An Update on Modifications to Water Treatment Plant Model

Jeff Yang

EPA, ORD, WSD

WQTC, Portland

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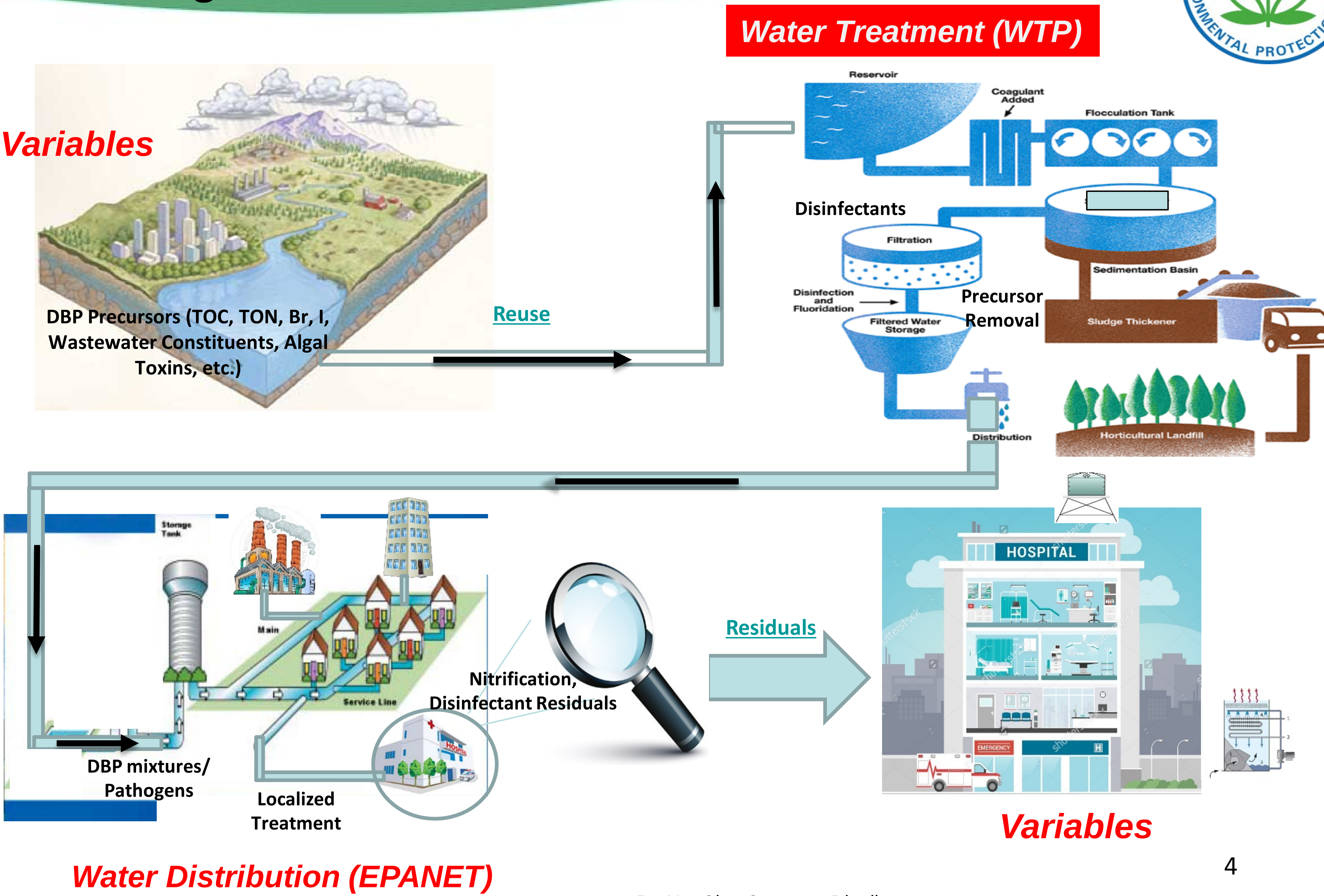
Main Points

- Water treatment plant (WTP) model is an EPA tool for informing regulatory options. WTP has a few versions.
- ***WTP2.2*** can help in regulatory analysis. An ***updated version (WTP3.0)*** will allow plant-specific analysis (***WTP-ccam***) and thus help meet plant-specific treatment objectives.
- WTP3.0 will have ***three distinct features***: 1) mechanistic model of Cl and TOC/DBP for conventional and GAC treatment; 2) Monte Carlo engine for source water variability; and 3) cost probability to meet given treatment objectives.
- WTP3.0 will have a GUI to ***run either updated WTP2.2 or WTP-ccam***.
- ***WTP3.0 development*** is ongoing ***with a focus on WTP-ccam enhancement using real plant data*** from case studies in the U.S. and China.

Source to Tap Considerations for Pathogens and DBPs Controls



Drinking Water Disinfection and WTP Focus

Current Disinfection Practices in U.S.

Type	No. of Entry Points into DS [a]	CL only (%)	CL/ CLM or CLM only (%)	Other Disinfectants (%)				
				O_3	ClO_2	UV	Other	No Disinfection
GW	> 10k (N=8,846)	81.3	9.1	0.5	0.5	0.2	1.2	6.8
SW	> 10k (N=2,886)	51.7	27.9	7.5	8.1	4.2	1.0	0

Data source: UCMR3, from Exhibit 6.2 in the SYR3 DBP Technical Support Document (2016)

[a] Note that the total number of entry points also includes entry points that did not use disinfectants.

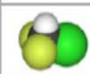
- Chlorine and chloramine disinfection is the dominant practice for GW and SW plants
- Disinfection by-products (DBP) and residual chlorine in finished water are being considered in WTP model simulations
- Other disinfection pathways such as UV are gaining traction in practice

DBP Formation and DBP Precursors in Water Plants

$$CH_3COCH_3 + 3HOCl \rightarrow CH_3COCCl_3 + 3H_2O$$ oxidation step

$$CH_3COCCl_3 + H_2O \rightarrow CH_3COOH + CHCl_3$$ hydrolysis step

Common trihalomethanes (ordered by molecular weight)

Molecular formula	IUPAC name	CAS registry number	Common name	Other names	Molecule
CHF_3	trifluoromethane	75-46-7	fluoroform	Freon 23, R-23, HFC-23	
$CHClF_2$	chlorodifluoromethane	75-45-6	chlorodifluoromethane	R-22, HCFC-22	
$CHCl_3$	trichloromethane	67-66-3	chloroform	R-20, methyl trichloride	
$CHBrCl_2$	bromodichloromethane	75-27-4	bromodichloromethane	dichlorobromomethane, BDCM	
$CHBr_2Cl$	dibromochloromethane	124-48-1	dibromochloromethane	chlorodibromomethane, CDBM	
$CHBr_3$	tribromomethane	75-25-2	bromoform	methyl tribromide	
CHI_3	triiodomethane	75-47-8	iodoform	methyl triiodide	

TTHM

- Specific DBP Considerations
  - THM, HAA
  - Br-THMs
  - Nitrosamines (NDMA)
- DBP precursors chemically oxidized and physically removed in multiple step
- DBP level and species in competitive multi-species reactions (e.g.,Cl-, Br-, etc.)
- Models to address these interactions and quantify residual Cl-- , DBP level and composition

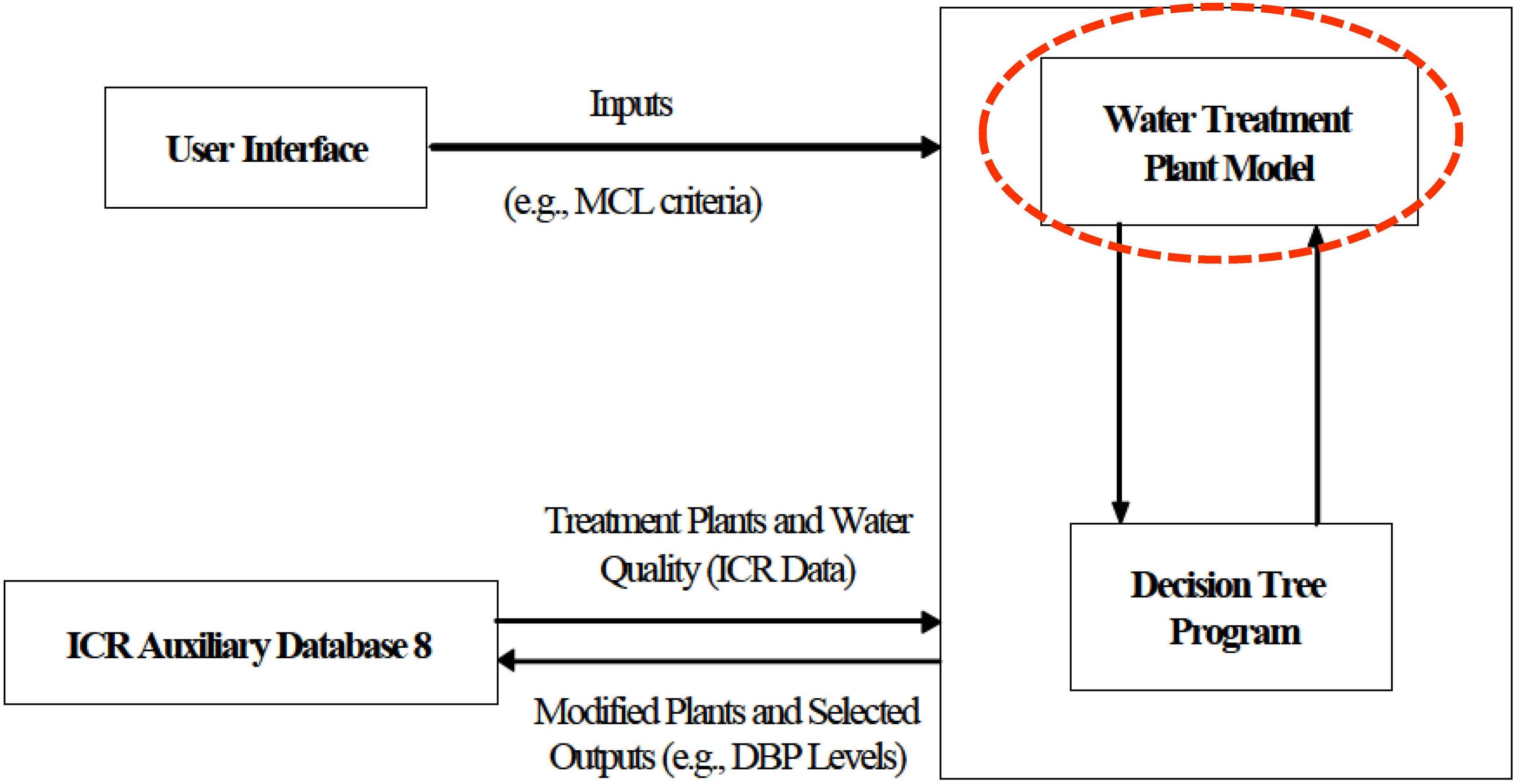
Tools for Analysis: SWAT/WTP Model

- Surface Water Analytical Tool (SWAT) is the primary tool used by EPA in developing Economic Analysis for the Stage 2 Disinfectants/Disinfection Byproducts Rule
  - Predicts treatment technology choices and resulting changes in water quality for different rule alternatives and input conditions based on the 1997-98 Information Collection Rule (ICR)

- WTP model is one of the four components of SWAT
  - Predicts the formation of DBPs given source water quality conditions and water treatment plant configuration
  - Calibrated with the 1997-98 ICR data.

The Stage 2 EA, SWAT and WTP manuals are available at https://www.epa.gov/dwreginfo/stage-1-and-stage-2-disinfectants-and-disinfection-byproducts-rules#additional-resources

Tools for Analysis: SWAT Components

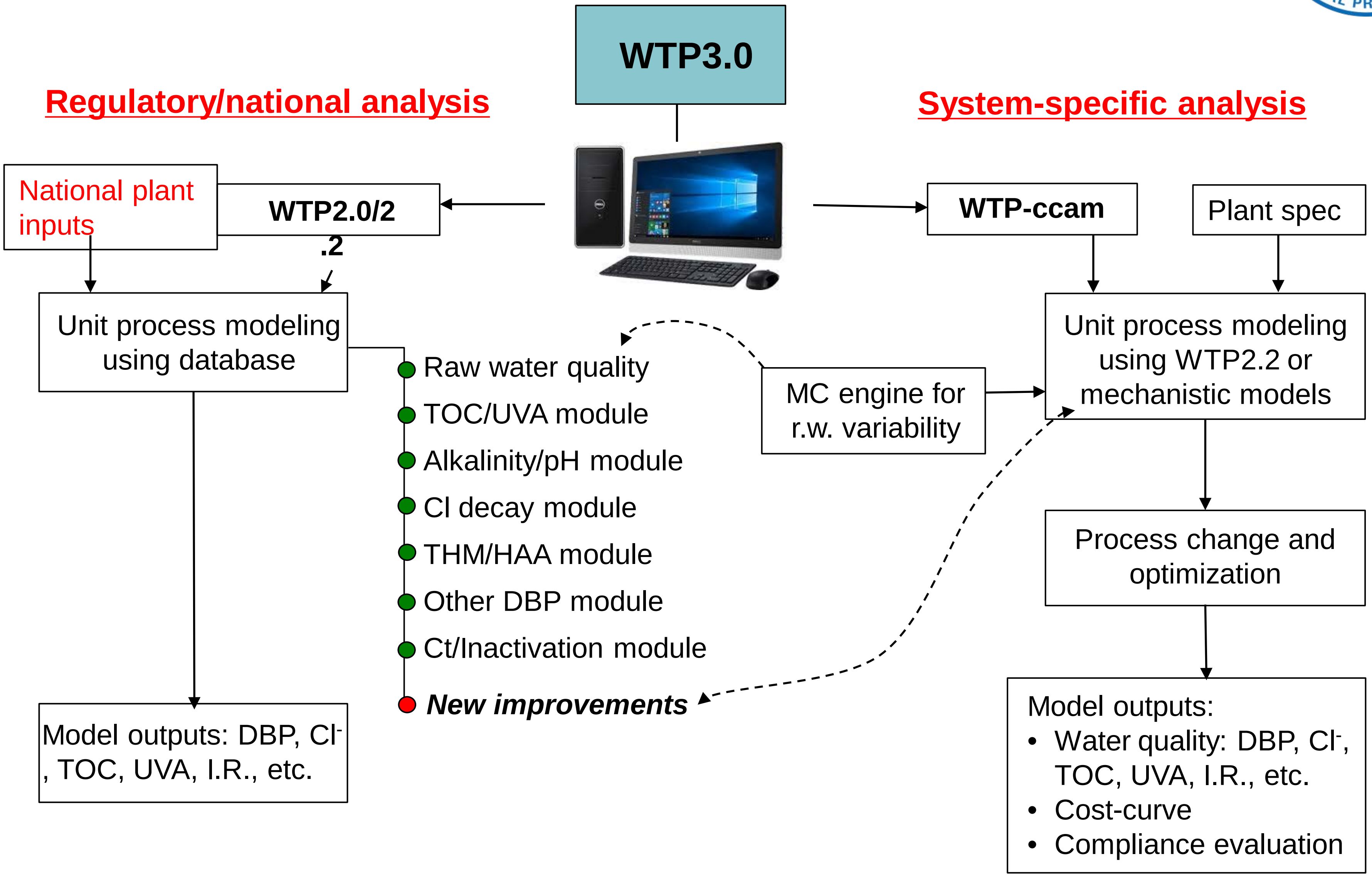


Source: Exhibit A.2 in Appendix A to the Economic Analysis for the Final Stage 2 D/DBPR, 2005

Tools for Analysis: WTP Development

- 1990s: WTP in Fortran
- 2001-2003: WTP2.0/2.2 in C. Empirical formulation for:
  - Conventional processes (coag. – floc. – filtrat.)
  - GAC, membrane, ozone
  - Cl disinfection, TOC removal, and DBP formation potential
  - Limitations
- 2011: WTP-ccam in C^{++}; full-function GUI; cost calculation, and treatment scenario analysis
  - All models and functions of WTP2.2
  - New developments:
    - Logistic model for GAC applicable for full-plant operation
    - Monte Carlo simulation to account for source water variability
    - Cost and optimization of GAC unit operation
- 2017-2018: WTP3.0 in C^{++} in ongoing R&D

Tools for Analysis: WTP3.0

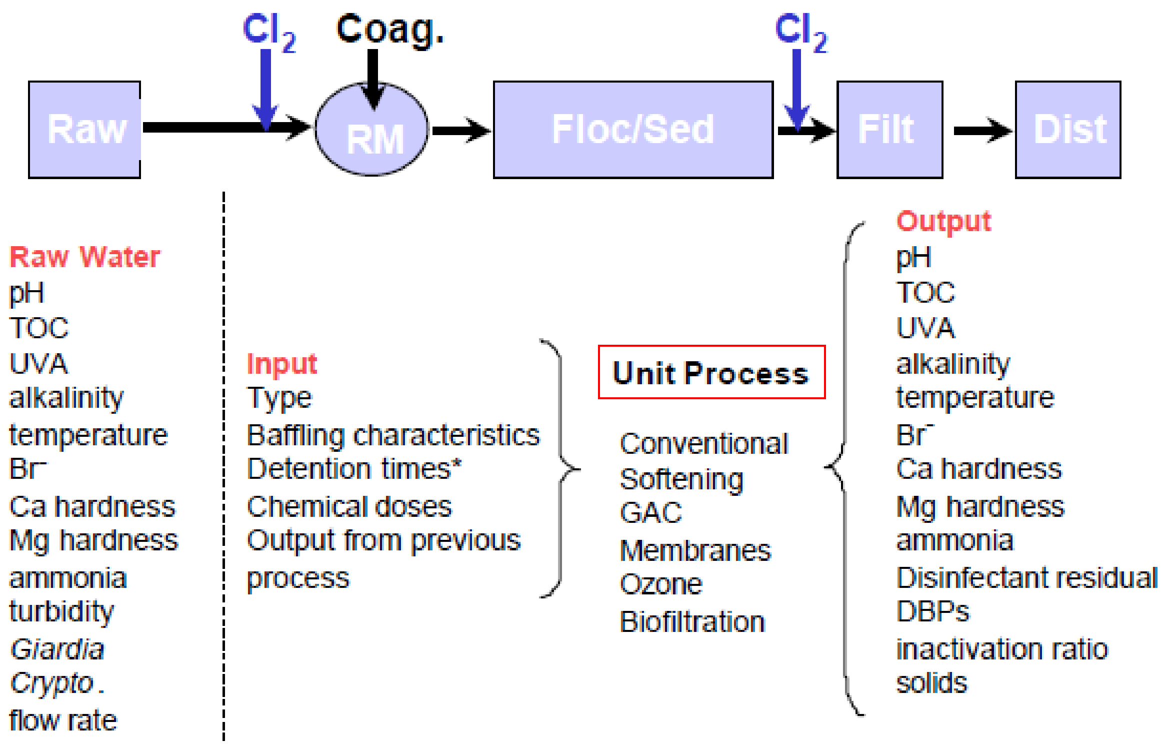


Tools for Analysis: WTP3.0

- 2017-2018: WTP3.0 in C^{++} for regulatory analysis and also for plant-specific analysis:
  - Programming for duo functions in national and plant-specific analysis (WTP2.2 + WTP-ccam)
  - WTP2.2: All generalized formulations in WTP2.2 remain (with some updating) for regulatory analysis
  - WTP-ccam: Mechanistic models for TOC removal and DBP formation in conventional treatment and GAC processes, and for scenario analysis.
    - Monte Carlo engine in WTP-ccam remains for source water variability and cost-curve analysis
    - TOC models applicable for Cl-DBP, and Br-DBP, using the GCWW Richard Miller plant, and two treatment plants in China
    - Modeling capability on cost curve
- Status and planning: Active R&D. The final product expected in 2018.

WTP2.0/2.2 for Regulatory/National Analysis

WTP2.2 Model Schematic



Source: Figure 1-1 in Water Treatment Model v. 2.0 Manual, 2001

A few footnotes:

- Empirical formula based on non-linear regression of plant and bench-scale data
- Obtained statistically significant relationships and models well calibrated in national scale
- Models confidence high in concentration ranges of trained data
- A few assumptions

WTP2.0 Models: NOM/DBP

Table. Model Equations for WTP2.0/2.2

Process	Type	TOC f(x)	TOC Data	UVA f(x)	UVA Data
Raw water					
Coag.-Floc.-Filtration					
Alum	Emperical	pH, Dose, SUVA, TOC_{raw}	39 waters	UVA_{raw}, Dose, pH	WITAF database
Ferric	Emperical	pH, Dose, SUVA, TOC_{raw}	21 waters	- Same as for Alum -	
Softening	Emperical	pH_{sft}, Dose, TOC_{raw}, Corr.	12 waters	UVA_{raw}, ΔTOC	36 data points
GAC					
Coag before GAC	Semi-empirical	EBCT, pH, T	Logistic	TOCeff, const.	ICR (4000 data pair)
Coag. O3, and biotr	Semi-empirical	EBCT, pH, T	Logistic	TOCeff, const.	4 waters, 4 colume
Chlorine decay					
Raw water		constants: a_1, a_2	48 waters		

All equations valid in data ranges, e.g.,

- TOC eq. in alum coag: TOC_{raw}: 1.8-26.5 mg/L;
- TTHM in raw water: TOC: 1.2-10.6 mg/L; UVA: 0.01-0.318 1/cm

THM species as %TTHM

Process	Chlorine Decay Type	Chlorine Decay f(x)	Chlorine Decay Data
Raw water	Mechanistic	a_1 (C_o), a_2 (TOC)	48 waters
Coag.-Floc.-Filtration	Mechanistic	a_1 (C_o) a_2 (C_o,TOC, UVA)	24 waters
GAC			
Coag before GAC			
Coag. O3, and biotr			
Chlorine decay			
Raw water			

Process	DBP (THM, HAA) Type	DBP (THM, HAA) f(x)	DBP (THM, HAA) Data
Raw water	Empirical	TOC, C_{l2}, Br^-, T, pH, t	13 Waters
Pre-chlorination	Empirical	ΔTOC	20 Waters
Post-chlorination	Empirical	DOC, UVA, C_{l2}, Br^-, T, pH, t	
GAC effluent	Empirical	DOC, UVA, C_{l2}, Br^-, T, pH, t	

Potential WTP2.0/2.2 Enhancements

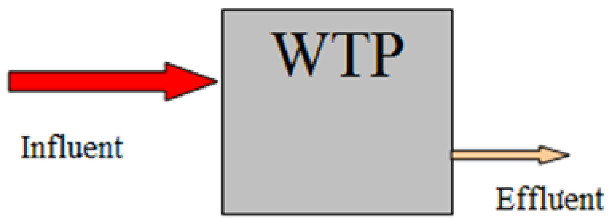
- Update existing predictive equations in WTP2.2
- Add biofiltration, UV and other unit processes (e.g., ozone-BAC)
- Predict formation of unregulated DBPs, such as chlorate, NDMA, HAA9, etc.
- Predict impacts of increasing chlorine residual thresholds

WTP-ccam for
System Engineering Analysis

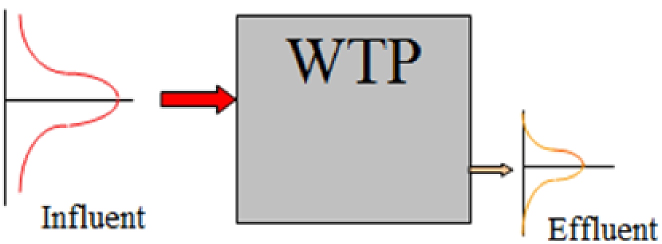
WTP-ccam: New Features

- **The Monte-Carlo simulation** for future variability of source water and for estimating cost-probability curve in process adjustment
- **Full-scale treatment plant study** at Richard Miller plant and China's plants
  - Full data for TOC, Cl- and Br-DBPs at process units
  - Mechanistic model for conventional unit process
  - Model reliability for extreme raw water in treatment trains
- Treatability data for emerging contaminants using data from China studies
  - Cynobacteria and microcystin
  - Pesticides and emerging contaminants
  - EPA treatability database and WTP3.0

WTP-ccam: Monte Carlo Simulation



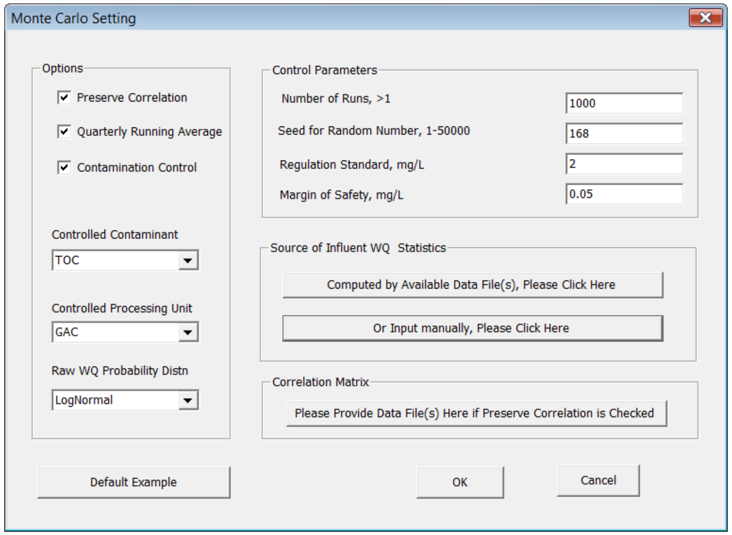
Original model

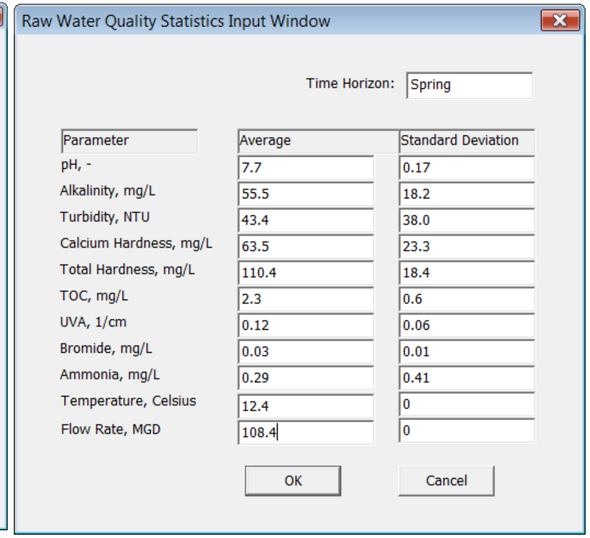


Modified model

- Source water variability in log-normal distribution
- The variability propagates in treatment train, resulting in variability in finished water
- Different from current engineering practice of using an single design parameter
- Allows evaluation of risk management, and application in forward projections

WTP-ccam: Monte Carlo Simulation





Source variability in input parameters

→

N=1000

WTP-ccam runs

Model outputs

→

N=1000

Number	Qin	Alk	Bro	Ca-H	Tt-H	NH3	Turb	PH	Temp	TOC	UVA
--	MGD	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	--	C	mg/L	1/cm
1	120.6	55.52	0.035	49.4	100.8	0.061	12.0	7.60	18.6	3.06	0.061
2	120.6	63.23	0.033	44.4	107.3	0.124	19.5	7.80	18.6	3.76	0.109
3	120.6	61.30	0.033	71.0	104.9	0.191	28.5	7.57	18.6	4.74	0.110
4	120.6	30.96	0.027	62.6	83.5	0.141	26.8	7.72	18.6	1.99	0.095
5	120.6	82.32	0.035	54.8	117.0	0.171	21.1	7.77	18.6	4.99	0.147
6	120.6	59.12	0.031	95.9	108.1	0.063	15.9	7.93	18.6	2.77	0.061
7	120.6	100.52	0.026	89.0	120.5	0.268	281.7	7.87	18.6	5.81	0.406
8	120.6	45.33	0.036	45.6	94.3	0.291	32.3	7.39	18.6	3.14	0.100
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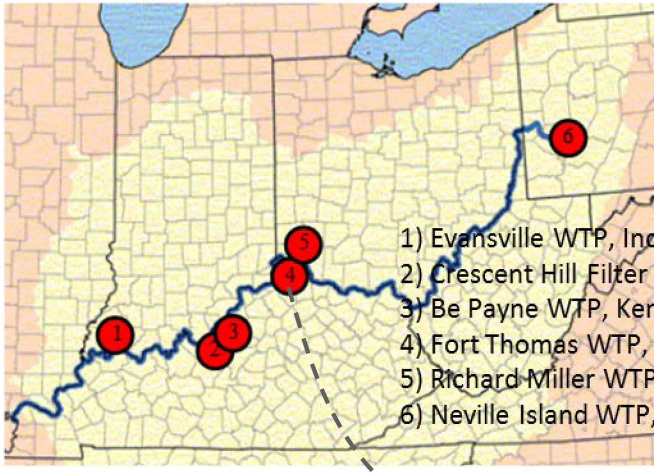
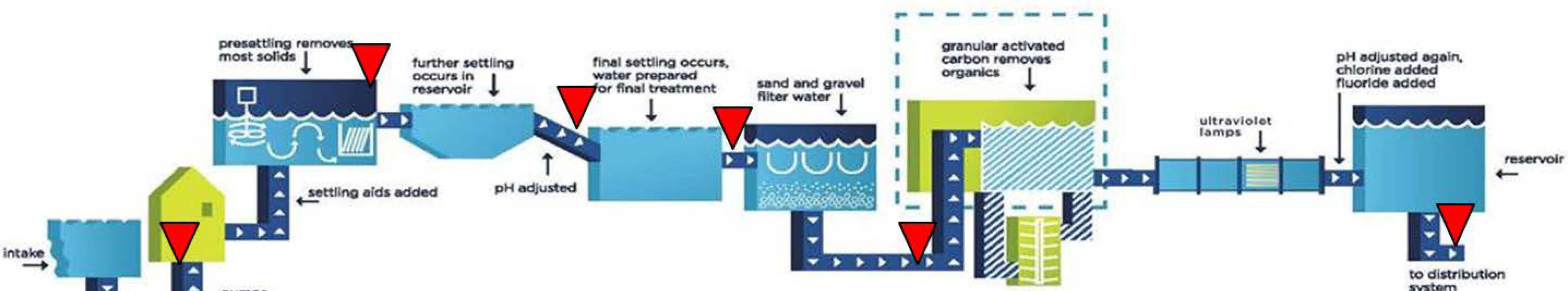
996	120.6	47.58	0.028	44.5	90.5	0.236	11.9	7.71	18.6	2.85	0.042
997	120.6	51.37	0.031	56.6	93.3	0.246	44.9	7.57	18.6	3.96	0.106
998	120.6	41.62	0.030	89.7	90.9	0.249	12.5	7.44	18.6	3.17	0.058
999	120.6	58.67	0.027	82.0	101.6	1.558	146.5	7.80	18.6	5.09	0.147
1000	120.6	40.39	0.031	72.4	94.3	0.351	18.1	7.60	18.6	2.14	0.041
Samples	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000	1000
Mean	120.6	58.18	0.030	62.6	98.9	0.359	43.7	7.71	18.6	3.83	0.113
St.dev	0.0	22.36	0.006	23.2	18.0	0.446	40.5	0.16	0.0	1.11	0.056
Min	120.6	15.48	0.014	23.8	49.5	0.003	2.1	7.14	18.6	1.36	0.024
Max	120.6	232.32	0.053	183.3	219.6	4.178	506.9	8.13	18.6	8.82	0.406

Case Study: Monte Carlo Simulation



1) Evansville WTP, Indiana.
2) Crescent Hill Filter WTP, Kentucky.
3) Be Payne WTP, Kentucky.
4) Fort Thomas WTP, Kentucky.
5) Richard Miller WTP, Ohio.
6) Neville Island WTP, Pennsylvania

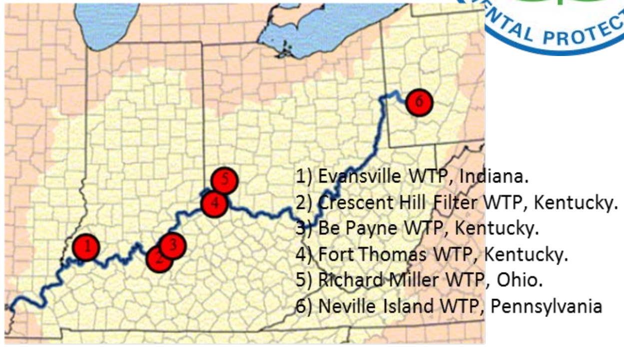
Miller Plant Treatment Model Development

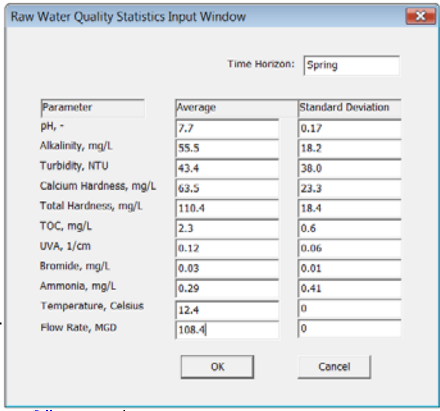


GCWW's treatment process at the Richard Miller Plant on the Ohio River

Case Study: Monte Carlo Simulation

- Probability distribution for projected source water variability in year 2030
- Based on statistical model using ICR data from Ohio River plants



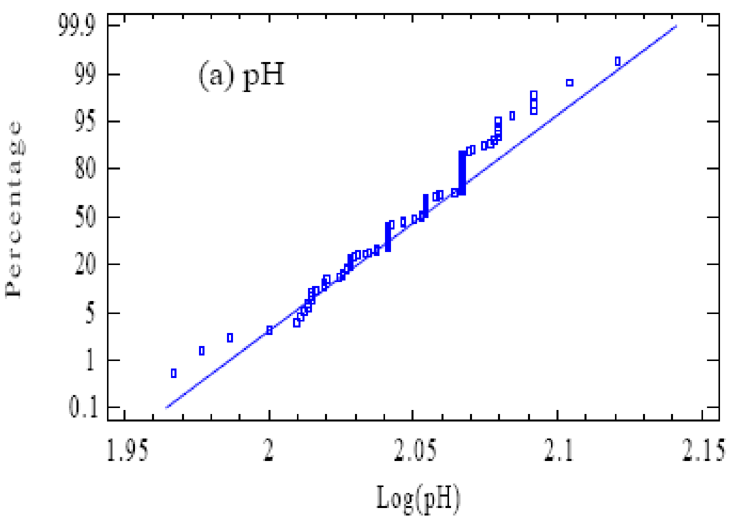


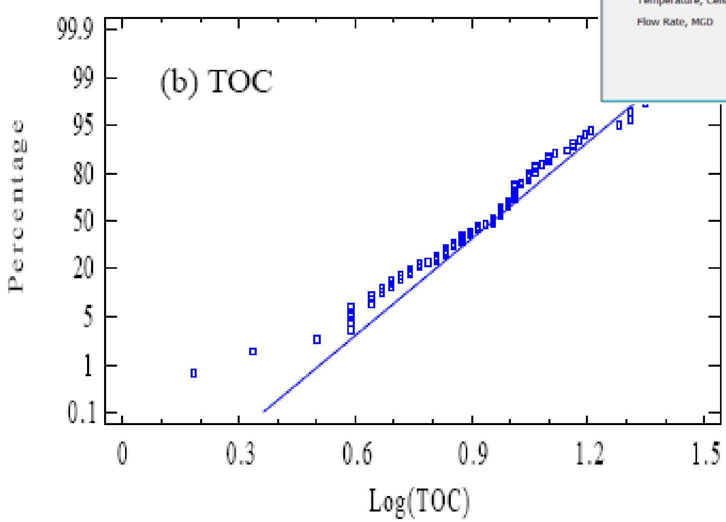
Raw Water Quality Statistics Input Window

Time Horizon: Spring

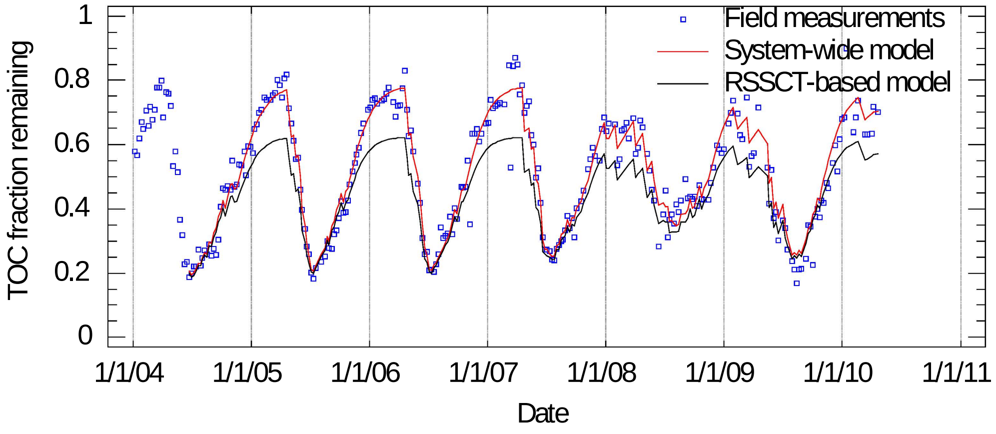
Parameter	Average	Standard Deviation
pH, -	7.7	0.17
Alkalinity, mg/L	55.5	18.2
Turbidity, NTU	43.4	38.0
Calcium Hardness, mg/L	63.5	23.3
Total Hardness, mg/L	110.4	18.4
TOC, mg/L	2.3	0.6
UVA, 1/cm	0.12	0.06
Bromide, mg/L	0.03	0.01
Ammonia, mg/L	0.29	0.41
Temperature, Celsius	12.4	0
Flow Rate, MGD	108.4	0

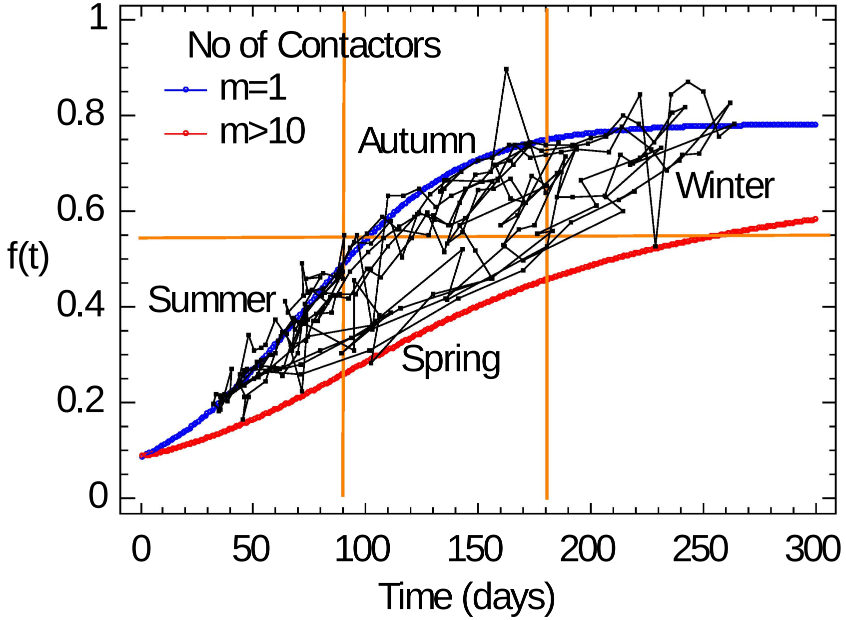
OK Cancel





Case Study: Monte Carlo Simulation





Probability of TOC variations in source water through the treatment train

- Source seasonal variation propagates passing through conventional treatment into GAC unit
- WTP-ccam simulates TOC removal and TTHM level by GAC
- The influent variability determines GAC treatment efficiency, the frequency of carbon regeneration, and thus operational cost
- One can optimize GAC for difference scenarios of reactor operation and carbon regeneration

Case Study: Monte Carlo Simulation

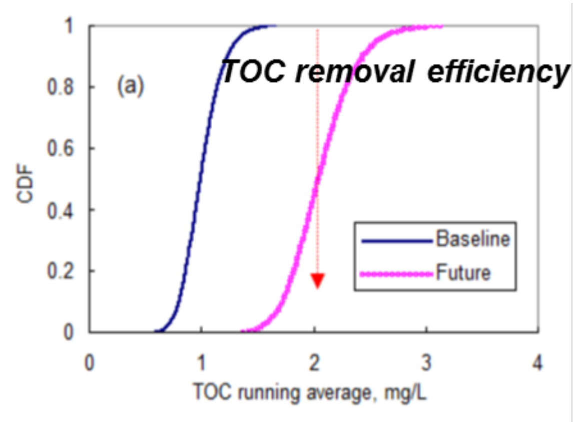
Removal rates in probability of source water variations

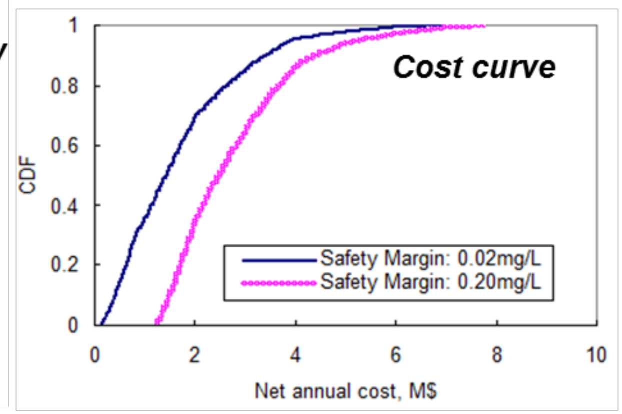
Two ways to characterize:

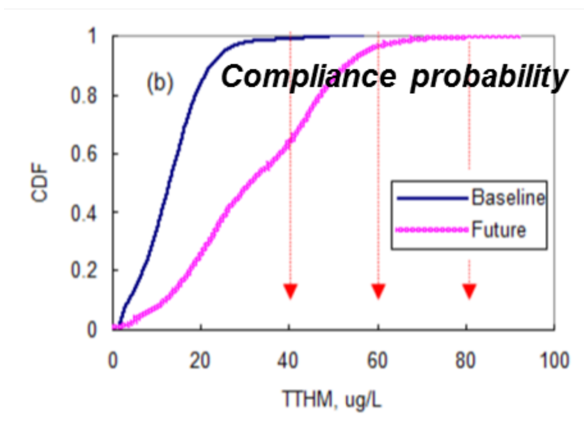
- Generalized formula for regional analysis (regulatory)
- **Model-based mechanistic formula for plant treatment analysis (compliance)**

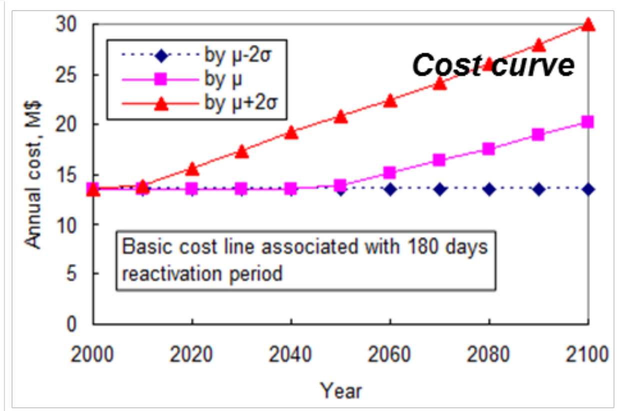
Treatment System Optimization:

- Optimize the staggered sequence of reactor reactivation
- Model the optimization point for seasonal variability







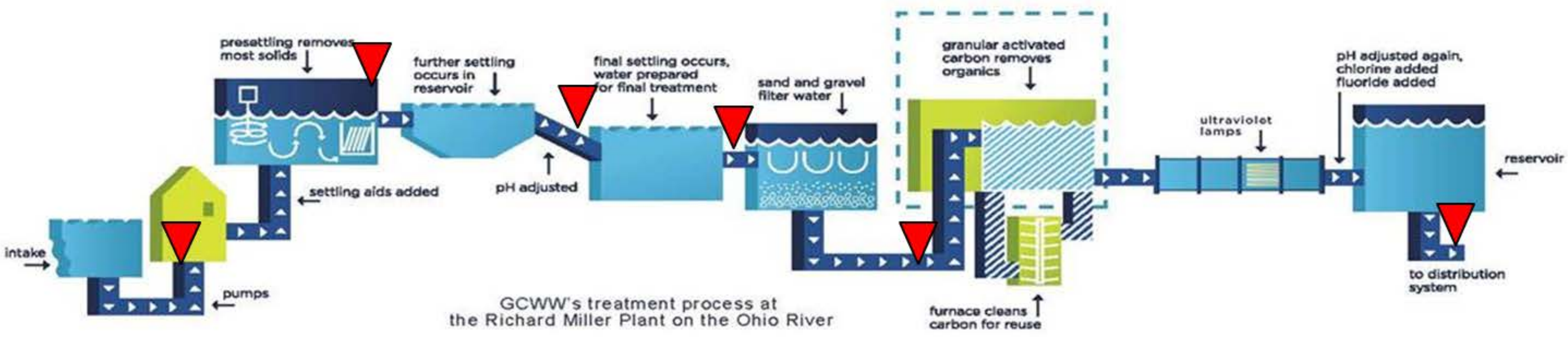


Ongoing Studies: Conventional Process Model

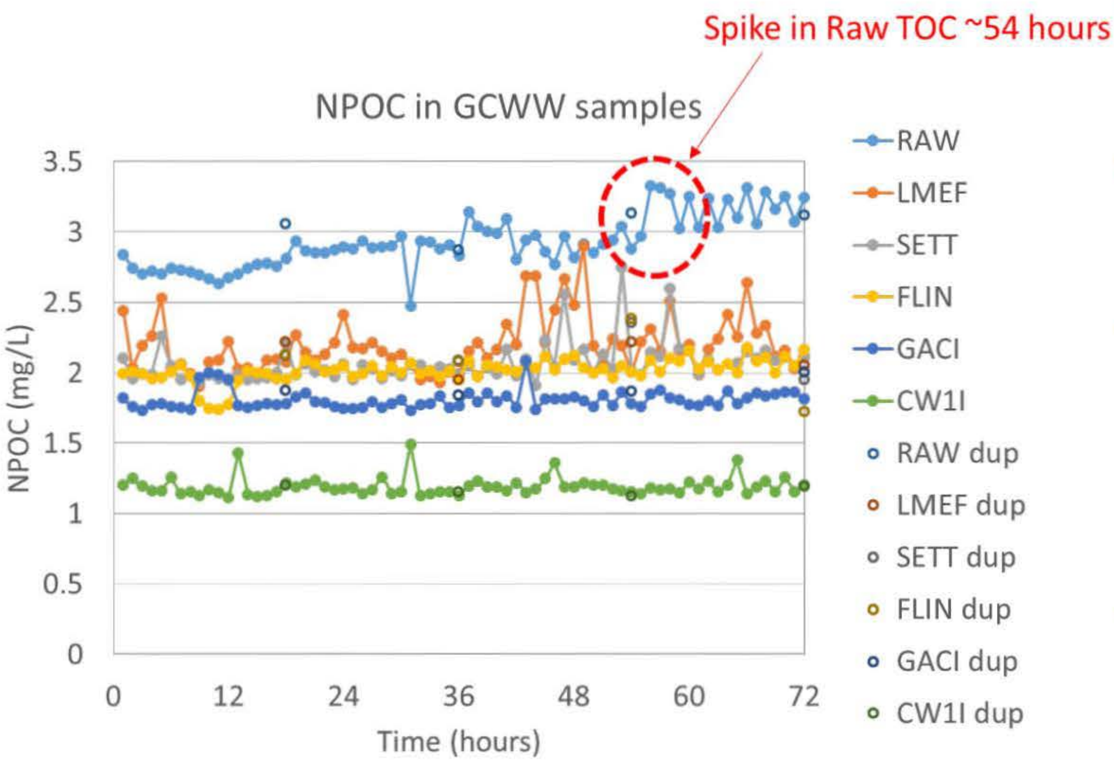
Objectives

- Develop TOC removal and TTHM formation models in conventional processes
- Evaluate applicability of the mechanistic models for Br-DBP generation
- Find general water quality parameters as model surrogates

- **Develop mechanistic models** for TOC, turbidity, and particulate removal in the conventional process units
- **72 Hours continuous sampling** at one-hr interval across the treatment train: coagulation/flocculation, sedimentation, sand filtration, GAC adsorption
- Capture a rain-induced perturbation in source water
- **Analyte includes** TOC, UV254 and UV spectrum, zeta potential, THM species, THM potential
- **Field measurements** include SCADA data (flow, dosage, turbidity, pH, temperature, etc.)



Ongoing Studies: Conventional Process Model

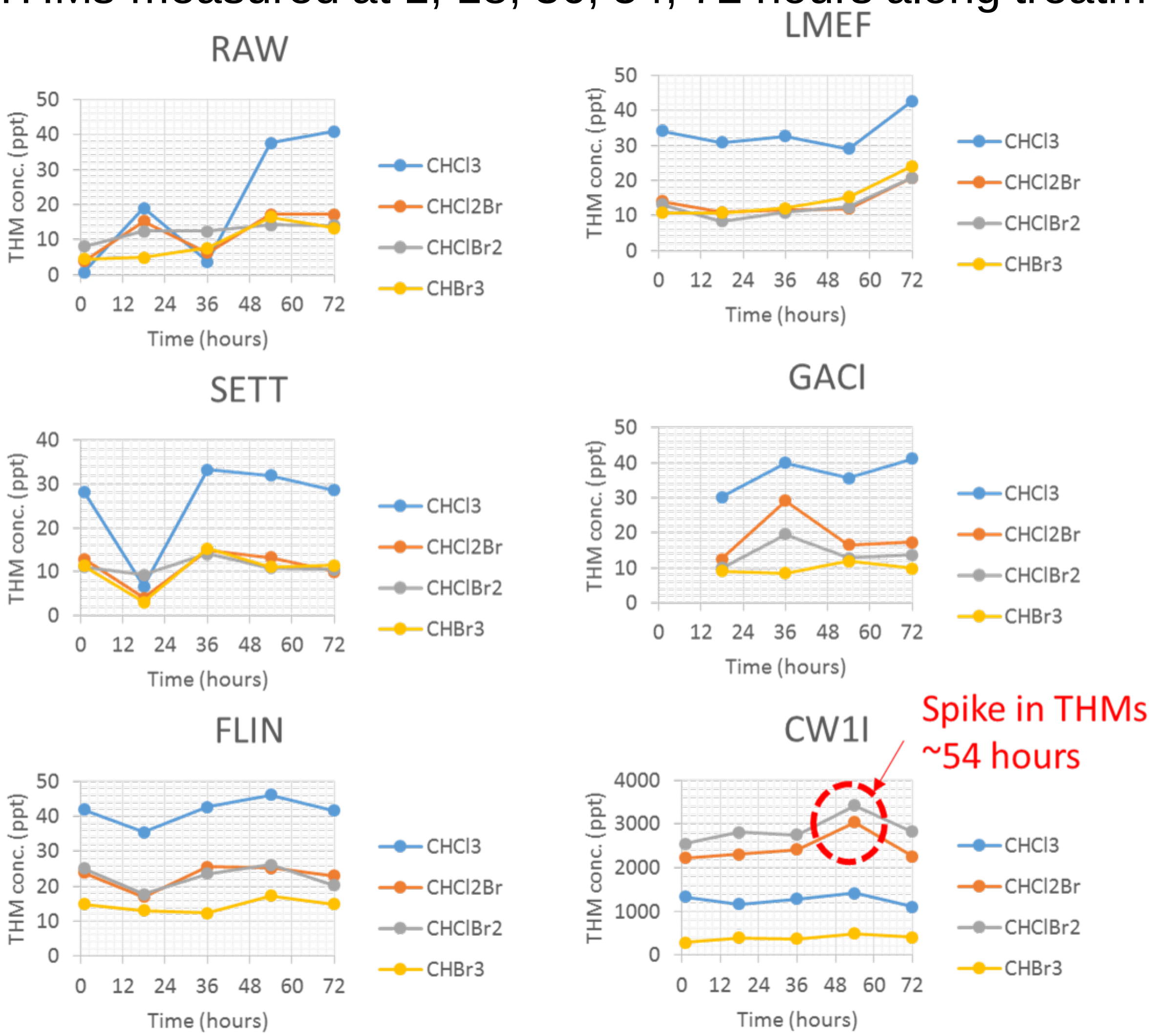


- **System response** in TOC, turbidity, zeta potential, and UV254 during the source water perturbation
- **Unit processes** differ in removal rates, and **system-wide coordination** in operation is very important
- **TOC removed** in sedimentation and, filtration. **GAC as key barrier** for removal of reactive TOC
- **Ongoing model development,** Focusing on TOC removal and THM formation potential
- **THM formation potential model established**. To be further calibrated with Miller plant data and the China water plant data

Ongoing Studies: Conventional Process Model

In situ measurement of THM formation

THMs measured at 1, 18, 36, 54, 72 hours along treatment process

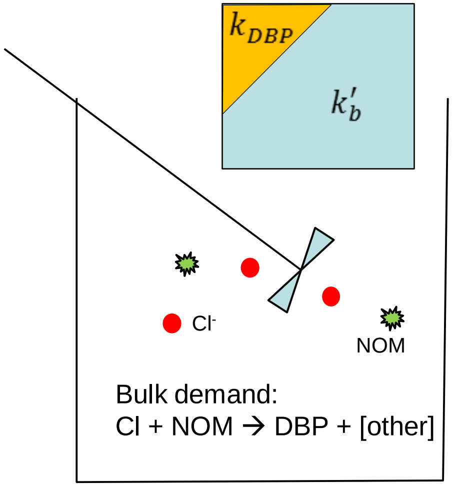


- Very low level for all treatment units until CW1I
- Before CW1I, chloroform in consistently the highest THM
- In CW1I, CHClBr2 is the highest, followed by CHCl2Br
- In RAW and LMEF, which have highest TOC, THMs increase with time
- Other systems have less temporal pattern

DBP Mechanistic Models

$CH_3COCH_3 + 3HOCl \rightarrow CH_3COCCl_3 + 3H_2O$ oxidation step

$CH_3COCCl_3 + H_2O \rightarrow CH_3COOH + CHCl_3$ hydrolysis step



Chlorine decay

$$\left(\frac{\partial C_A}{\partial t}\right)_{b1} = -k_b^{'} C_A \cdot C_{OM}$$

$$\left(\frac{\partial C_A}{\partial t}\right)_{b2} = -k_{DBP} C_A C_E = -k_{DBP} C_A \left[C_{E,0} - \overline{\theta}\left(C_{A,0} - C_A\right)\right]$$

Solving for DBP analytical solution

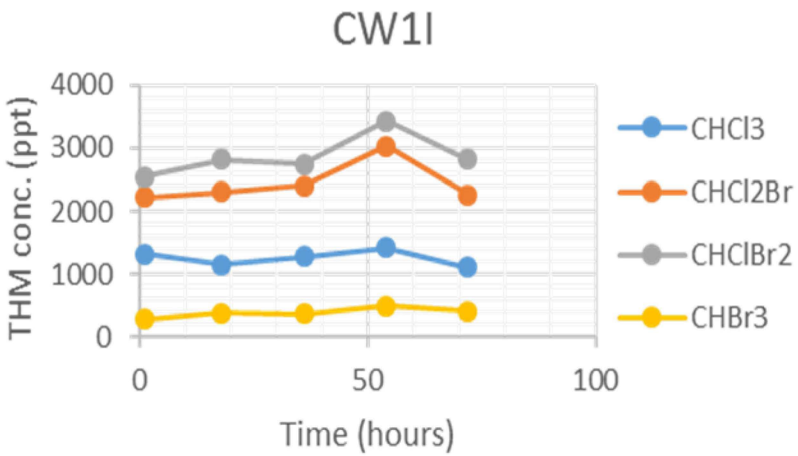
$$C_{DBP} = \int k_{DBP} \frac{\gamma C_{A,0}}{\left(\gamma + \theta C_{A,0}\right) e^{k_E t} - \theta C_{A,0}} \left(C_{E,0} - \theta C_{A,0}\right) \partial t + $$

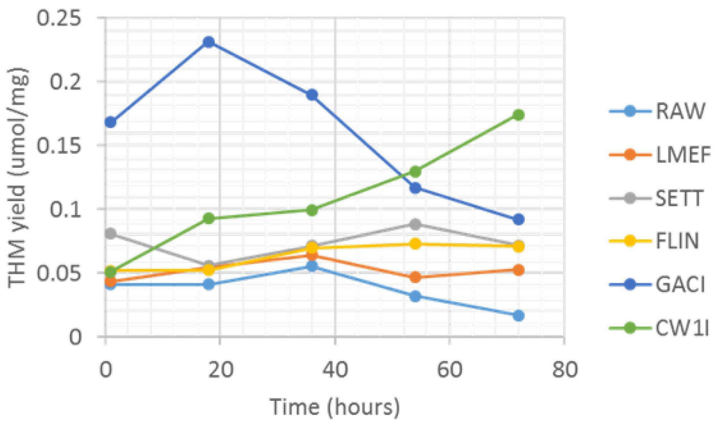
$$+ \int k_{DBP} \left[\frac{\gamma C_{A,0}}{\left(\gamma + \theta C_{A,0}\right) e^{k_E t} - \theta C_{A,0}}\right]^2 \partial t$$

DBP formation

$$\frac{\partial C_{DBP}}{\partial t} = k_{DBP} C_A \cdot C_E = k_{DBP} C_A \cdot \left[C_{E,0} - \overline{\theta}\left(C_{A,0} - C_A\right)\right]$$

DBP Mechanistic Models





THM Formation Potential: Model Development

$$\frac{\Delta C_{DBP,0}}{C_{A,0}} = \bar{\theta}\frac{\left(e^{k_E t} - 1\right)}{e^{k_E t} - \left(\frac{\theta C_{A,0}}{\theta C_{A,0} + \gamma}\right)1}$$

$$t \to \infty$$

$$\left(\Delta C_{DBP,0}\right)_p = \bar{\theta} C_{A,0}$$

TBP formation potential

Can this model be for general use?

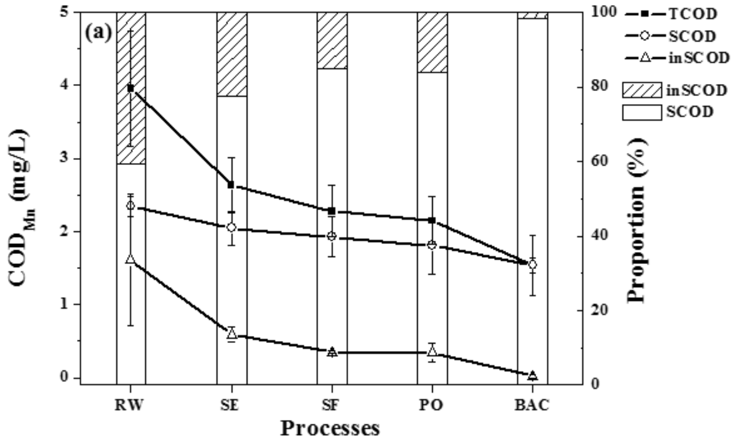
Ongoing Studies: Conventional Process Model

Ongoing Br-THM model development:

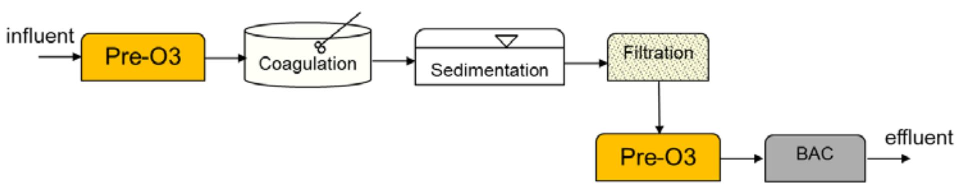
- All samples in the plant study are being analyzed for bromide concentrations
- The results will be calculated in molar equivalence to reconcile with measured Br-THM species
- Kinetic models will be developed for each of the treatment units
- Special attention to the effect of source water perturbation and the plant operational parameters

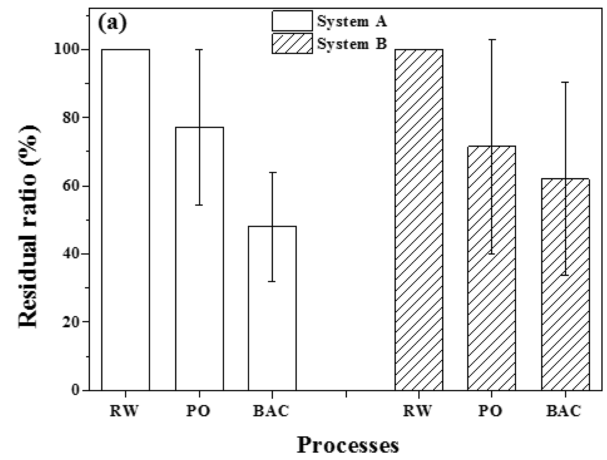
Treatment Plant Analysis in China

- Test and further develop WTP with different water sources and treatment processes in China
- Comparative studies on parameters: turbidity, particle size, TCOD, COD_{Mn}, and odor compounds
- Research ongoing

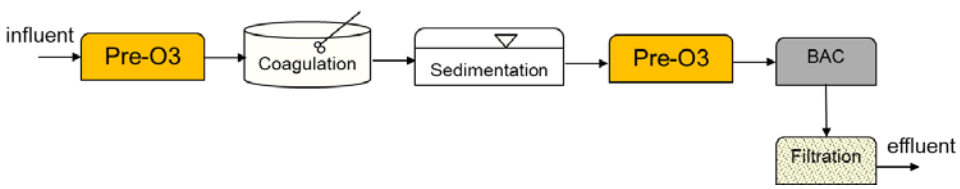


- Conventional O3-BAC Process (System A)





- Rear Sand Filtration Process (System B)



Future Developments

Incorporate DBP-related NOM indicators in modeling of DBP formation potentials

- Zeta potentials
- UV-vis
- NOM fractions

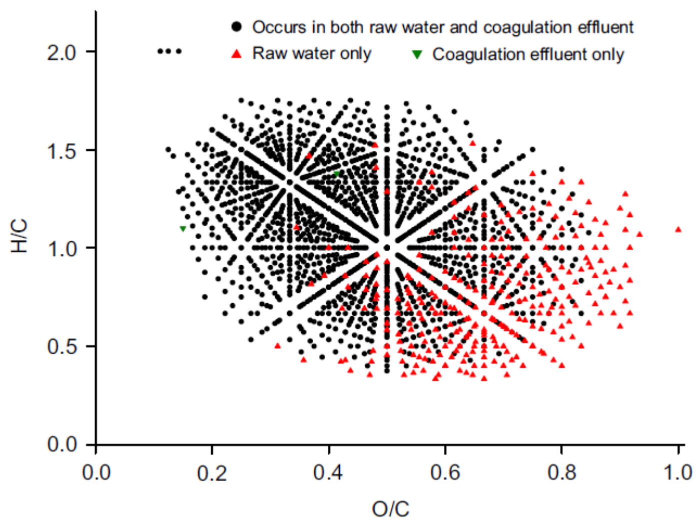
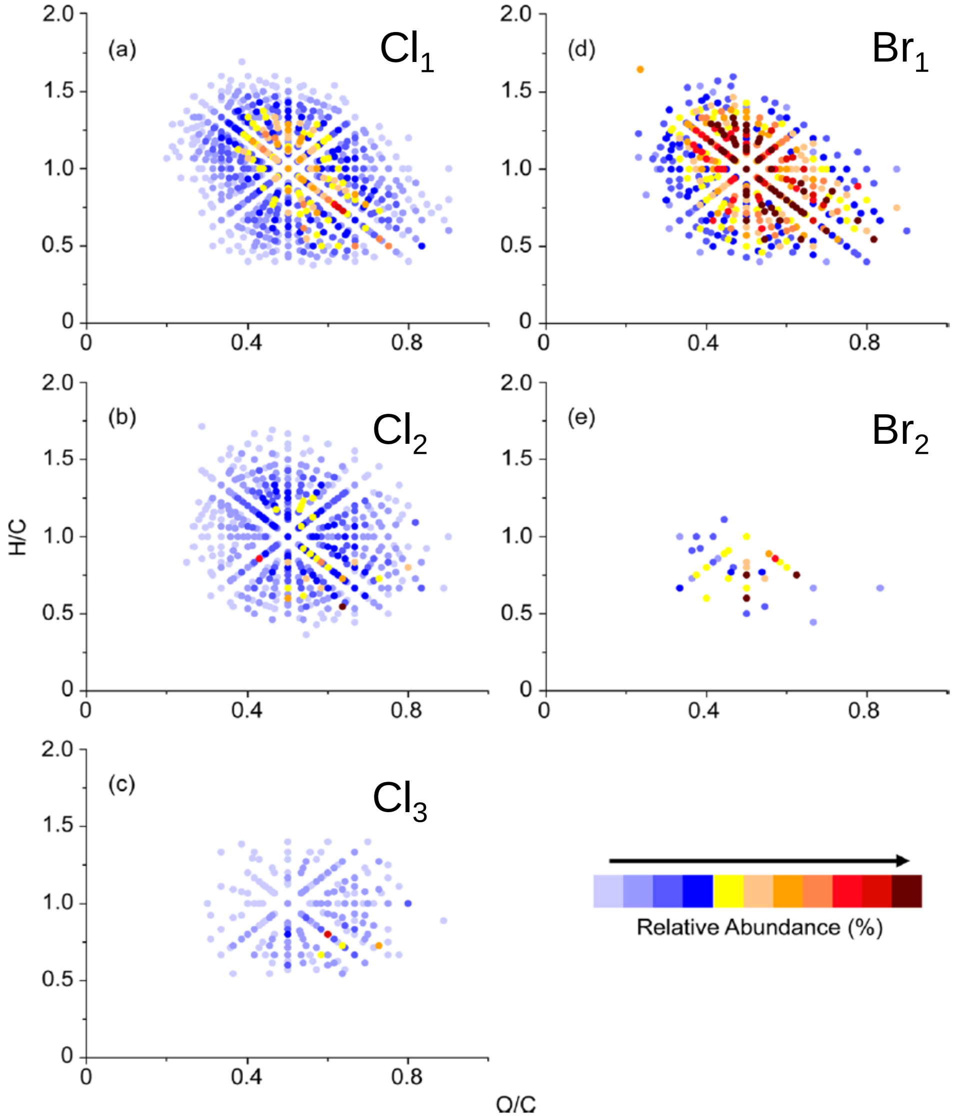
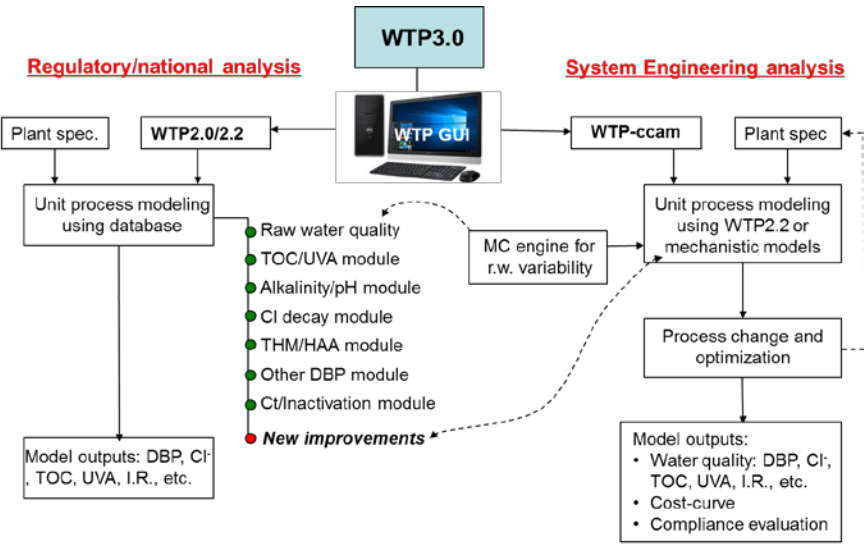


Fig. 2 — The van Krevelen diagram of the raw water DOM overlain with the coagulation effluent DOM.



Zhang et al. (2012, 2014)

Summary



- WTP3.0 expected in 2018
- Options for applications
  - Improved WTP2.0/2.2 for regulatory/national analysis
  - Enhanced WTP-ccam for model-based engineering analysis
- Capability simulating TOC, TTHM, Br-DBP, HAA and TOX for a given plant configuration and operation scenarios
- Future developments with data on emerging concerns (microcystins, pesticides, etc.)
- Treatment adaptation key to manage the risk from source water variations

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- Zhejiang University: Yu Shao

Disclaimer:

The content and views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA.

Thank you!

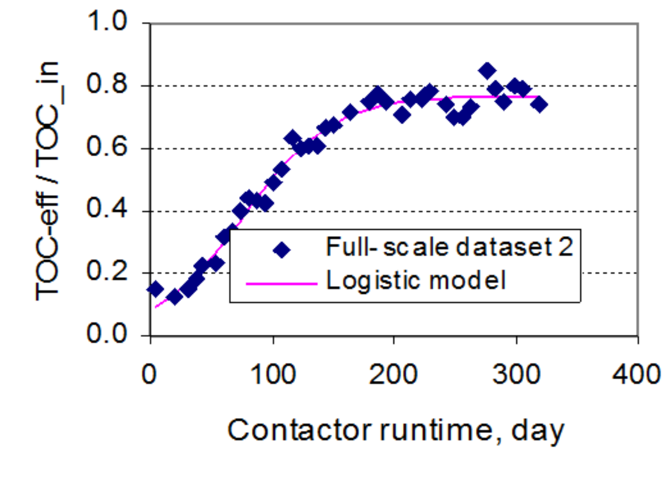
- Questions and comments

Estimation of Logistic Model Parameters

- Logistic model parameters *a, b* and *d* were estimated based on a non-linear regression algorithm (Hartley,1961).
  - Objective function using least square analysis.

Min $$Q(a',b',d') = \sum_{k=1}^{n} \left(y_k - f(t_k;a',b',d')\right)^2$$

    - t_k and y_k are observed GAC service time and ratio of TOC_{-eff} over TOC_{-in}
    - n is field sample size
  - Corrections to parameters during iterations using Gauss-Newton method.



System-Wide Logistic Model for Miller Plant

- Logistic model parameters were first averaged for each contactor.
- Values in each column were then averaged.

These values were used to build up the system-wide logistic model

Contactor ID	$\bar{a}$	$\bar{b}$	$\bar{d}$ (1/day)
1	0.832	8.334	0.027
2	0.741	9.557	0.031
3	0.759	8.124	0.029
4	0.770	9.419	0.030
5	0.773	7.502	0.032
6	0.795	6.440	0.032
7	0.811	8.838	0.027
8	0.801	7.478	0.028
9	0.799	7.176	0.027
10	0.765	6.988	0.026
11	0.776	8.588	0.027
12	0.767	9.843	0.031
System-wide average	0.782	8.191	0.029
Coefficient of variation	0.03	0.13	0.08