

Updated: 13 November 2013

CEE697K Lecture #17 1

[Print version](#)

CEE 697K

ENVIRONMENTAL REACTION KINETICS

Lecture #17

Kinetic Modeling: Computer Models

Case Study: Chloramination II

Brezonik, pp.

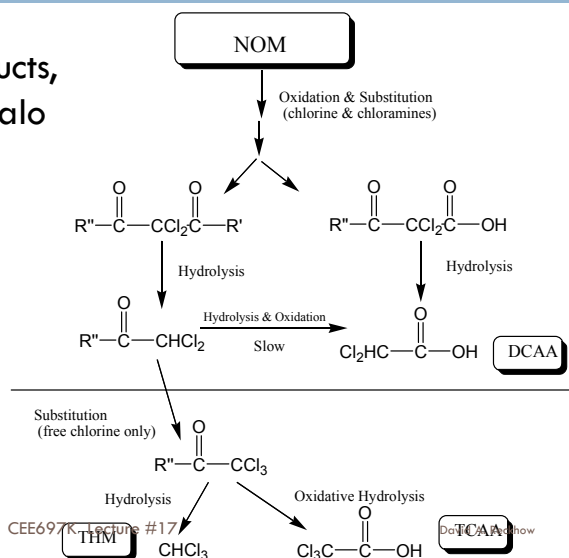
David A. Reckhow

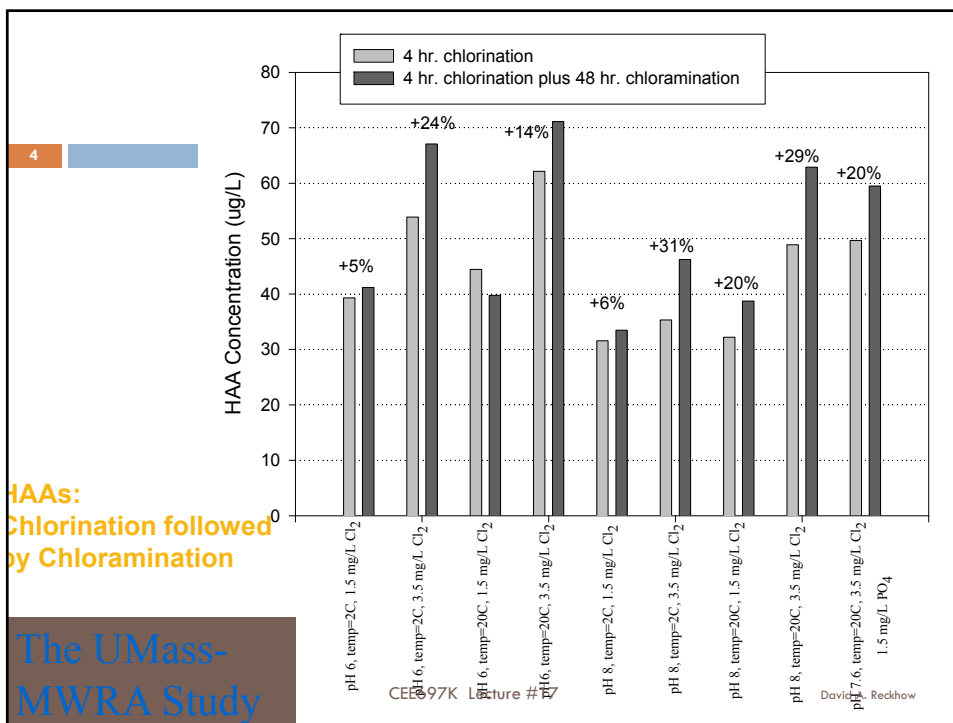
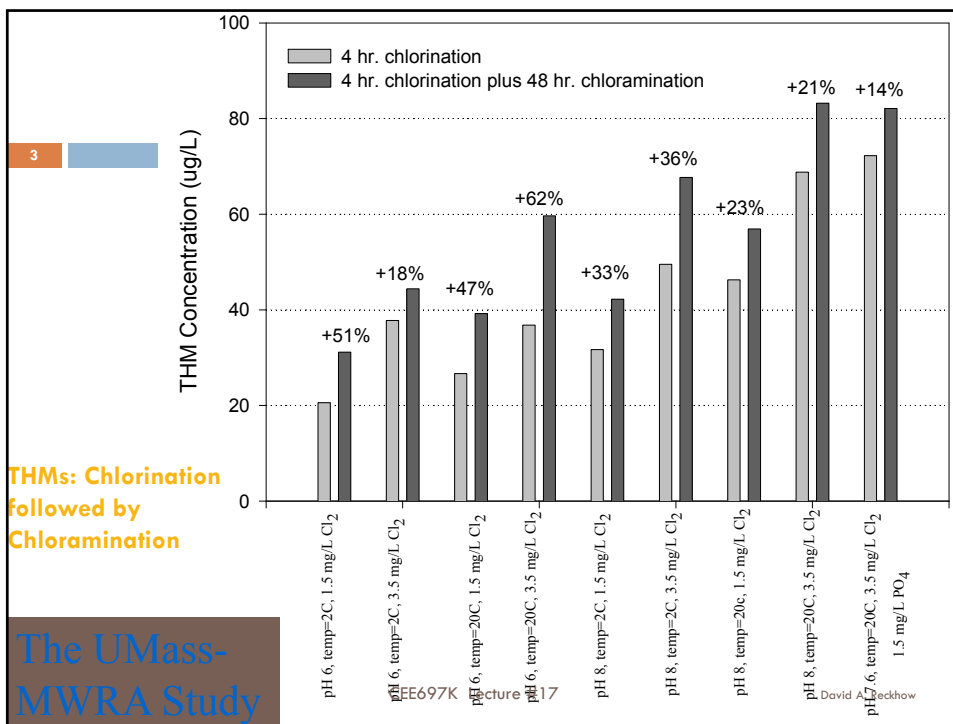
Introduction

HAA: Chlorine vs Chloramine

2

- Dihalo products, but little trihalo





Precursors & Behavior

General Trends

Mono & Dihalo-DBPs	Trihalo-DBPs	Precursor Origins	Removal by:	
			Coag. or Oxidation	Biodegradation
Haloacids (DCAA)	THMs	General NOM	Average	Average
Aldehydes	Aldehydes (Chloral Hydrate)	Oxidized NOM (bacterial, solar, ozone)	Poor	Good
Ketones (Dichloropropanone)	Ketones (Trichloropropanone)			
Nitroalkanes	Nitroalkanes (Chloropicrin)	reactive Nitrogen species		
Nitriles (Dichloroacetonitrile)	Nitriles (Trichloroacetonitrile)	Algal (autochthonous)	Average	Average
Amides (Dichloroacetamide)	Amides (Trichloroacetamide)			
Cyanogen Halides (CNCl, CNBr)				
Halobenzoquinones?	Haloacids (TCAA)	Terrestrial - Lignin (allochthonous)	Good	Poor

CEE697K Lecture #17
Preferentially formed by Chloramination

DBP control with DS management

6

Parameter	THM	Tri-HAAs	Di-HAAs	HANs	TCP	DCP	CP	Iodo-DBPs
Time ↓	↓	↓	↓	↑	↑	↑	↓	↑
Cl ₂ Dose ↓	↓	↓~	↓	↑	↑	↑↑	↓	↑
pH ↓	↓	↑	~	↑	↑	↑		↑
Cl ₂ to NH ₂ Cl ↑	↓	↓↓	↓~	~	~	↑	↑	↑
Temp ↓	↓	~	↓	↑	↑	↑	↓	↑

Notes:

HANs: haloacetonitriles, including DCAN

TCP: trichloropropanone, a halo ketone

DCP: dichloropropanone: a halo ketone

CP: chloropicrin: a halonitromethane

Iodo-DBPs: include iodinated THMs, HAAs, etc

David A. Reckhow

Chloramines vs Free Chlorine

7

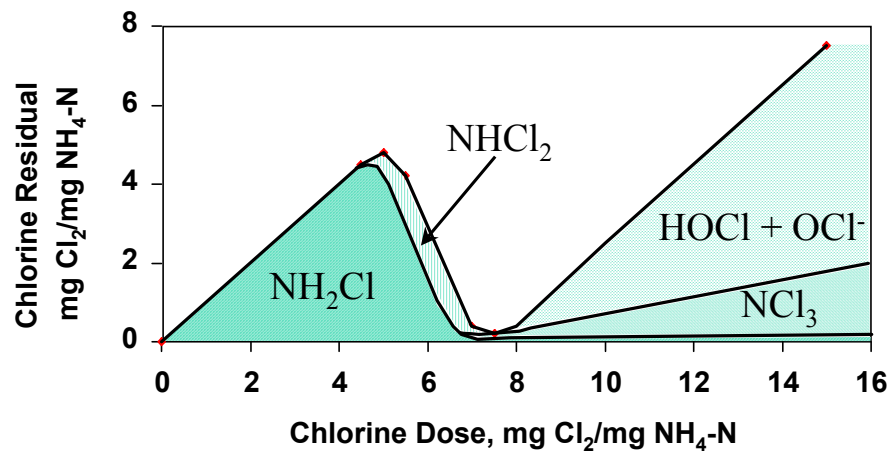
- DBPs
 - Lower levels of trihalogenated byproducts
 - Easier to meet current DBP regulations
 - Less impact on dihalogenated compound
 - Some are higher with chloramines
 - More of some types of N-DBPs
 - Organic chloramines, nitriles, amides, nitro compds
- Other concerns
 - Growth of ammonia oxidizing bacteria
 - Loss of residual, formation of reactive intermediates
 - Reduction of Lead (IV)
 - Public perception & direct health effects

CEE697K Lecture #17

David A. Reckhow

Theoretical Breakpoint Curve

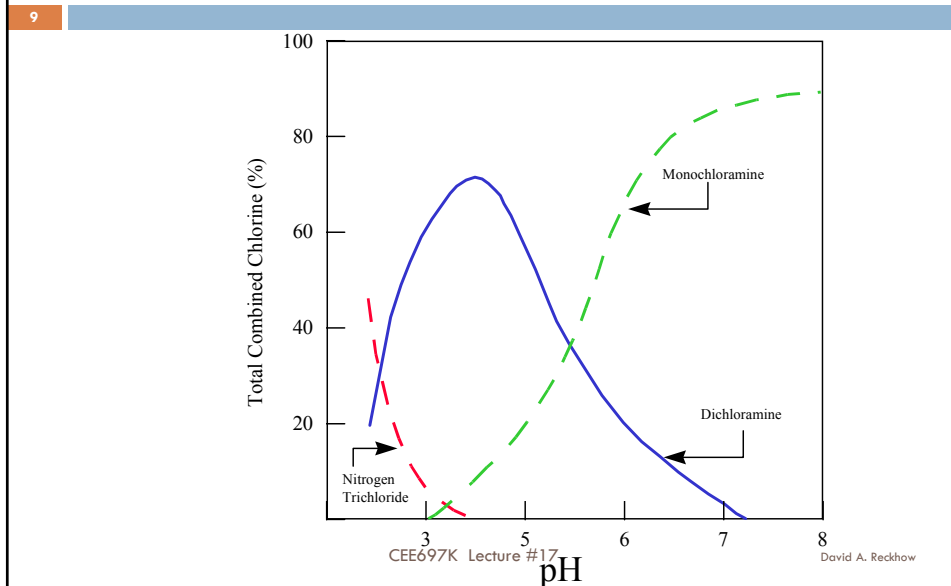
8



CEE697K Lecture #17

David A. Reckhow

Distribution Diagram for Chloramine Species with pH



Jafvert & Valentine Model

10

Jafvert, C. T. and R. L. Valentine (1992). "Reaction Scheme for the Chlorination of Ammoniacal Water." *Environmental Science & Technology* **26(3): 577-586.**

Table I. Reactions and Associated Constants

reaction stoichiometry	rate expression	rate constant (25 °C)	ref
(1) HOCl + NH ₃ → NH ₂ Cl + H ₂ O	$k_{am}[\text{HOCl}][\text{NH}_3]$	$k_{am} = 1.5 \times 10^{10} \text{ M}^{-1} \text{ h}^{-1}$	18
(2) NH ₂ Cl + H ₂ O → HOCl + NH ₃	$k_{ma}[\text{NH}_2\text{Cl}]$	$k_{ma} = 7.6 \times 10^{-2} \text{ h}^{-1}$	18
(3) HOCl + NH ₂ Cl → NHCl ₂ + H ₂ O	$k_{md}[\text{HOCl}][\text{NH}_2\text{Cl}]$	$k_{md} = 1.0 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$	4, 17
(4) NHCl ₂ + H ₂ O → HOCl + NH ₂ Cl	$k_{dm}[\text{NHCl}_2]$	$k_{dm} = 2.3 \times 10^{-3} \text{ h}^{-1}$	17
(5) NH ₂ Cl + NH ₂ Cl → NHCl ₂ + NH ₃	$k_{ammd}[\text{NH}_2\text{Cl}]^2$	$k_{ammd}^a = k_{d1}[\text{H}^+] + k_{H_3\text{P}}[\text{H}_3\text{PO}_4^-] + k_{H_3\text{P}}[\text{H}_3\text{PO}_4]$	20, 21
(6) NHCl ₂ + NH ₃ → NH ₂ Cl + NH ₂ Cl	$k_{dmm}[\text{NHCl}_2][\text{NH}_3][\text{H}^+]$	$k_{dmm} = 2.16 \times 10^8 \text{ M}^{-2} \text{ h}^{-1}$	9
(7) NHCl ₂ + H ₂ O → I	$k_{di}[\text{NHCl}_2][\text{OH}^-]$	$k_{di} = 4.0 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$	20, 28
(8) I + NHCl ₂ → HOCl + products ^b	$k_{idp}[I][\text{NHCl}_2]$	$k_{idp} = 1.0 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$	6
(9) I + NH ₂ Cl → products ^b	$k_{imp}[I][\text{NH}_2\text{Cl}]$	$k_{imp} = 3.0 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$	6
(10) NH ₂ Cl + NHCl ₂ → products ^b	$k_{mdp}[\text{NH}_2\text{Cl}][\text{NHCl}_2]$	$k_{mdp} = 55.0 \text{ M}^{-1} \text{ h}^{-1}$	6, 8
(11) HOCl + NHCl ₂ → NCl ₃ + H ₂ O	$k_{at}[\text{NHCl}_2][\text{HOCl}]$	$k_{at}^c = k_{HP}[\text{HPO}_4^{2-}] + k_{OCl}[\text{OCl}^-] + k_{OH}[\text{OH}^-]$	9
(12) NHCl ₂ + NCl ₃ + 2H ₂ O → 2HOCl + products ^b	$k_{atp}[\text{NHCl}_2][\text{NCl}_3][\text{OH}^-]$	$k_{atp} = 2.0 \times 10^{14} \text{ M}^{-2} \text{ h}^{-1}$	9, d
(13) NH ₂ Cl + NCl ₃ + H ₂ O → HOCl + products ^b	$k_{mtp}[\text{NH}_2\text{Cl}][\text{NCl}_3][\text{OH}^-]$	$k_{mtp} = 5.0 \times 10^{12} \text{ M}^{-2} \text{ h}^{-1}$	d
(14) NHCl ₂ + 2HOCl + H ₂ O → NO ₃ ⁻ + 5H ⁺ + 4Cl ⁻	$k_{dhp}[\text{NHCl}_2][\text{OCl}^-]$	$k_{dhp} = 8.3 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$	d

^a $k_H = 2.5 \times 10^7 \text{ M}^{-2} \text{ h}^{-1}$; $k_{HP} = 1.3 \times 10^8 \text{ M}^{-2} \text{ h}^{-1}$; $k_{H_3\text{P}} = 3.2 \times 10^6 \text{ M}^{-2} \text{ h}^{-1}$. In carbonate-buffered systems additional terms include $k_{H_2\text{CO}_3}[\text{H}_2\text{CO}_3] + k_{\text{HCO}_3^-}[\text{HCO}_3^-]$, where $k_{\text{H}_2\text{CO}_3} = 2.7 \times 10^8 \text{ M}^{-2} \text{ h}^{-1}$ and $k_{\text{HCO}_3^-} = 7.2 \text{ M}^{-2} \text{ h}^{-1}$ (21). ^b Products may include N₂, H₂O, Cl⁻, H⁺, NO₃⁻, and unidentified reaction products. For purposes of d[H⁺] calculation, products were assumed to contain 3H⁺ for each reaction, consistent with N₂ formation. ^c $k_{HP} = 5.72 \times 10^7 \text{ M}^{-2} \text{ h}^{-1}$; $k_{OCl} = 3.24 \times 10^5 \text{ M}^{-2} \text{ h}^{-1}$; $k_{OH} = 1.18 \times 10^{13} \text{ M}^{-2} \text{ h}^{-1}$. In carbonate-buffered systems an additional term is $k_{\text{CO}_3}[\text{CO}_3^{2-}]$, where $k_{\text{CO}_3} = 2.16 \times 10^{10} \text{ M}^{-2} \text{ h}^{-1}$ (9). ^d This work.

CEE697K Lecture #17

David A. Reckhow

Model Equations

Vikesland, P. J., K. Ozekin, et al. (2001).
 "Monochloramine decay in model and distribution
 system waters." *Water Research* **35(7)**: 1766-1776.

#	Reaction	Rate coefficient/equilibrium constant (25°C)	References
1.1	$\text{HOCl} + \text{NH}_3 \rightarrow \text{NH}_2\text{Cl} + \text{H}_2\text{O}$	$k_{1.1} = 1.5 \times 10^{10} \text{ M}^{-1} \text{ h}^{-1}$	Morris and Isaac (1981)
1.2	$\text{NH}_2\text{Cl} + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{NH}_3$	$k_{1.2} = 7.6 \times 10^{-2} \text{ h}^{-1}$	Morris and Isaac (1981)
1.3	$\text{HOCl} + \text{NH}_2\text{Cl} \rightarrow \text{NHCl}_2 + \text{H}_2\text{O}$	$k_{1.3} = 1.0 \times 10^6 \text{ M}^{-1} \text{ h}^{-1}$	Margerum et al. (1978)
1.4	$\text{NHCl}_2 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{NH}_2\text{Cl}$	$k_{1.4} = 2.3 \times 10^{-3} \text{ h}^{-1}$	Margerum et al. (1978)
1.5	$\text{NH}_2\text{Cl} + \text{NH}_2\text{Cl} \rightarrow \text{NHCl}_2 + \text{NH}_3$	k_d^a	Vikesland et al. (2001)
1.6	$\text{NHCl}_2 + \text{NH}_3 \rightarrow \text{NH}_2\text{Cl} + \text{NH}_2\text{Cl}$	$k_{1.6} = 2.2 \times 10^8 \text{ M}^{-2} \text{ h}^{-1}$	Hand and Margerum (1983)
1.7	$\text{NHCl}_2 + \text{H}_2\text{O} \rightarrow \text{I}$	$k_{1.7} = 4.0 \times 10^5 \text{ M}^{-1} \text{ h}^{-1}$	Jafvert and Valentine (1987)
1.8	$\text{I} + \text{NHCl}_2 \rightarrow \text{HOCl} + \text{products}$	$k_{1.8} = 1.0 \times 10^8 \text{ M}^{-1} \text{ h}^{-1}$	Leao (1981)
1.9	$\text{I} + \text{NH}_2\text{Cl} \rightarrow \text{products}$	$k_{1.9} = 3.0 \times 10^7 \text{ M}^{-1} \text{ h}^{-1}$	Leao (1981)
1.10	$\text{NH}_2\text{Cl} + \text{NHCl}_2 \rightarrow \text{products}$	$k_{1.10} = 55.0 \text{ M}^{-1} \text{ h}^{-1}$	Leao (1981)
1.11	$\text{HOCl} \rightarrow \text{H}^+ + \text{OCl}^-$	$\text{p}K_a = 7.5$	Snoeyink and Jenkins (1980)
1.12	$\text{NH}_4^+ \rightarrow \text{NH}_3 + \text{H}^+$	$\text{p}K_a = 9.3$	Snoeyink and Jenkins (1980)
1.13	$\text{H}_2\text{CO}_3 \rightarrow \text{HCO}_3^- + \text{H}^+$	$\text{p}K_a = 6.3$	Snoeyink and Jenkins (1980)
1.14	$\text{HCO}_3^- \rightarrow \text{CO}_3^{2-} + \text{H}^+$	$\text{p}K_a = 10.3$	Snoeyink and Jenkins (1980)

Vikesland modification

12

□ Modified version of equation #5 for carbonate

$$\square k_d = k_H^+ [\text{H}^+] + k_{\text{H}_2\text{CO}_3} [\text{H}_2\text{CO}_3] + k_{\text{HCO}_3} [\text{HCO}_3^-]$$

□ Where

■ $k_H^+ = 2.5 \times 10^7 \text{ M}^{-2} \text{ h}^{-1}$

■ $k_{\text{H}_2\text{CO}_3} = 4 \times 10^4 \text{ M}^{-2} \text{ h}^{-1}$

■ $k_{\text{HCO}_3} = 800 \text{ M}^{-2} \text{ h}^{-1}$

- I is the unidentified monochloramine auto-decomposition intermediate

Vikesland, P. J., K. Ozekin, et al. (2001).
 "Monochloramine decay in model and distribution
 system waters." *Water Research* **35(7)**: 1766-1776.

Temperature Effects

13

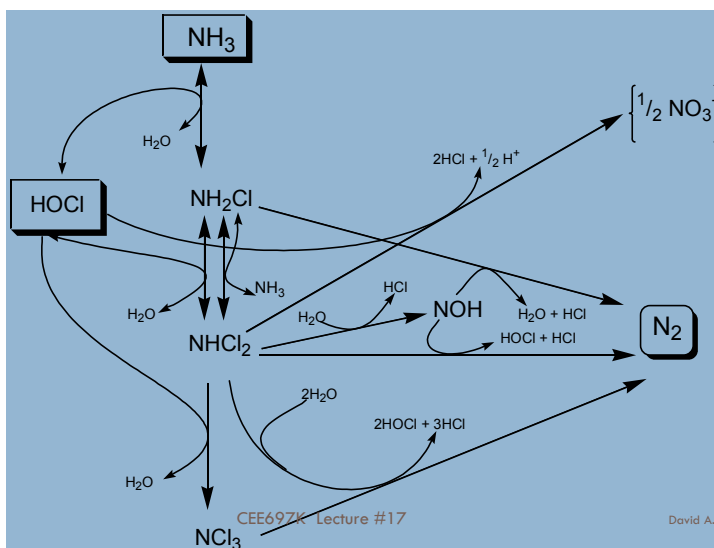
Reaction	Rate coefficient/equilibrium constant	References
$\text{HOCl} + \text{NH}_3 \rightarrow \text{NH}_2\text{Cl} + \text{H}_2\text{O}$	$k_{1,1} = 2.37 \times 10^{12} \exp(-1510/T) \text{ M}^{-1} \text{ h}^{-1}$	Morris and Isaac (1981)
$\text{NH}_2\text{Cl} + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{NH}_3$	$k_{1,2} = 6.7 \times 10^{11} \exp(-8800/T) \text{ h}^{-1}$	Morris and Isaac (1981)
$\text{HOCl} + \text{NH}_2\text{Cl} \rightarrow \text{NHCl}_2 + \text{H}_2\text{O}$	$k_{1,3} = 1.08 \times 10^9 \exp(-2010/T) \text{ M}^{-1} \text{ h}^{-1}$	Margrumei et al. (1978)
$\text{NH}_2\text{Cl} + \text{NH}_2\text{Cl} \rightarrow \text{NHCl}_2 + \text{NH}_3$	$k_{1,5} = k_H[H^+] + k_{\text{HCO}_3}[HCO_3^-] + k_{\text{H}_2\text{CO}_3}[H_2CO_3]$	
	$k_{\text{H}^+} = 3.78 \times 10^{10} \exp(-2169/T) \text{ M}^{-2} \text{ h}^{-1}$	Granstrom (1954)
	$k_{\text{HCO}_3} = 1.5 \times 10^{35} \exp(-22144/T) \text{ M}^{-2} \text{ h}^{-1}$	Vikesland et al. (2001)
	$k_{\text{H}_2\text{CO}_3} = 2.95 \times 10^{10} \exp(-4026/T) \text{ M}^{-2} \text{ h}^{-1}$	Vikesland et al. (2001)
$\text{H}_2\text{CO}_3 \rightleftharpoons \text{HCO}_3^- + \text{H}^+$	$\text{pka} = 1.48 \times 10^{-4} (T) - 9.39 \times 10^{-2} (T) + 21.2$	Snoeyink and Jenkins (1980)
$\text{HCO}_3^- \rightleftharpoons \text{H}^+ + \text{CO}_3^{2-}$	$\text{pka} = 1.19 \times 10^{-4} (T) - 7.99 \times 10^{-2} (T) + 23.6$	Snoeyink and Jenkins (1980)
$\text{NH}_4^+ \rightleftharpoons \text{NH}_3 + \text{H}^+$	$\text{pka} = 1.03 \times 10^{-4} (T) - 9.21 \times 10^{-2} (T) + 27.6$	Bates and Pinching (1950)
$\text{HOCl} \rightleftharpoons \text{OCl}^- + \text{H}^+$	$\text{pka} = 1.18 \times 10^{-4} (T) - 7.86 \times 10^{-2} (T) + 20.5$	

CEE697K Lecture #17

David A. Reckhow

Chloramine Decay

14



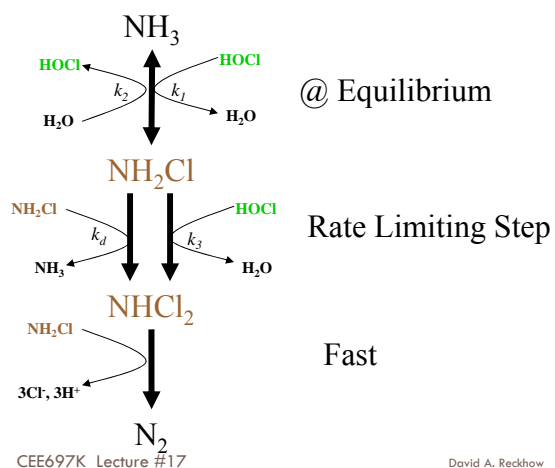
CEE697K Lecture #17

David A. Reckhow

Valentine Model #1

15

- Chloramine Formation and Decay pathway

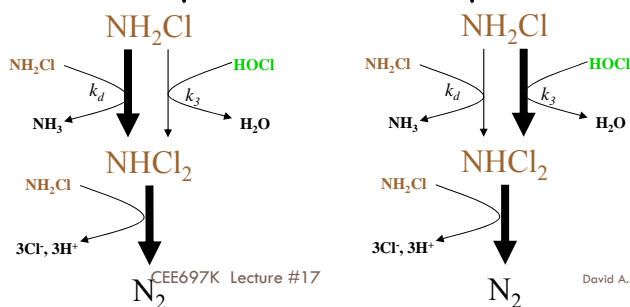


Valentine Model #2

16

- Looking at the Rate Limiting Step

$$-\frac{d[NH_2Cl]}{dt} = 3k_d[NH_2Cl][NH_2Cl] + 2k_3[NH_2Cl][HOCl]$$



Valentine Model #3

17

- Re-arranging:

$$-\frac{d[NH_2Cl]}{dt} = 3k_d[NH_2Cl][NH_2Cl] + 2k_3[NH_2Cl][HOCl]$$

$$-\frac{d[NH_2Cl]}{dt} = 3k_d[NH_2Cl]^2 + 2k_3[NH_2Cl][HOCl]$$

$$-\frac{d[NH_2Cl]}{dt} = \left(3k_d + 2k_3 \frac{[HOCl]}{[NH_2Cl]} \right) [NH_2Cl]^2$$

CEE697K Lecture #17

David A. Reckhow

Valentine Model #4

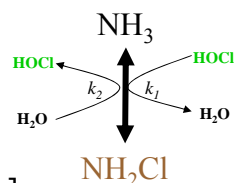
18

- Looking at the first step
 - Forward reaction rate equals reverse rate
 - equilibrium

$$k_1[HOCl][NH_3] = k_2[NH_2Cl]$$

- Which leads to

$$\frac{[HOCl]}{[NH_2Cl]} = \frac{\left(\frac{k_2}{k_1} \right)}{[NH_3]}$$



CEE697K Lecture #17

David A. Reckhow

Valentine Model #5

19

- Combining

$$-\frac{d[NH_2Cl]}{dt} = \left(3k_d + 2k_3 \frac{[HOCl]}{[NH_2Cl]} \right) [NH_2Cl]^2 \quad \frac{[HOCl]}{[NH_2Cl]} = \frac{\left(\frac{k_2}{k_1} \right)}{[NH_3]}$$

- We get:

$$-\frac{d[NH_2Cl]}{dt} = \left(3k_d + \frac{2k_3 \left(\frac{k_2}{k_1} \right)}{[NH_3]} \right) [NH_2Cl]^2$$

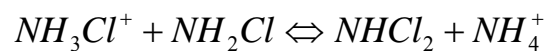
CEE697K Lecture #17

David A. Reckhow

pH effects

20

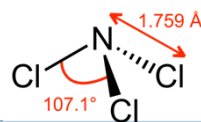
- Ammonia and chloramine species are prone to protonation
- Dichloramine is more prevalent at low pH
 - Why?
 - The protonated form of monochloramine reacts more quickly than the neutral form or the reverse reaction is slower



CEE697K Lecture #17

David A. Reckhow

Nitrogen Trichloride



21

□ Acute Human toxicity ??

□ Drinking Water, showers and swimming pools

□ Blatchley's group:

Weng, S.C., W.A. Weaver, M.Z. Afifi, T.N. Blatchley, J.S. Cramer, J. Chen, and E.R. Blatchley. 2011. Dynamics of gas-phase trichloramine (NCl₃) in chlorinated, indoor swimming pool facilities. *Indoor Air* 21:391-399.

- "Trichloramine (NCl₃), which is often associated with the 'chlorine odor' of swimming pools, has been identified as a common by-product of chlorination of many organic-N compounds that are common to swimming pools, including urea, creatinine, and amino acids.
- NCl₃ is a respiratory irritant to mice, and more recent studies have indicated NCl₃ to contribute to acute ocular and respiratory irritation symptoms in lifeguards and swimming pool workers.
- Retrospective studies have shown positive correlation between irritation symptoms among swimmers and patrons and high gas-phase NCl₃ concentration at indoor pool facilities."

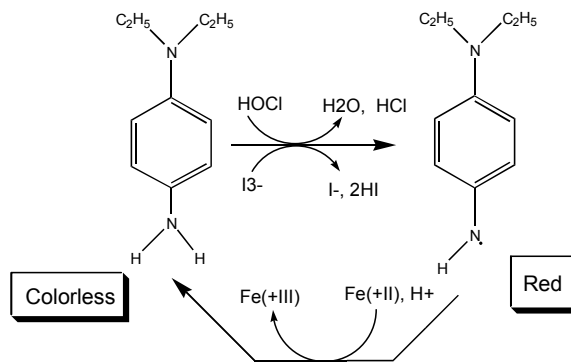
CEE697K Lecture #17

David A. Reckhow

Measuring chloramines

22

□ DPD titrimetric method



CEE697K Lecture #17

David A. Reckhow

Oxidation of DPD

23

- Reaction with free chlorine or iodine

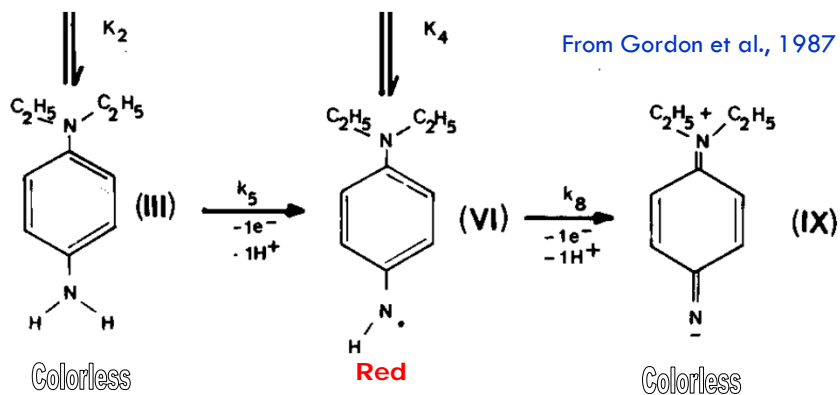


Figure 2.6 Oxidation-reduction/acid-base reaction of DPD

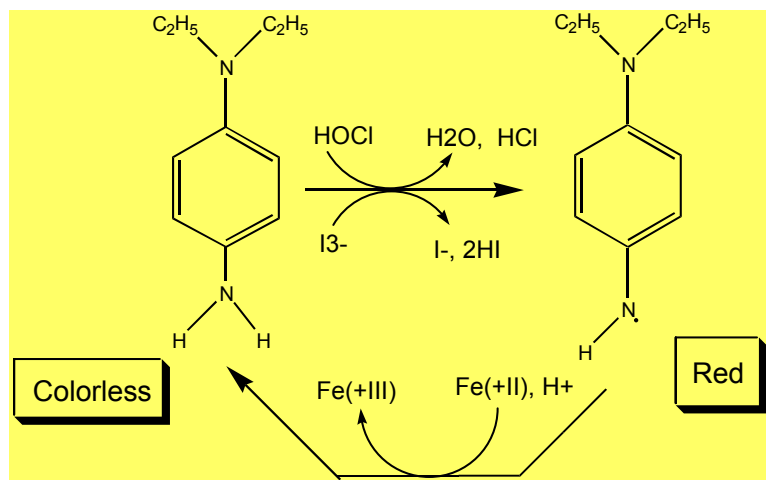
Speciation with DPD

24

- FRC
 - Direct reaction of HOCl/OCl⁻ with DPD
- Monochloramine
 - Oxidation of I⁻ to I₃⁻ by NH₂Cl, and subsequent oxidation of DPD
 - Require only a small amount of iodide
- Dichloramine
 - Oxidation of I⁻ to I₃⁻ by NHCl₂, and subsequent oxidation of DPD
 - Require a large amount of iodide and longer reaction time

DPD titrimetric method

25



CEE697K Lecture #17

David A.
Reckhow

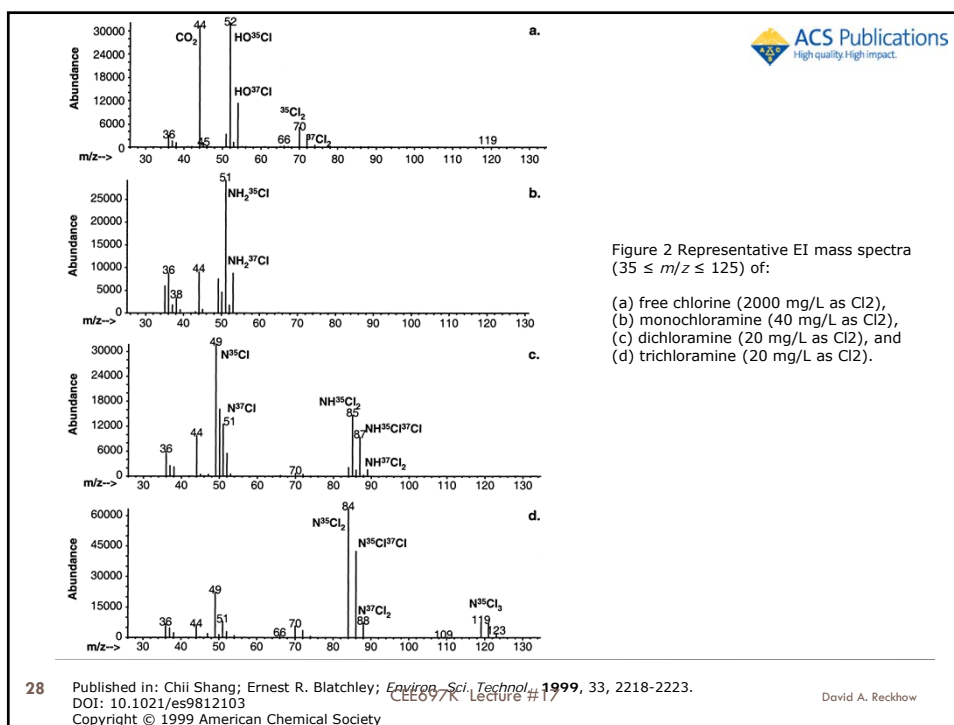
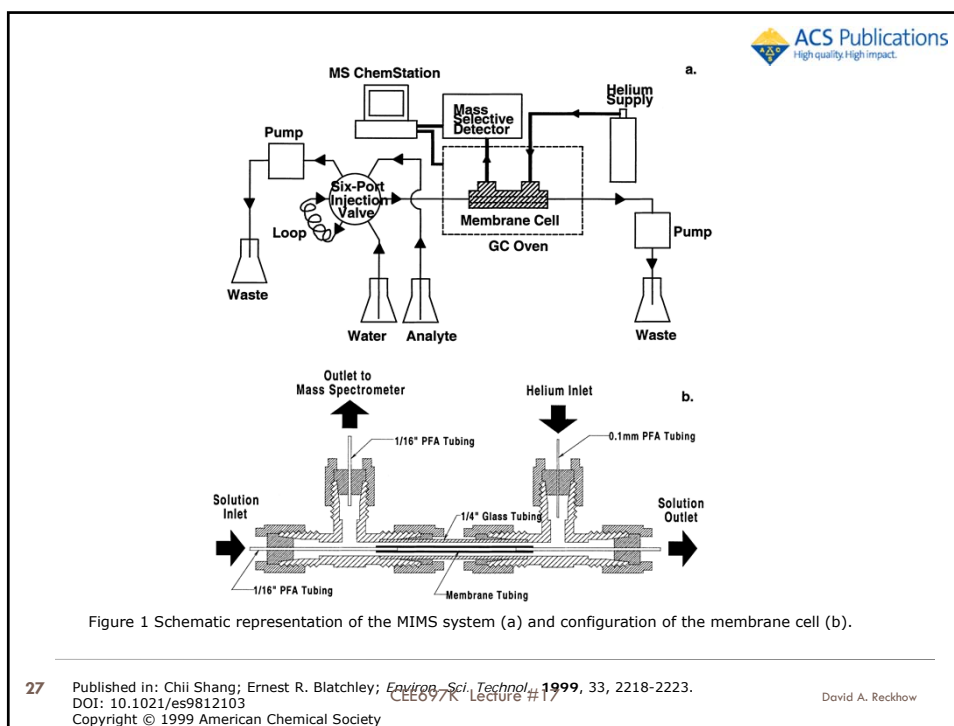
DPD titrimetric method

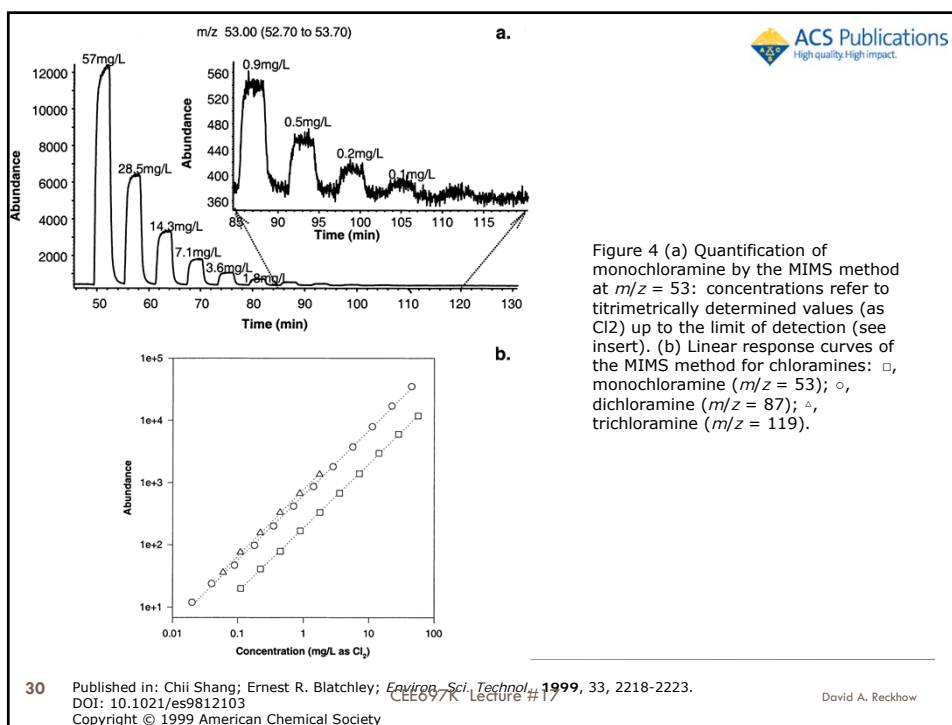
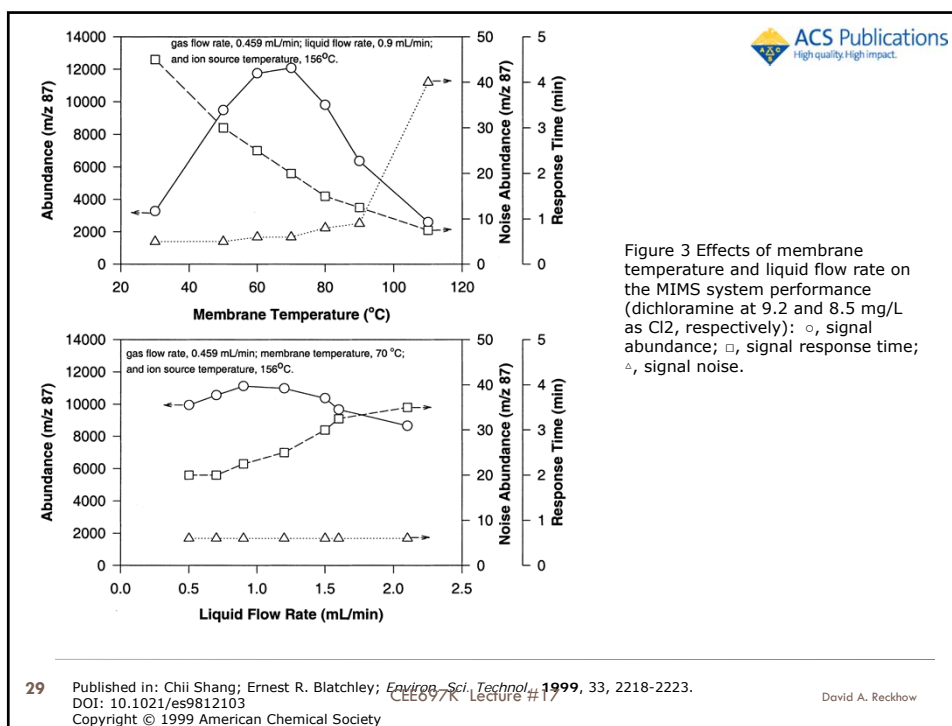
26

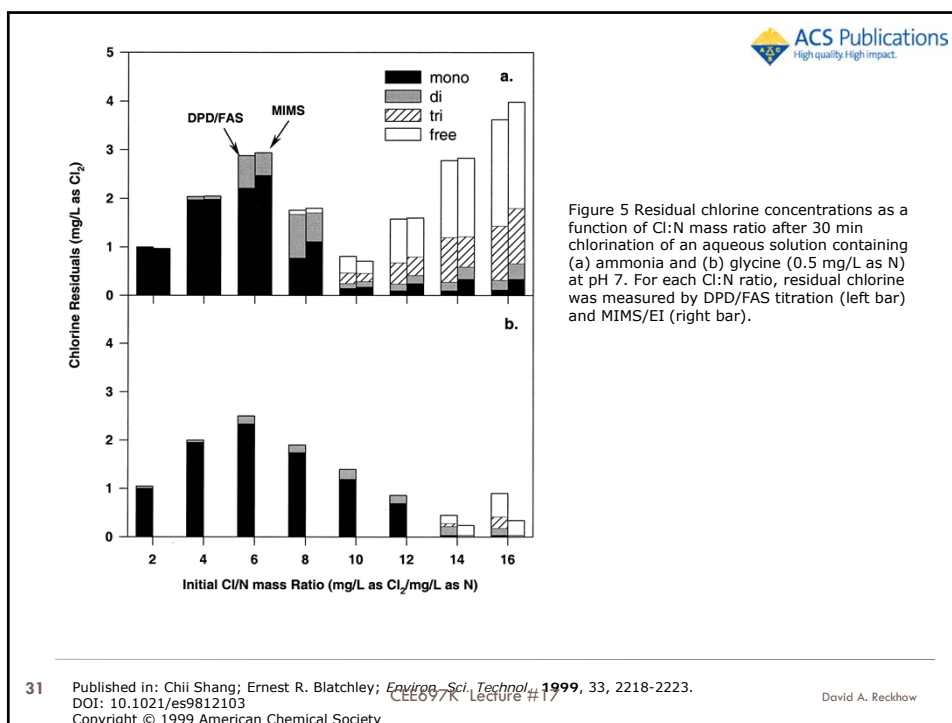
- pH control
 - Low pH leads to protonated forms
 - High pH catalyzes DPD oxidation by atmospheric oxygen
- Potential interference
 - Any substance that can directly oxidize DPD
 - MCA can do this a bit, so we sometimes add HgCl_2
 - Any substance that can oxidize iodide
 - Hydrogen peroxide, persulfate

CEE697K Lecture #17

David A.
Reckhow







32	Chlorine dose	species	DPD		MIMS		Lafayette wastewater (NH ₄ ⁺ -N, 12.2 mg/L; org-N, 13.1 mg/L)		Purdue p otable wa ter (NH ₄ ⁺ - N, 0.05 m g/L; org- N, 0.35 m g/L)
			mean	RSD ² (%)	mean	RSD ² (%)	DPD	MIMS	DPD
1.0	free	0		0		0	0	0.38	
	mono	0.12	4 (n=6)	0		0.08	0.07	0.09	
	di	0.05	12 (n=6)	0.03	2 (n=6)	0.04	0.02	0.02	
	tri	0		0		0	0	0	
5.0	free	0.16	14 (n=6)	0.17	5 (n=6)	0.16	0	4.28	
	mono	0.15	17 (n=6)	0		1.94	2.05	0.14	
	di	0.40	2 (n=6)	0.22	1 (n=6)	0.08	0.03	0	
	tri	0		0		0	0	0.04	
10.0	free	2.92	2 (n=3)	2.58	1 (n=3)	0.16	0	9.00	
	mono	0.15	15 (n=3)	0.13	5 (n=3)	4.64	5.17	0.20	
	di	0.77	8 (n=3)	0.37	0 (n=3)	0.40	0.24	0	
	tri	0		0.08	3 (n=3)	0	0	0.04	

CEE697K Lecture #17

David A. Reckhow

33

chlorine dose	species	DPD		MIMS		Lafayette waste-water (NH ₄ ⁺ -N, 12.2 mg/L; org-N, 13.1 mg/L)		Purdue potable water (NH ₄ ⁺ -N, 0.05 mg/L; org-N, 0.35 mg/L)	
		mean	RSD ^b (%)	mean	RSD ^b (%)	DPD	MIMS	DPD	MIMS
1.0	free	0		0		0	0	0.38	0.13
	mono	0.12	4 (n=6)	0		0.08	0.07	0.09	0
	di	0.05	12 (n=6)	0.03	2 (n=6)	0.04	0.02	0.02	0
	tri	0		0		0	0	0	0
5.0	free	0.16	14 (n=6)	0.17	5 (n=6)	0.16	0	4.28	3.22
	mono	0.15	17 (n=6)	0		1.94	2.05	0.14	0.26
	di	0.40	2 (n=6)	0.22	1 (n=6)	0.08	0.03	0	0.02
	tri	0		0		0	0	0.04	0
10.0	free	2.92	2 (n=3)	2.58	1 (n=3)	0.16	0	9.00	7.33
	mono	0.15	15 (n=3)	0.13	5 (n=3)	4.64	5.17	0.20	0.56
	di	0.77	8 (n=3)	0.37	0 (n=3)	0.40	0.24	0	0.05

CEE697K Lecture # 17 David A. Reckhow

DPD based method for NCl₃

34

□ Schematic of impinger method for gas-phase NCl₃ measurement. The arrows indicate the air flow pattern

□ Validation experiment setup. A gas-washing bottle containing an aqueous solution of the target compound was prepared and connected to the air entrance of measuring impinger system

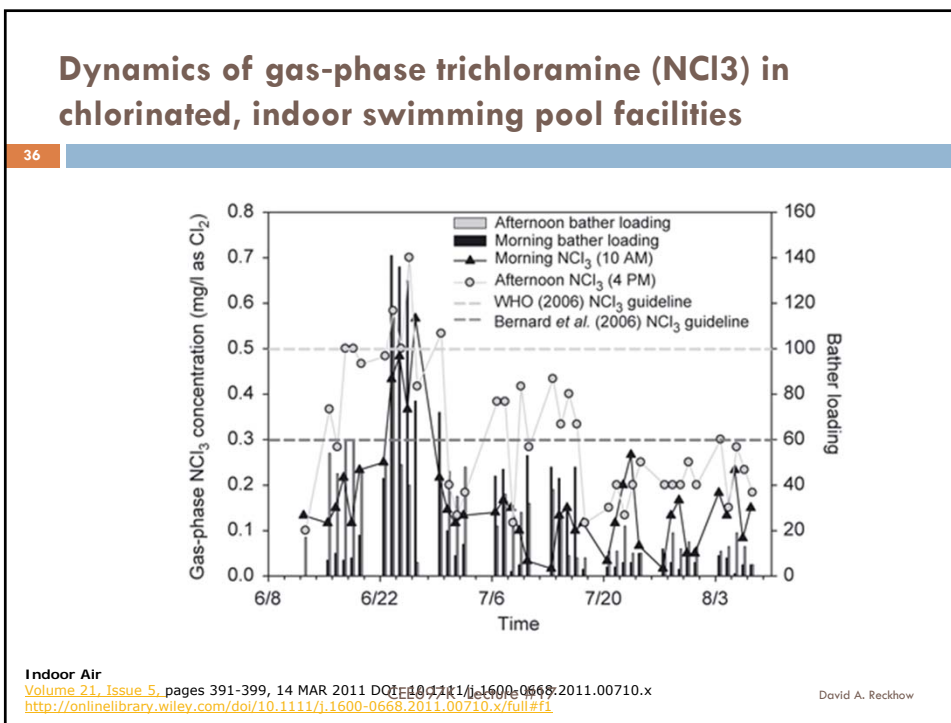
Weng, S.C., W.A. Weaver, M.Z. Affi, T.N. Blatchley, J.S. Cramer, J. Chen, and E.R. Blatchley. 2011. Dynamics of gas-phase trichloramine (NCl₃) in chlorinated, indoor swimming pool facilities. *Indoor Air* 21:391-399.

CEE697K Lecture # 17 David A. Reckhow

35

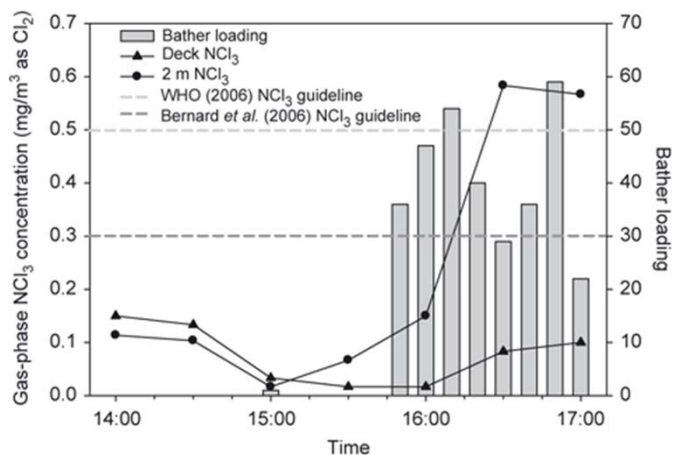
Compound	Typical liquid-phase concentration (mg/l) ^a	Henry's law constant (atm, 20°C) ^b	Equilibrium gas-phase Concentration (mg/m ³)	Reported gas-phase concentration at pool area (mg/m ³)
HOCl ^c	1.2	0.060	0.053	N.A
Cl ₂ ^c	0.000012	767	0.0067	N.A
NH ₂ Cl	0.30	0.45	0.10	N.A
NHCl ₂	0.10	1.52	0.11	N.A
NCl ₃	0.070	435	23	0.1–0.7 ^d
CHCl ₃	0.080	185	11	0.009–0.058 ^e
CHBr ₂ Cl	0.0040	57.3	0.17	0.002–0.003 ^e
CHBr ₃	0.0010	21.5	0.016	0.0008 ^e
CNCl	0.0030	108	0.24	N.A
CNCHCl ₂	0.00080	0.21	0.00013	N.A
CH ₃ NCl ₂	0.020	154	2.3	0.016–0.07 ^f

CEE697K Lecture #17 David A. Reckhow



Dynamics of gas-phase trichloramine (NCl₃) in chlorinated, indoor swimming pool facilities

37

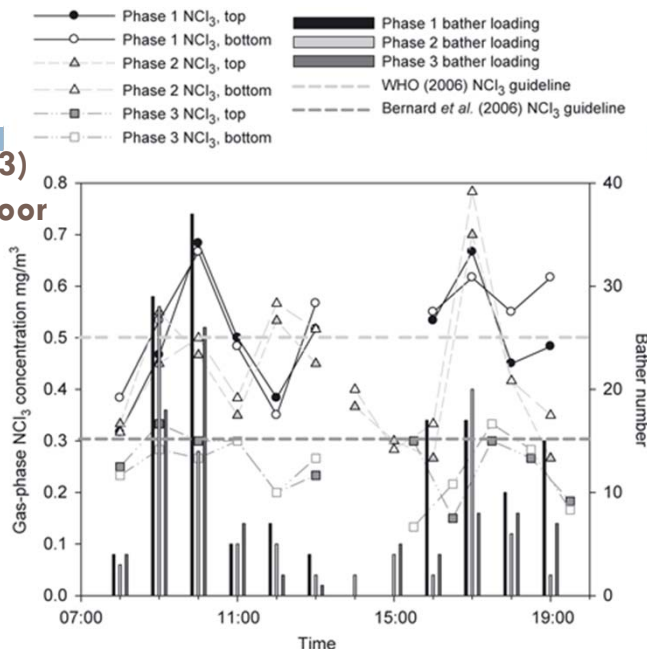


Indoor Air
 Volume 21, Issue 5, pages 391-399, 14 MAR 2011 DOI:10.1111/j.1600-0668.2011.00710.x
<http://onlinelibrary.wiley.com/doi/10.1111/j.1600-0668.2011.00710.x/full#f2>

David A. Reckhow

Dynamics of gas-phase trichloramine (NCl₃) in chlorinated, indoor swimming pool facilities

38



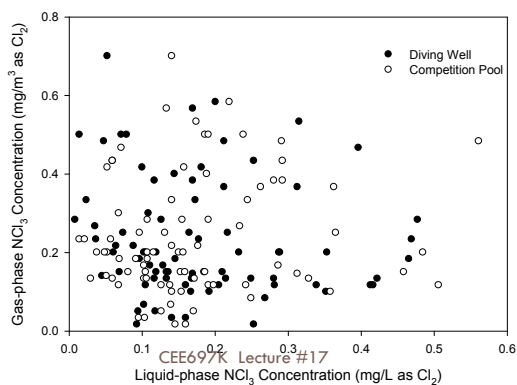
Indoor Air
 Volume 21, Issue 5, pages 391-399, 14 MAR 2011 DOI:10.1111/j.1600-0668.2011.00710.x
<http://onlinelibrary.wiley.com/doi/10.1111/j.1600-0668.2011.00710.x/full#f4>

David A. Reckhow

Liquid vs gas concentration

39

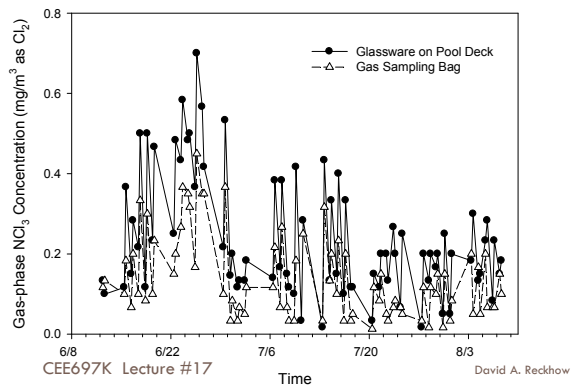
- Relationship between DPD-based liquid-phase NCl_3 concentration and gas-phase NCl_3 concentration in Pool A facility. The results showed no significant correlation between these two parameters for this facility. The correlation coefficients between liquid-phase and gas-phase NCl_3 concentrations were -0.140 and 0.154 for the diving well and competition pool, respectively.



Loss in Tedlar bag

40

- Comparison of gas-phase NCl_3 measurement at pool deck and in the laboratory with a Tedlar gas-sampling bag. The results showed apparent loss of NCl_3 from the gas-sampling bag during transport.



41

□ To next lecture