

Reaction Mechanisms for the Degradation of NDMA Through Advanced Oxidation Processes

Erica Coscarelli and Dr. Daisuke Minakata

Department of Civil and Environmental Engineering



Background

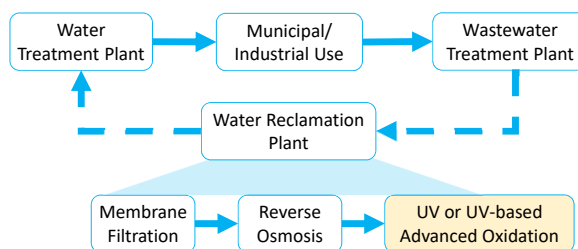


Figure 1. Direct Potable Reuse

N-nitrosodimethylamine (NDMA)

- Neutral low MW compound present in RO permeate
- Byproduct of free chlorine/chloramine disinfection
- Potential human carcinogen, EPA cancer risk level is 0.7 ng/L

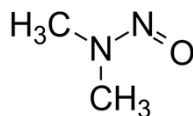


Figure 2. NDMA

Goal

Understand and predict the fate of NDMA degradation in the aqueous-phase UV treatment for direct potable reuse

Objectives

- Identify the elementary degradation pathways of NDMA induced by UV photolysis;
- Generate the ordinary differential equations based on the elementary reactions and the kinetic and solve the ODEs ; and
- Predict the concentration profiles of NDMA and the degradation products and compare with experiments.

Results

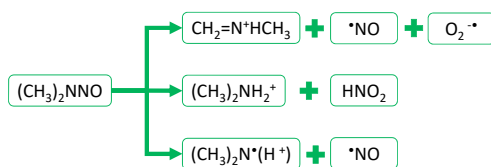


Figure 3. Initial elementary reactions for NDMA induced by UV

Table 1.
Experimental and model parameters

	pH = 3	pH = 7
Initial NDMA conc.	0.0001 M	0.01 M
Reaction time	15 min	300 min
Lamp	13 W low pressure mercury vapor lamp at 253.7 nm	
Optical pathlength	2 cm	
UV intensity	1.87×10^{-6} einstein/L/s	

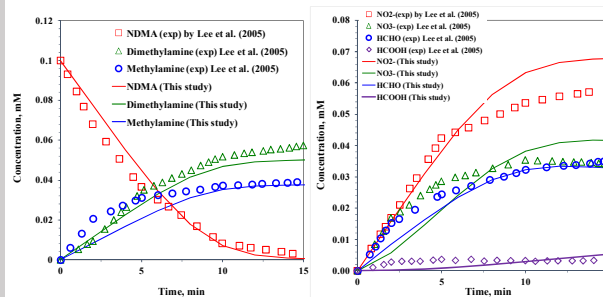


Figure 4. Time-dependent concentration profiles for NDMA and transformation products at pH 3

Results

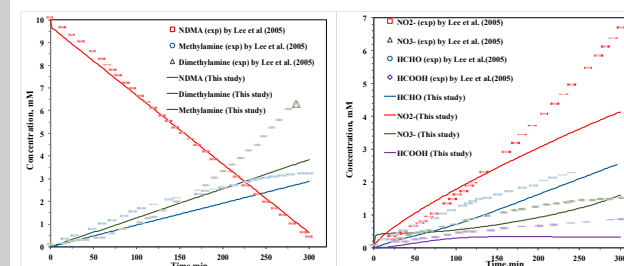


Figure 5. Time-dependent concentration profiles for NDMA and transformation products at pH 7

Future Research/ Model Improvements

- Identify the elementary reaction pathways and kinetics that have not been considered at pH 7 based on computational studies and literature reviews.
- Include full photolysis pathways and kinetics for nitrate and nitrite

Literature Cited

- C. Lee, W. Choi and J. Yoon. 2005. *ES & Tech*, vol. 39, no. 24, pp. 9702-9709.
- C. Lee, W. Choi, Y. Kim and J. Yoon. 2005. *ES & Tech*, vol. 39, no. 7, pp. 2101-2106.
- M. Stefan and J. Bolton. 2002. *Helvetica Chimica Acta*, vol. 85, no. 5, p. 1436.
- W. Mitch, A. Gerecke and D. Sedlak. 2003. *Water Research*, vol. 37, no. 15, pp. 3733-3741.

Acknowledgments

National Science Foundation Award: CBET-1435926.