Modeling Nicotine Induced Chlorine Loss with EPANET-MSX

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EWRI 2023

Henderson, NV

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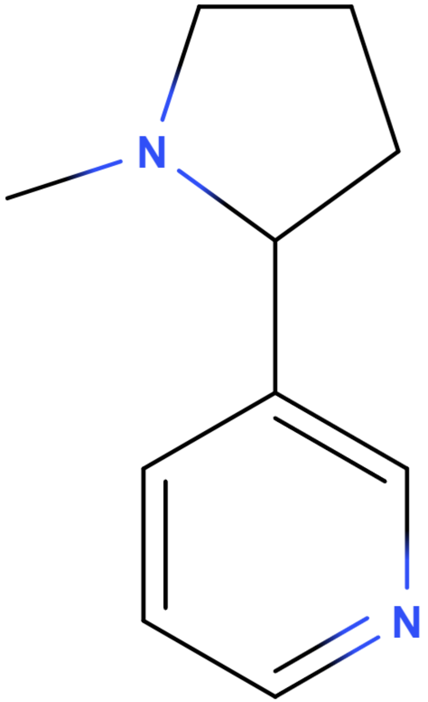
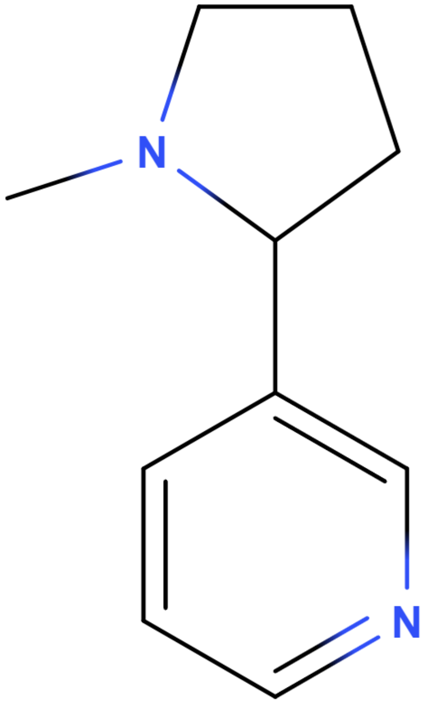
Nicotine Basics

- Commercially available
- Nicotine acts as a human stimulant and is used as an insecticide
- Expected to have slower reaction kinetics with chlorine than other tested chemicals



Study Basics

- Two Phases
  - Batch kinetics
  - Pipe injection study
- Modeling
  - Fit batch kinetic study
  - Apply parameters to pipe injection with EPANET-MSX



USEPA, 2016. Degradation of Nicotine in Chlorinated Water: Pathways and Kinetics. Technical Report. U.S. Environmental Protection Agency, Washington, DC, EPA/600/R-16/073, 2016.

Reaction Models

- Model 1: No Reactive Intermediate

$$\frac{dCl}{dt} = -(k_d[Cl] + k_1[Nic][Cl])$$

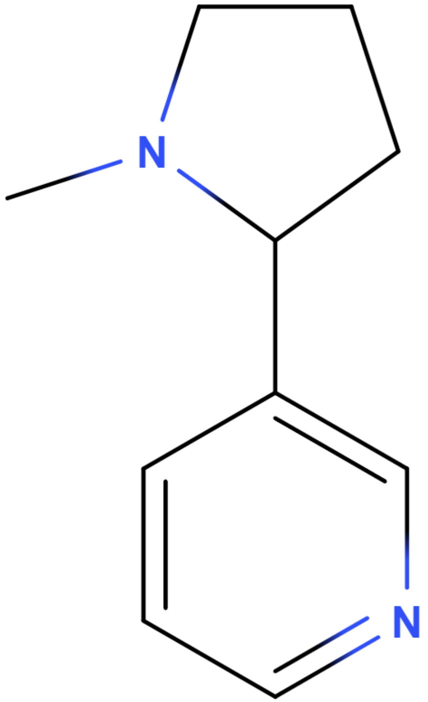
$$\frac{dNic}{dt} = -k_2[Nic][Cl]$$

- Model 2: With Reactive Intermediate

$$\frac{dCl}{dt} = -(k_d[Cl] + k_1[Nic][Cl] + k_3[N2][Cl])$$

$$\frac{dNic}{dt} = -k_2[Nic][Cl]$$

$$\frac{dN2}{dt} = k_2[Nic][Cl] - k_4[N2][Cl]$$

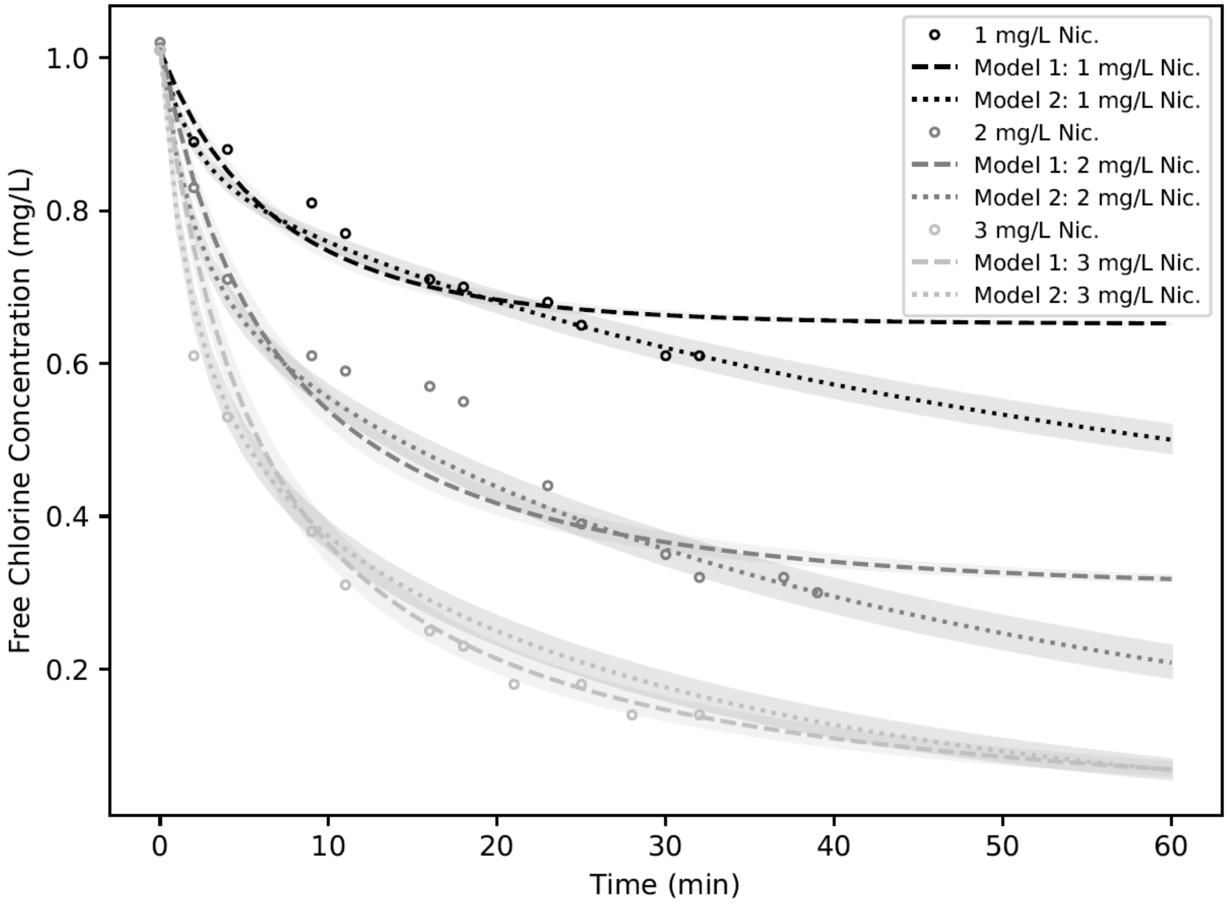


USEPA, 2016. Degradation of Nicotine in Chlorinated Water: Pathways and Kinetics. Technical Report. U.S. Environmental Protection Agency, Washington, DC, EPA/600/R-16/073, 2016.

Batch Experiments

- Model 1: Sharper initial loss, plateaus
- Model 2: Slower initial loss, more decay at later times

Coefficient	Model 1	Model 2	Units
k_d	3×10^{-5}	3×10^{-5}	min^{-1}
k_1	0.0560	0.0975	L/(mgNic · min)
k_2	0.157	0.573	L/(mgCl · min)
k_3	-	0.0134	L/(mgN2 · min)
k_4	-	0.0219	L/(mgCl · min)

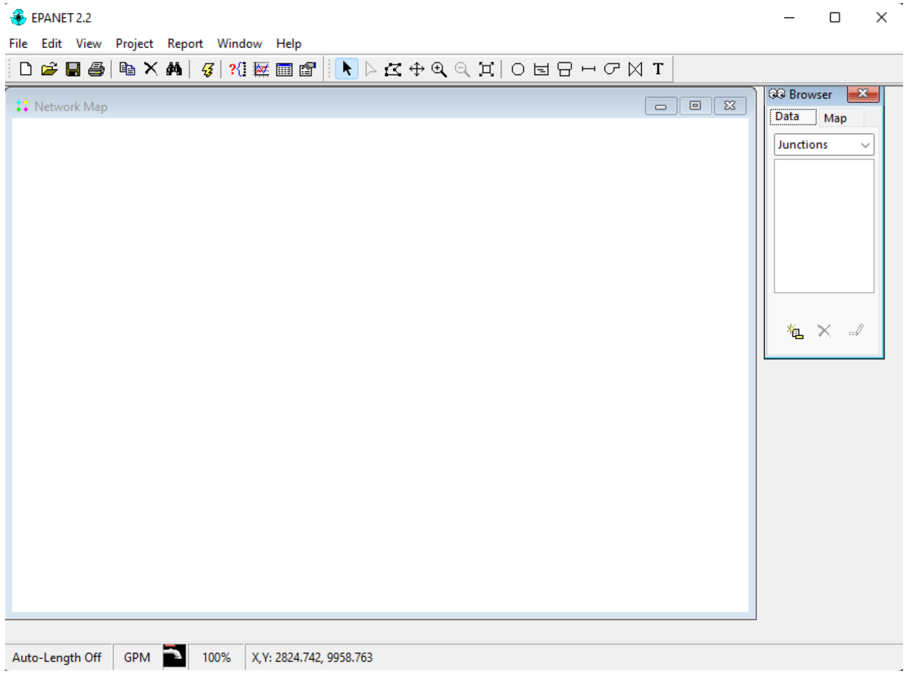


Shaded Region: ±10%

Updated EPANET-MSX

- Updates to EPANET 2.2's engine made it incompatible with EPANET-MSX 1.1

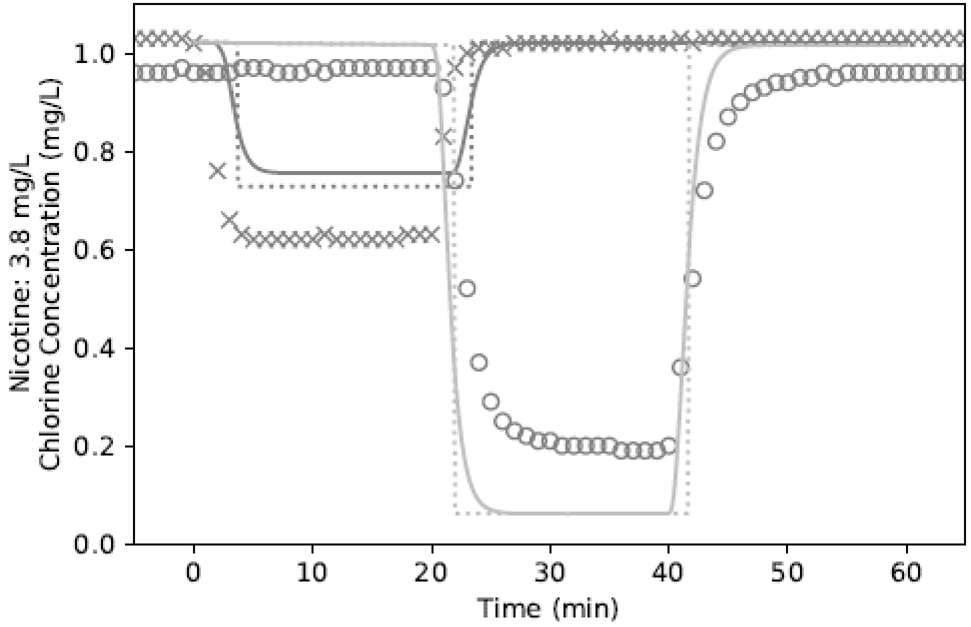
- New Version of EPANET-MSX was developed
  - Compatible with EPANET 2.2
  - Added dispersion
  - Added parallelization



https://github.com/USEPA/EPANET2.2

MSX_tools

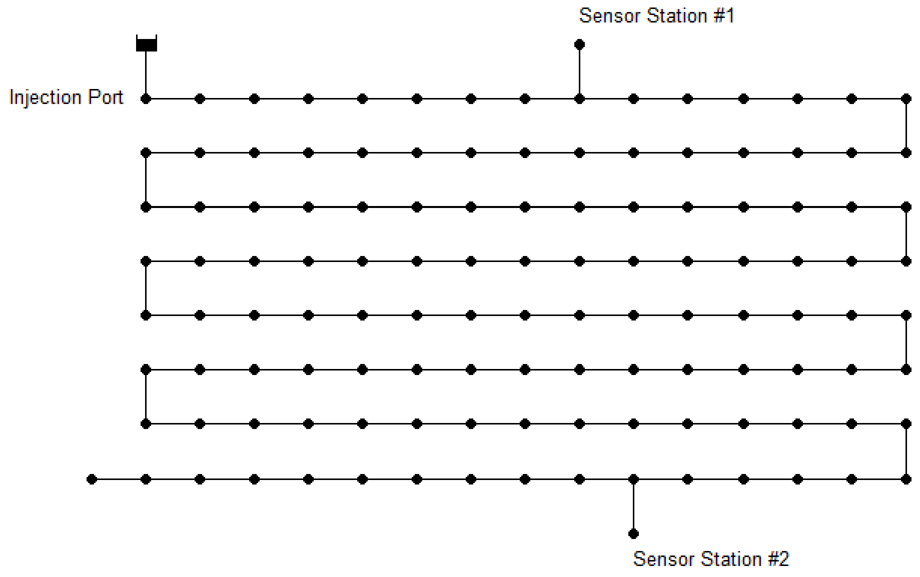
- Open-source Python-based EPANET-MSX handler
- Uses WNTR for EPANET file handling
- Adds reaction library features
- Automates MSX file generation and simulations
- Compatible with EPANET-MSX 1.1 and 2.0
- Access to all Python scripts for analysis, graphing, and data handling



https://github.com/USEPA/msx_tools

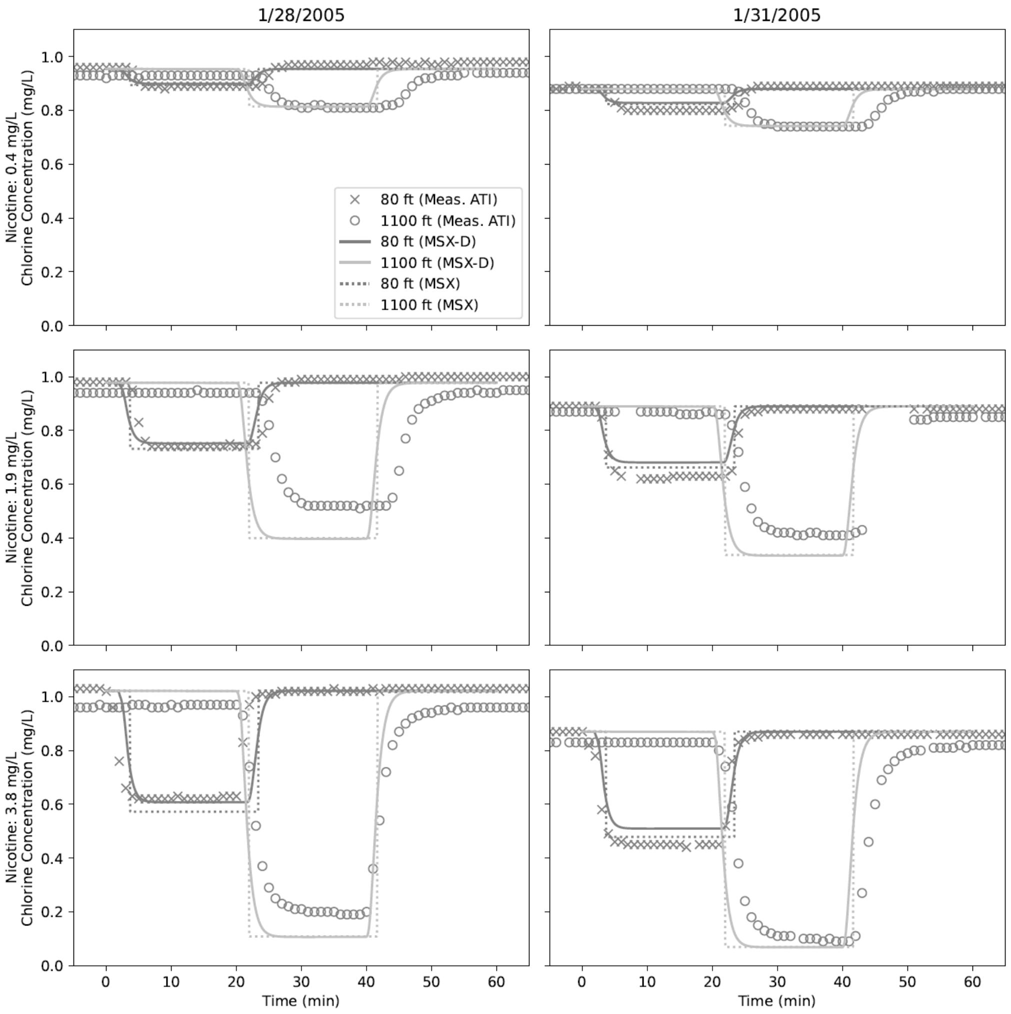
Injection Study

- 1,200 ft fiberglass lined 3” pipes
- 1,100 ft between sensor stations
- Locally supplied chlorinated tap water
  - ~1 mg/L chlorine
- 0.4, 1.9, 3.8 mgNic/L target final concentrations
- 20-minute injections
- ~1 ft/s or 22 gpm target flow

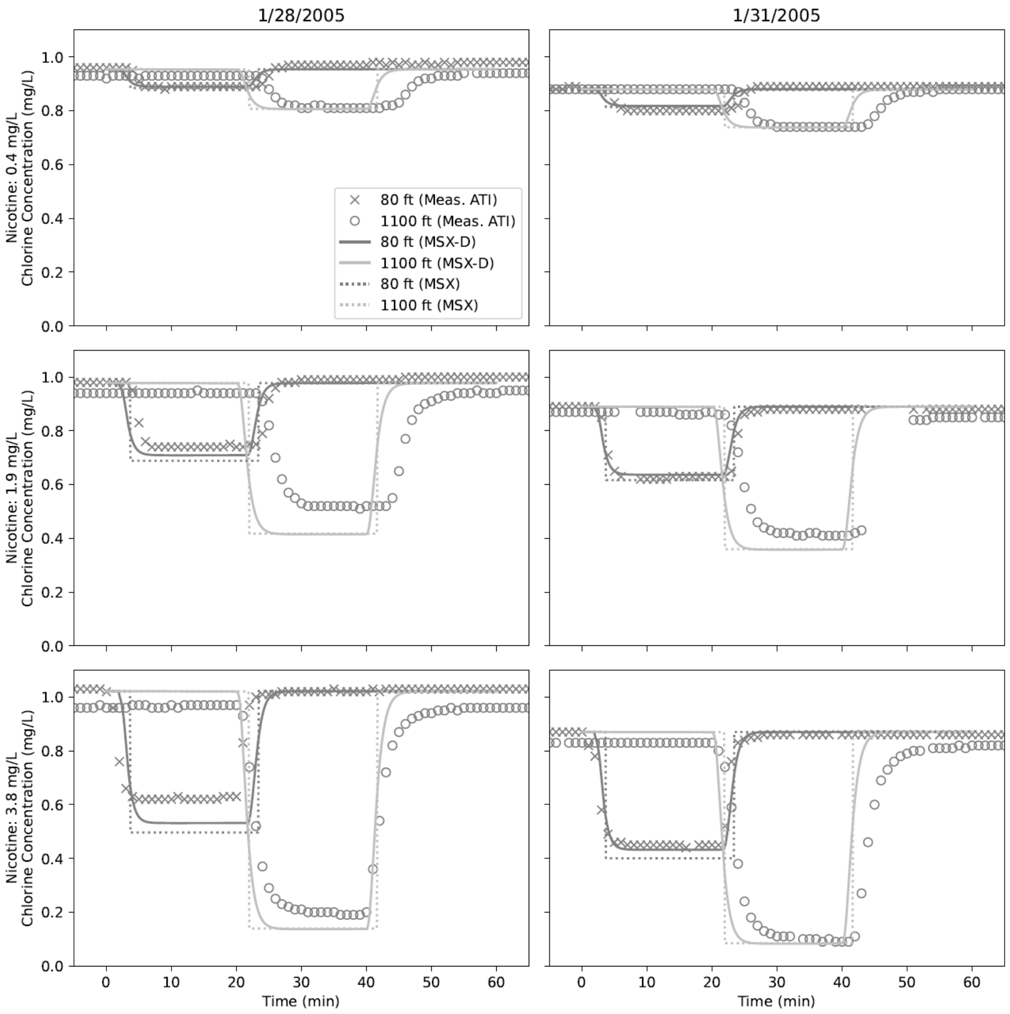


Injection Study: Results

Model 1

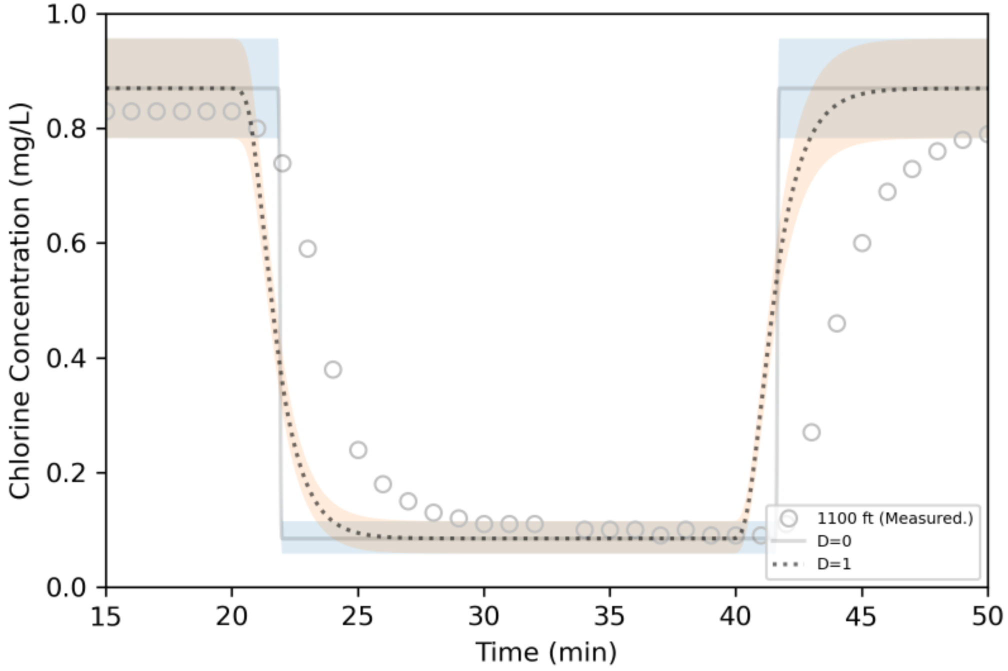


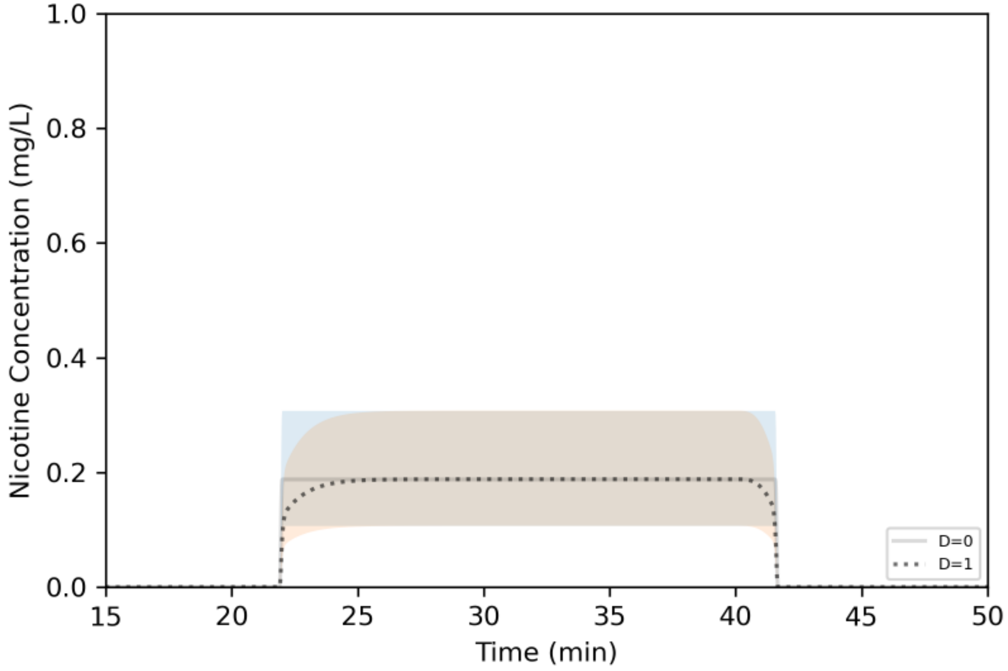
Model 2



Injection Study: Uncertainty in Initial Cl Conc.

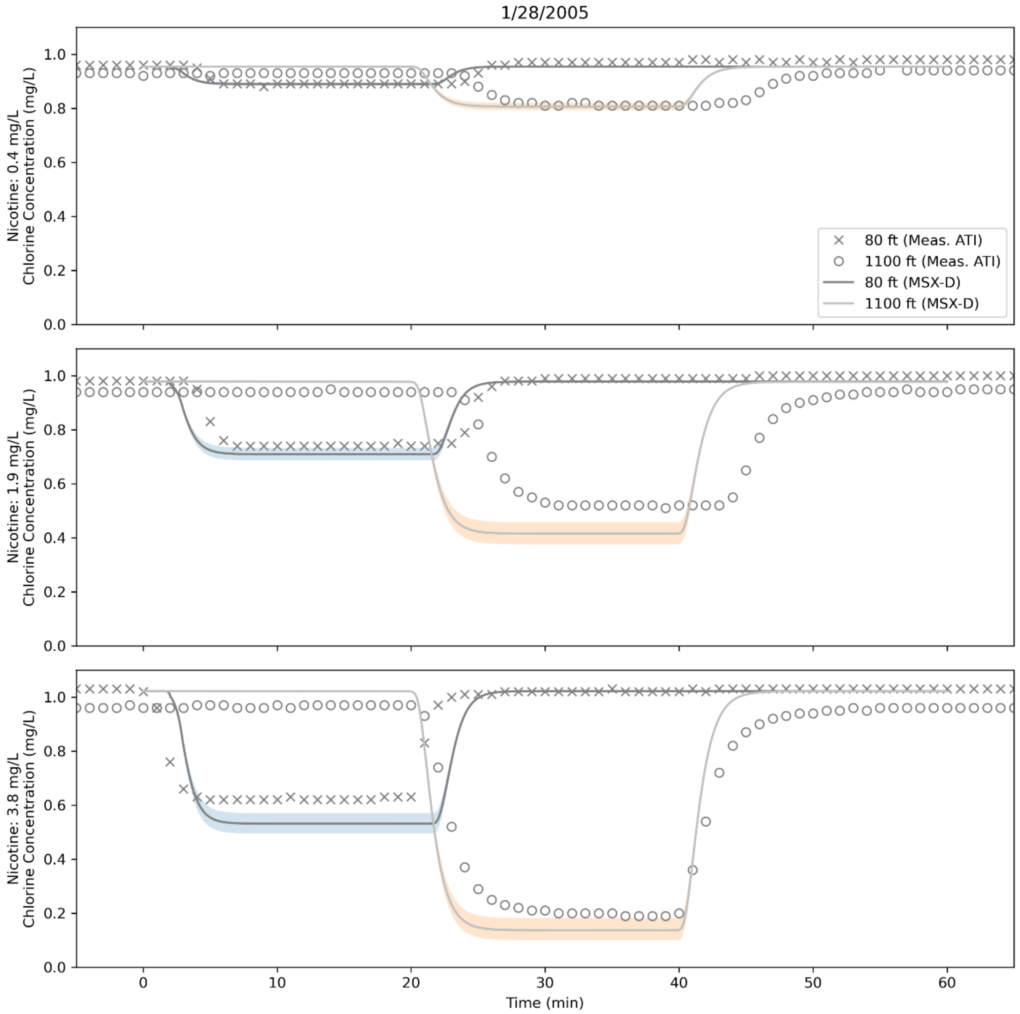
Model 2 Only (±10% in chlorine concentration) @ 1,100 ft sensor





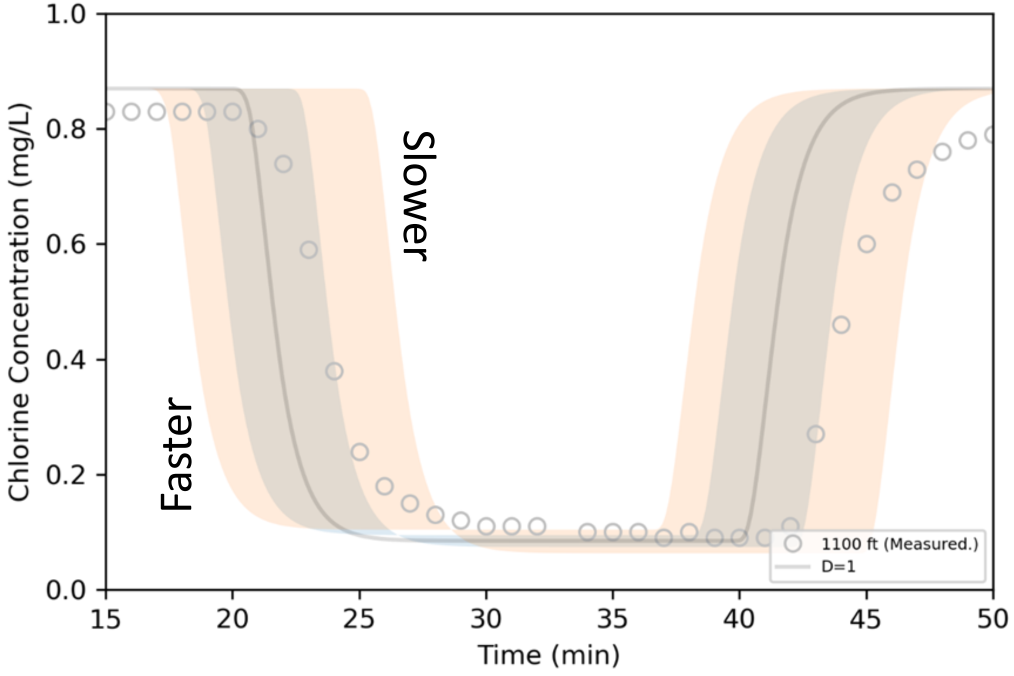
Injection Study: Uncertainty in Nicotine Conc.

Model 2 Only (±10% Nicotine Conc.) @ 1,100 ft sensor



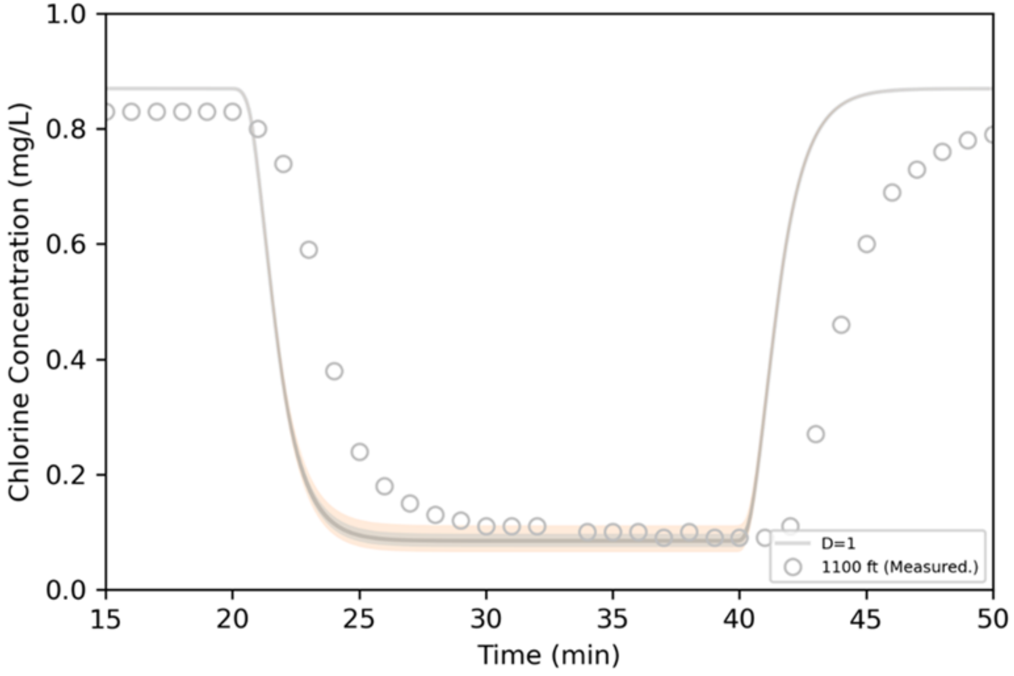
Injection Study: Uncertainty in System Flow

Model 2 Only (±10% and ±20% in flow rate) @ 1,100 ft sensor



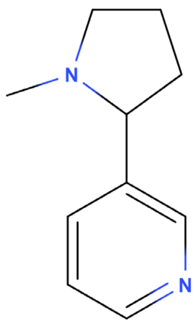
Injection Study: Uncertainty in Kinetic Parameters

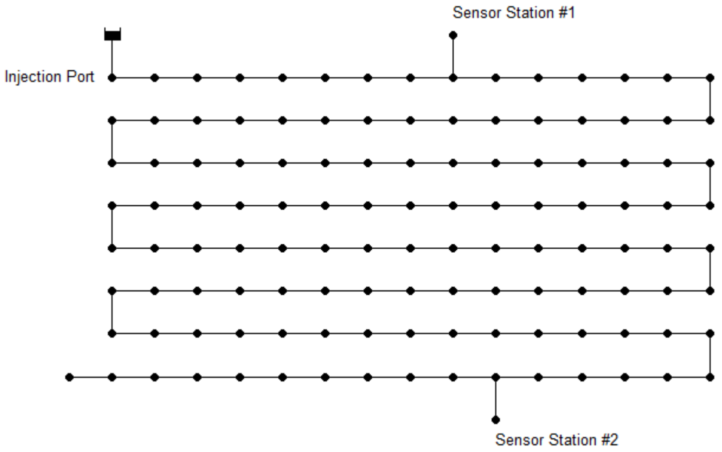
Model 2 Only (±10% and ±20% in kinetic parameters) @ 1,100 ft sensor

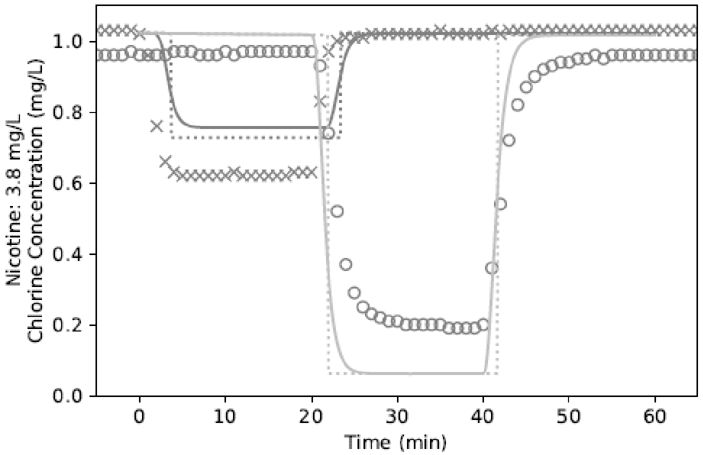


Conclusions

- Model 2 produced better agreement with both batch and injection experiments
- Dispersion model had smoother transitions than without dispersion (closer to experimental observations)
- MSX_tools allowed for automated testing and easy inclusion of uncertainty







Questions

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Models Used

https://github.com/USEPA/msx_tools
https://github.com/USEPA/WNTR
https://github.com/USEPA/EPANETMSX
https://github.com/USEPA/EPANET2.2