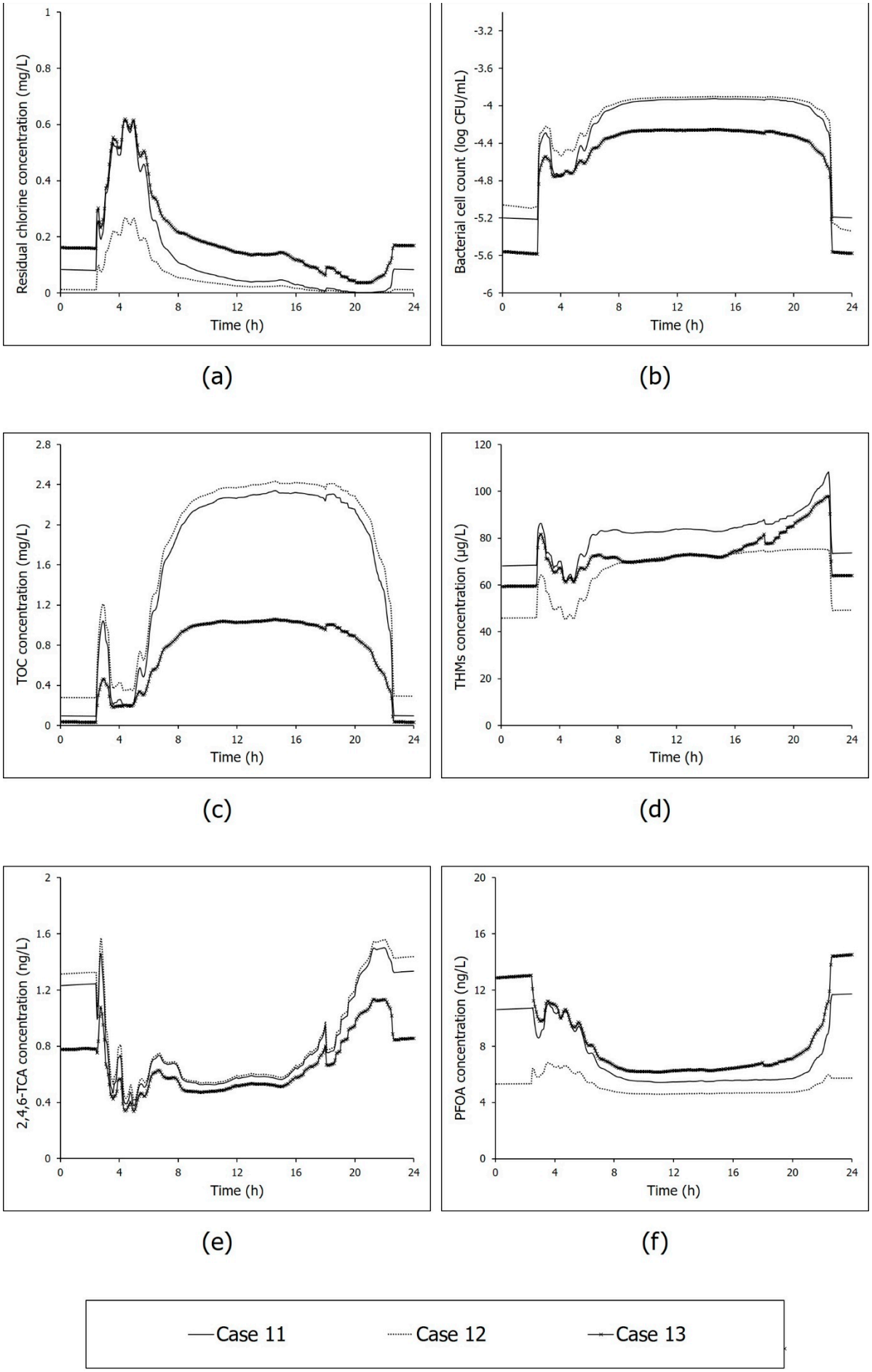

Figure S7. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 11, 12, and 13 at network location J255 of Test network 1.

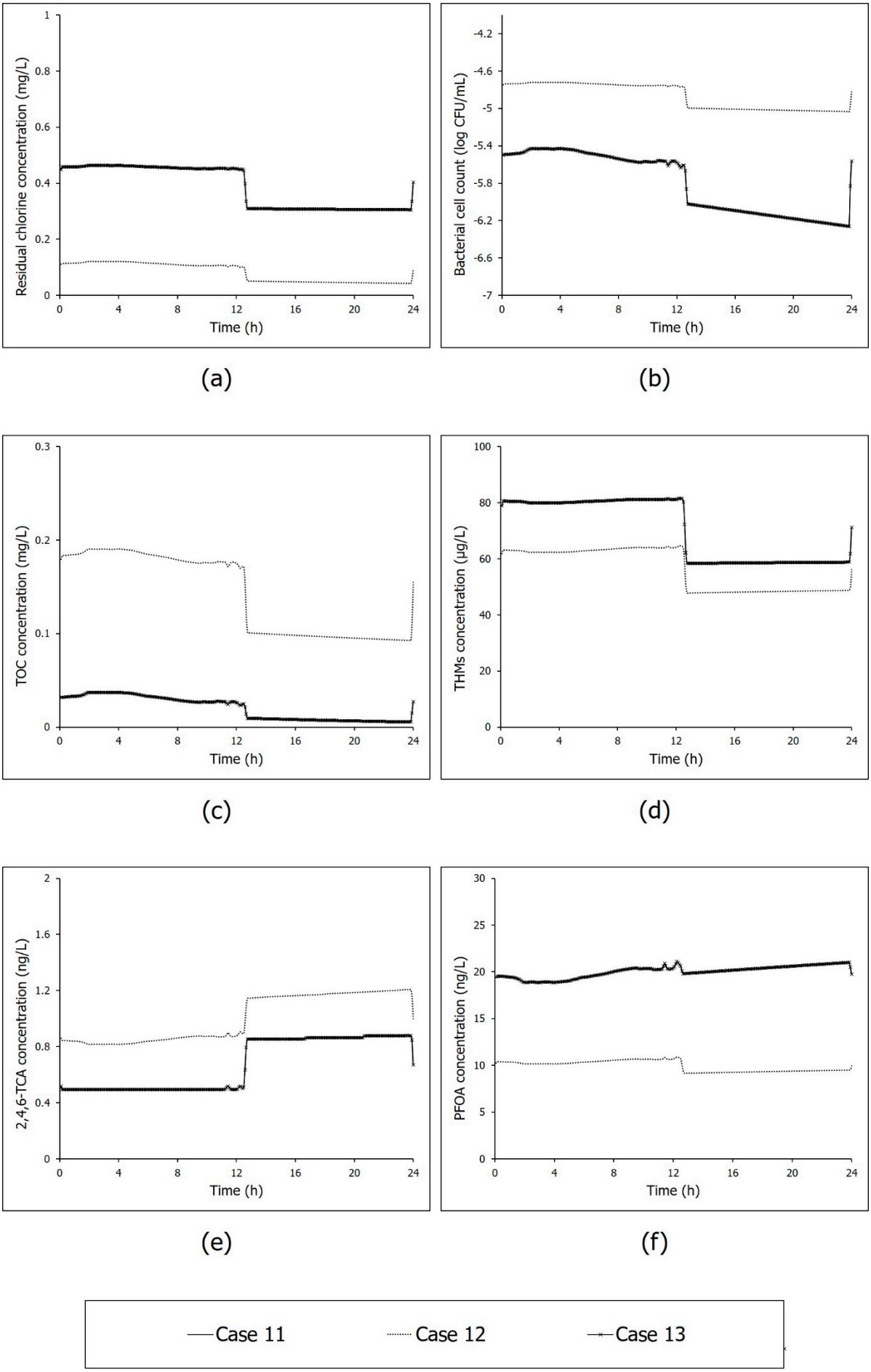

Figure S8. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 11, 12, and 13 at network location J131 of Test network 1.

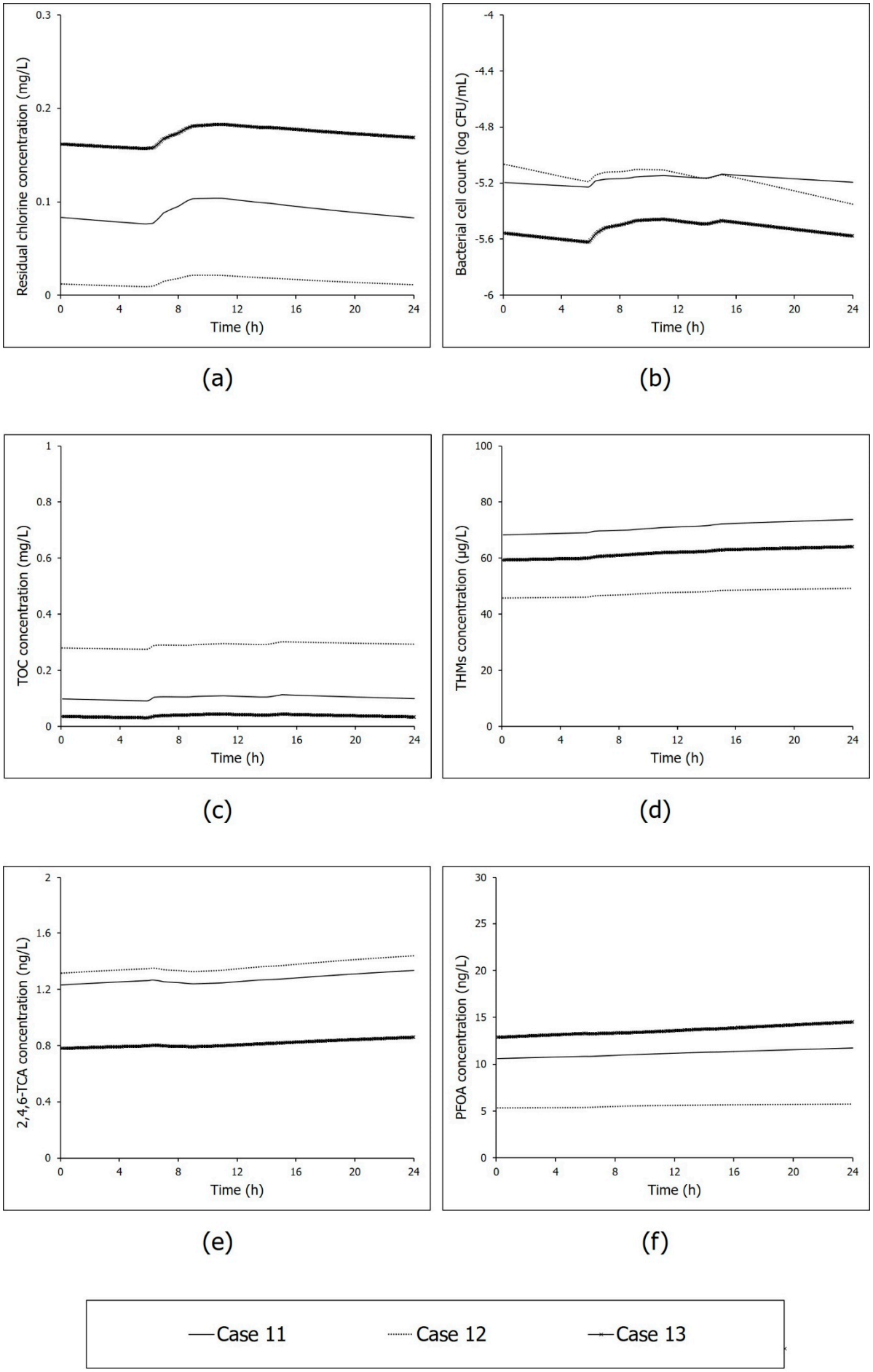

Figure S9. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 11, 12, and 13 at network location Tank 2 of Test network 1.

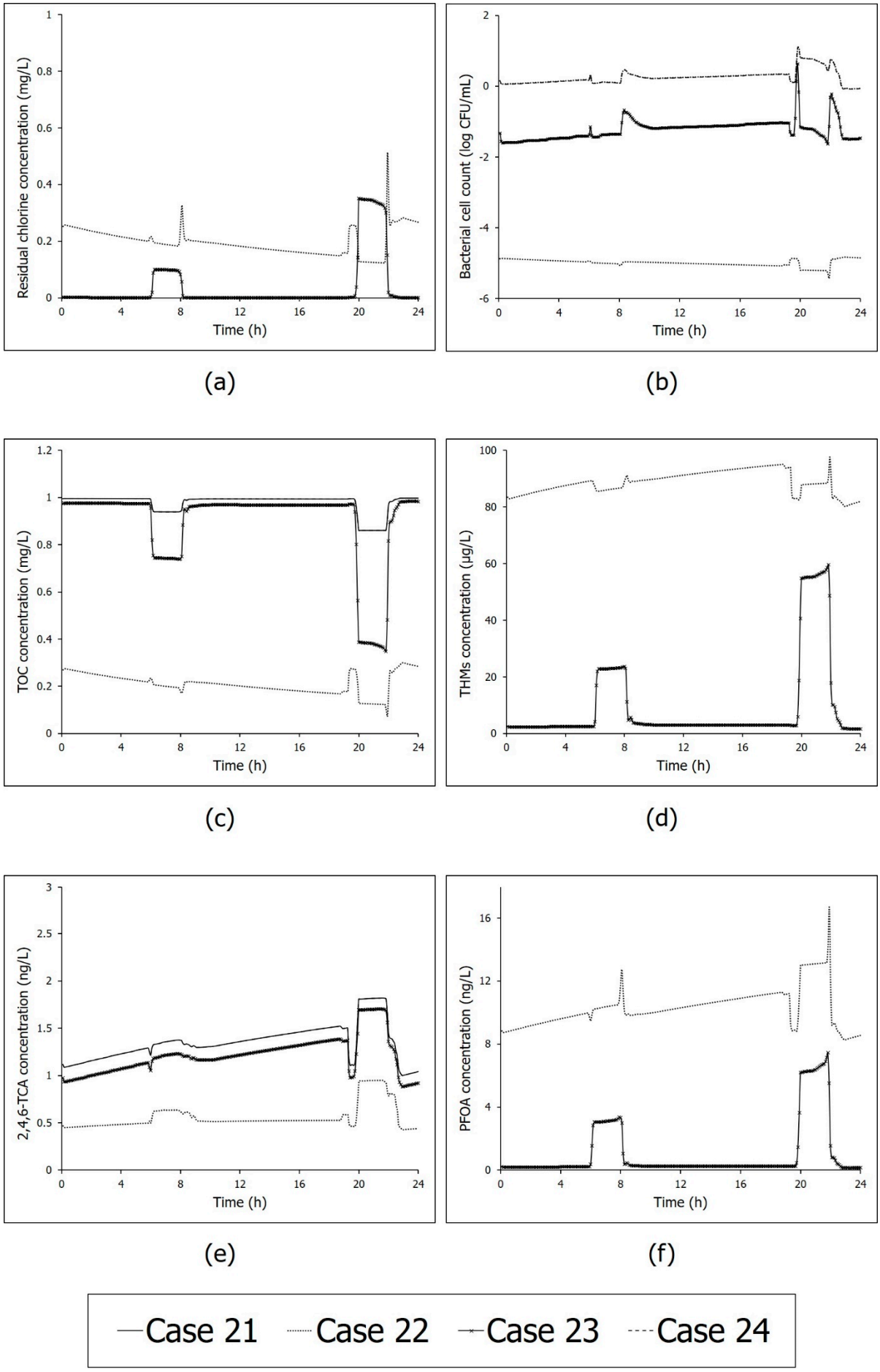

Figure S10. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 21, 22, 23, and 24 at network location J45 of Test network 2.

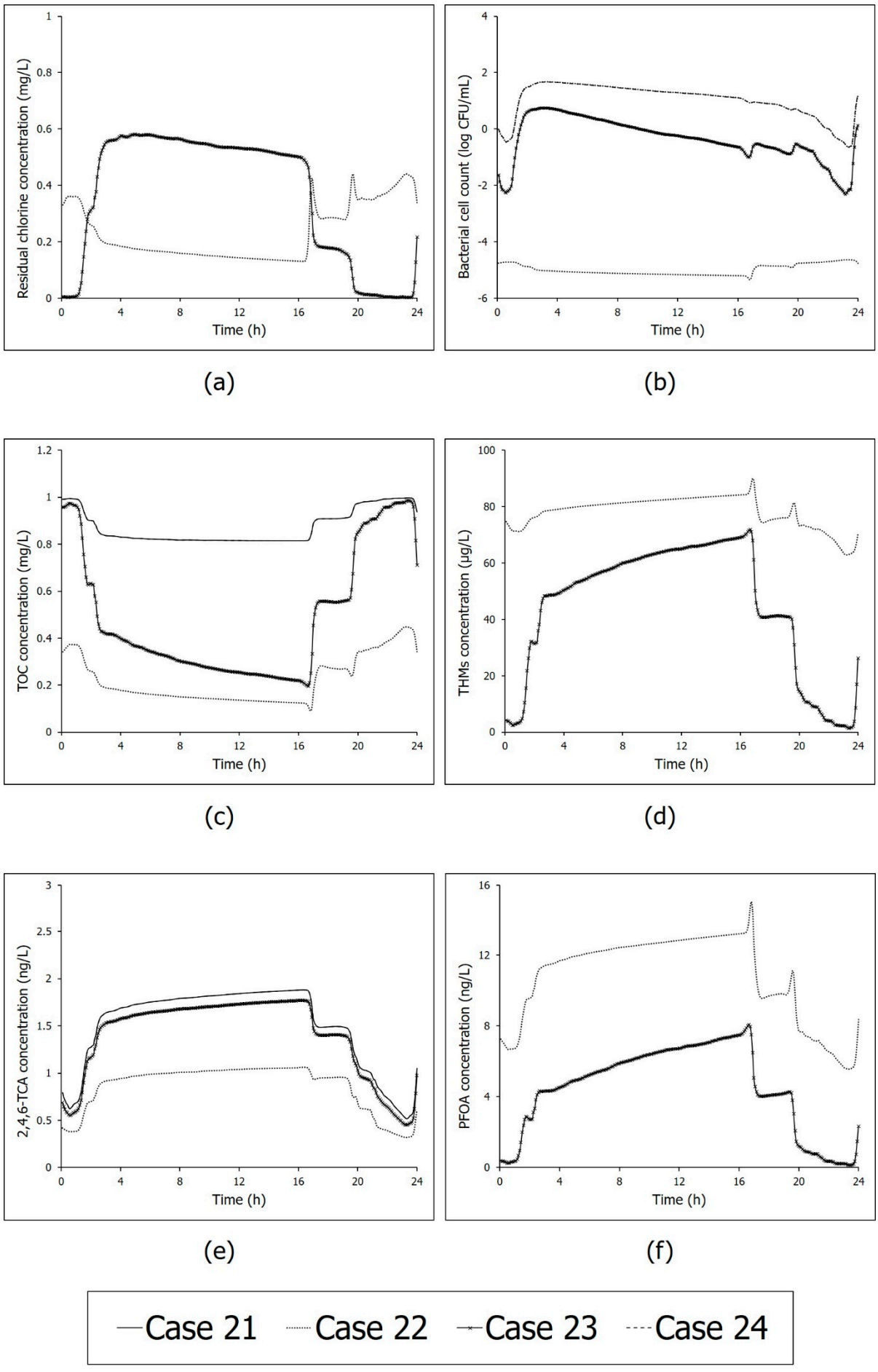

Figure S11. 24-h variations in (**a**) residual chlorine concentration, (**b**) planktonic bacterial cell count, (**c**) TOC concentration, (**d**) THMs concentration, (**e**) 2,4,6-TCA concentration, and (**f**) PFOA concentration simulated with EPANET-C Module 1234 under Cases 21, 22, 23, and 24 at network location J4 of Test network 2.

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