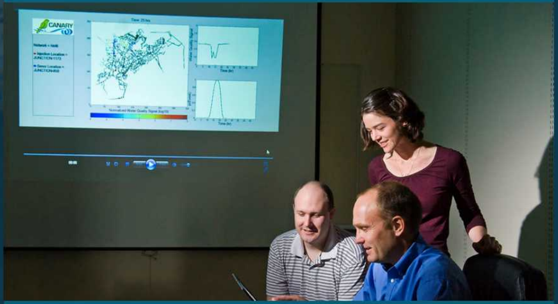
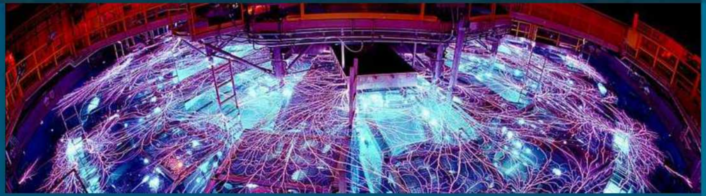
SAND2020-2126C

Water Quality Modeling: Transport and Uncertainty





Presented by David Hart, February 24, 2020 at the

Intelligent Water Technology Solutions for Disinfection and Public Health Protection and Water Security [Knowledge Development Forum]

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Why do modeling?

"The most that can be expected from any model is that it can supply a useful approximation to reality: all models are models are wrong; ***some models are useful****."* – George George Box, 2005

Water network models **are** useful for water flow and water quality approximations – as long as we recognize the limitations and account for them.

Modeling a Water Distribution System (WDS)

Two core types of models

1. **Conceptual or structural models**
   - Represent physical objects, places, connections, etc.
   - Describe behavior; e.g., usage of water
2. **Numerical models**
   - Equations for physical processes; e.g., reactions
   - Statistical models of behaviors or processes

Modeling a Water Distribution System (WDS)

WDS conceptual & structural models

- **Network model**
  - Pipes, tanks, valves, etc., and how they connect
- **Operations model**
  - Demand (usage) and rules/controls for equipment
- **Water quality**
  - What is the chemical and where did it start

Combined, often called ”the system model”

Modeling a Water Distribution System (WDS)

The numerical models

- **Hydraulic model**
  - Flow rates, pressures, statuses
- **Reaction model**
  - Chemical reactions and/or biological growth
- **Transport model**
  - Where does the mass go in the system?

Modeling a Water Distribution System (WDS)

Solvers

- **Free/open source**
  - EPANET – the standard workhorse

- **Commercial solvers**
  - Numerous companies offer very good products with their own special tools or features

Network Model

The EPANET sample network "Net3"

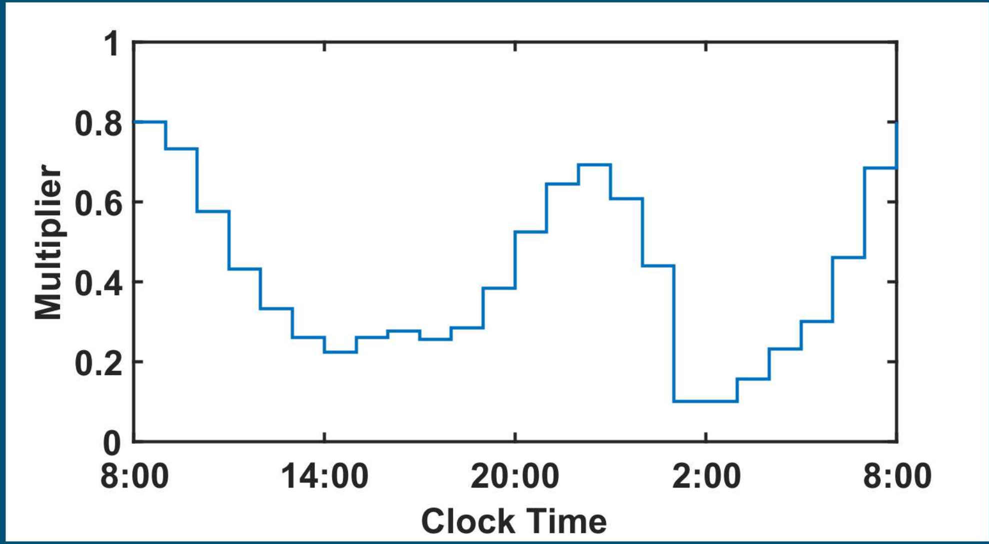
D.1 $H_i - H_j = h_{ij} = rQ_{ij}^n + mQ_{ij}^2$

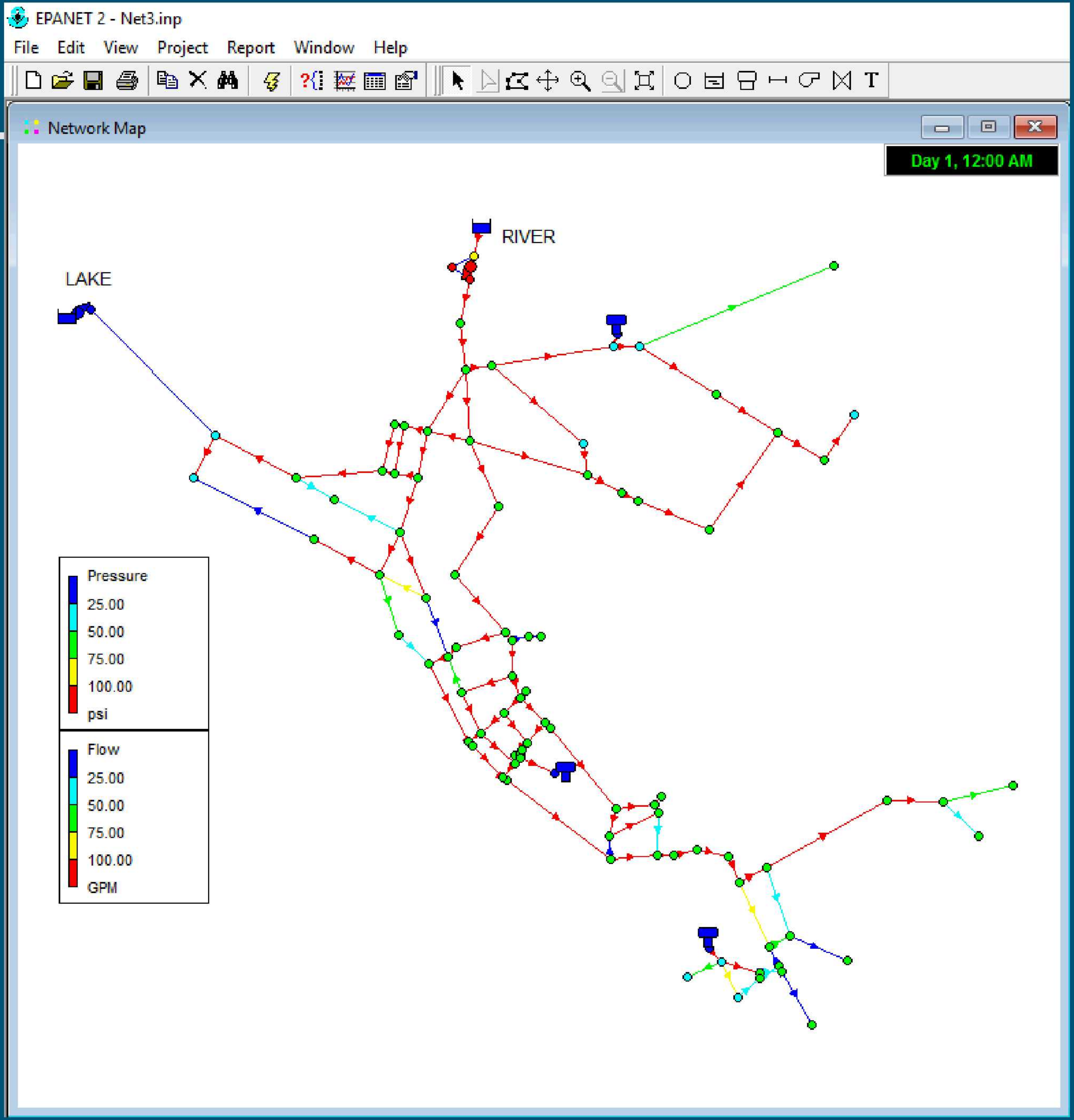
D.2 $\sum_j Q_{ij} - D_i = 0\,,\quad \text{for } i = 1,2,\ldots,N$

D.3 $\mathbf{AH} = \mathbf{F}$

D.4 $Q_{ij} = Q_{ij} - \left(y_{ij} - p_{ij}\left(H_i - H_j\right)\right)$

Rossman, L. (2000), *EPANET 2 Users Manual*, EPA/600/R-00/057.





EPANET 2.0, Lewis Rossman, 2000. Network 3 example network from software

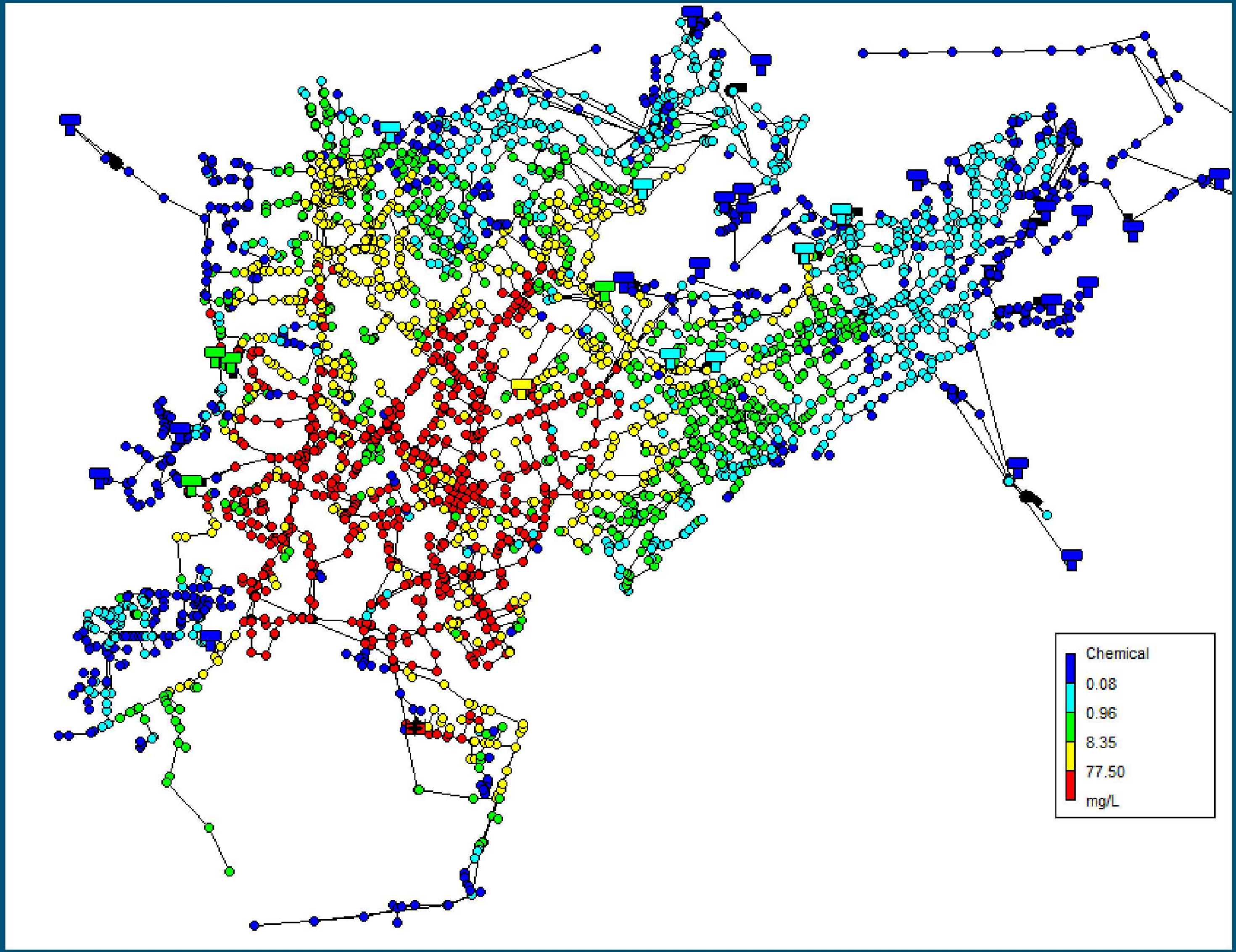
Network Model

Network "Net6"

Water Quality

D.5 $\frac{\partial C_i}{\partial t} = -u_i \frac{\partial C_i}{\partial x} + r(C_i)$

Rossman, L. (2000), *EPANET 2 Users Manual*, EPA/600/R-00/057.



Sources of uncertainty (hydraulics)

What are the approximations and limitations?

1. Are the pipes, valves, pumps, nodes located correctly?
2. Are the parameters (diameter, roughness, power) of the elements correct?
3. **Water Usage (Demands)!**

Sources of uncertainty (water quality)

What are the approximations and limitations?

4. Where is the source of contamination?
5. What is it?
6. When did it start?
7. **Where did it go?**

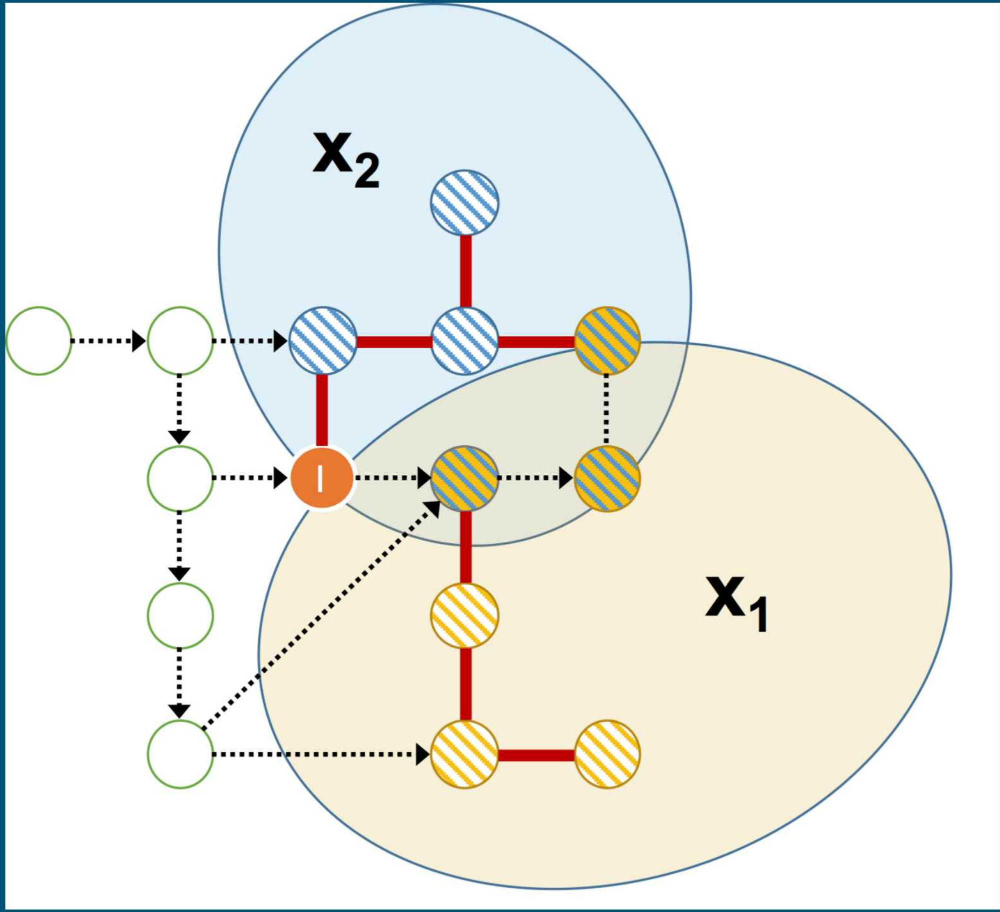
Uncertainty analyses

Two scenarios:

- Where did contaminant go?

Overlapping areas are definitely contaminated

Other two areas may, or may not, be affected



Sources of uncertainty studied

Possible hydraulic parameters

- **Demand at nodes**
- Pipe roughness
- **Network topology (valve closures)**
- Pump curves
- Initial conditions (tanks, valves)
- Solver discretization

Possible water quality parameters

- **Bulk reaction rate**
- Wall reaction rate
- Chemical interactions
- **Source location**
- Source mass
- **Injection start time**
- **Injection duration**

Experimental design

Design of experiments (DOE)

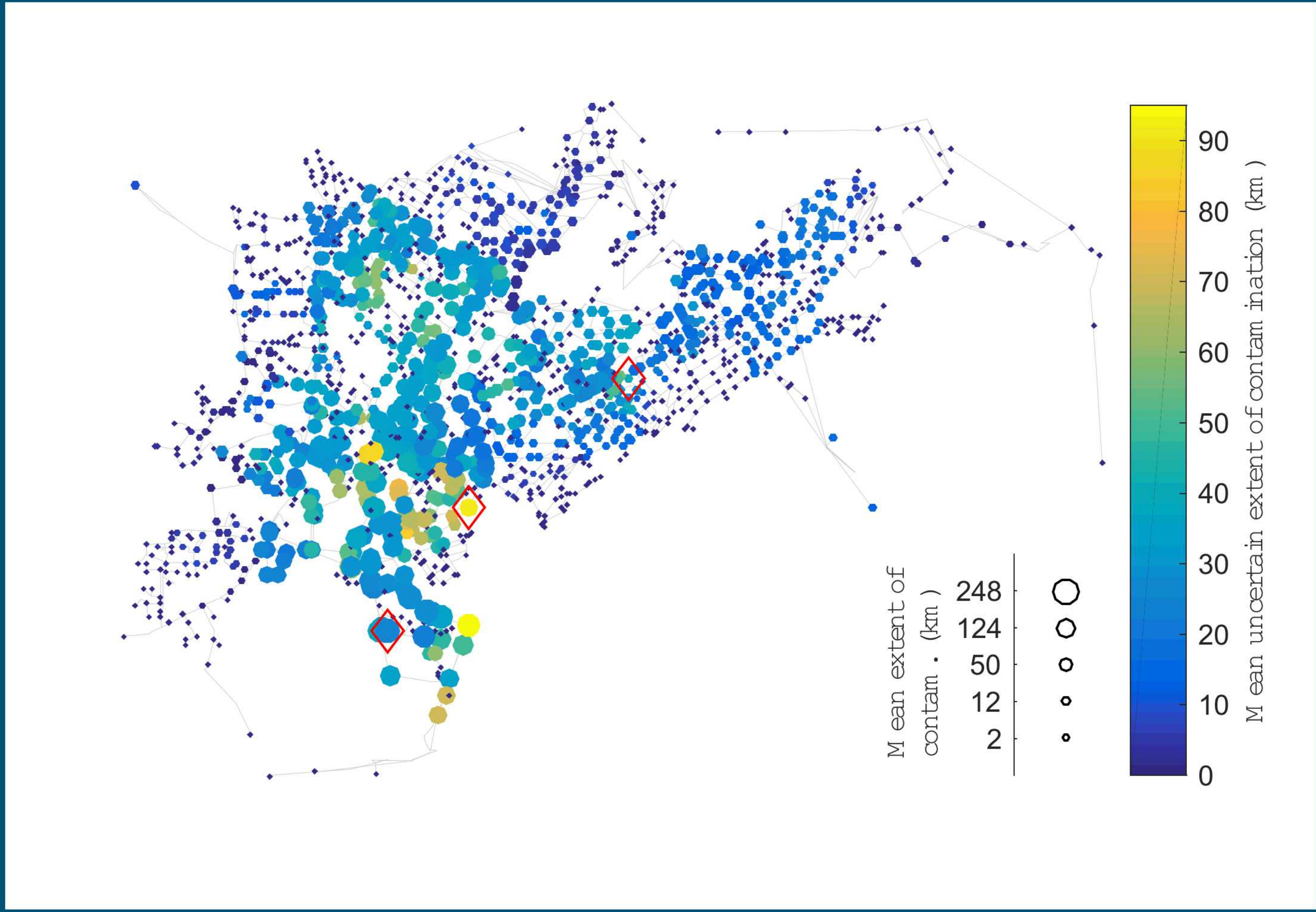
Three levels per parameter, any junction with a demand

50 stochastic realizations per factorial parameter combo.

Just under 18 million water quality simulations for a full-factorial experiment.

Parameter	Values
σ_d	0, 0.2, 0.4
β_f	0, 0.0025, 0.005
K_b	0, -0.1, -5.0
a_{inj}	see *map*
$t_{0,inj}$	24, 32, 40 hrs
Δt_{inj}	1, 12, 24 hours
r_c	0.1 to 10^{-4} mg/L

Average uncertainty

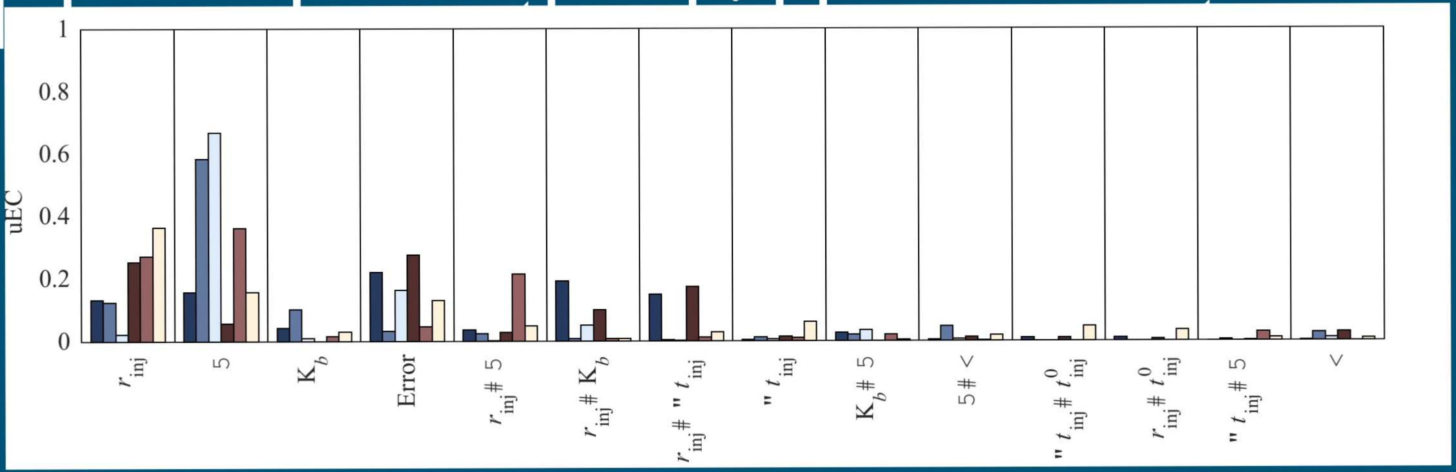


Most important parameters

The most important factor is the source location

The next most important factors were:

- Network topology errors (unknown valve statuses, for ex.)
- Rate of contamination or initial contamination mass
- Actual



Where does AI fit?

Source identification requires lots of simulations combined with field samples

BUT

We can use AI to pick the most likely and important simulations to focus sampling and speed up identification

Acknowledgements/Disclaimers

The current Sandia/EPA team members: Katherine Klise, David Hart, Joseph Hogge, Michael Bynum at SNL; Terra Haxton, Jonathan Burkhardt, Regan Murray at US EPA.

The many other scientists and engineers at Sandia, the U.S. EPA, and students of Carl Laird from Perdue University who have worked on the Sandia/EPA Water Security and Water Resilience projects over the years.

Many thanks to the WNTR user community and the EPANET developer community that have made the software better and enhanced the science of water distribution modeling.

This presentation describes objective technical results and analysis. Any subjective views or opinions that might be expressed here do not necessarily represent the views of the U.S. Department of Energy, the U.S. Environmental Protection Agency, or the United States Government.

The U.S. Environmental Protection Agency through its Office of Research and Development funded and collaborated in the research described here under an Interagency Agreement with the Department of Energy's Sandia National Laboratories.

Mention of trade names products, or services does not convey official approval, endorsement, or recommendation by the U.S. Government or any agency thereof.

Resources - Open Source Software and Tools

EPANET Application for Modeling Drinking Water Distribution Systems

- EPANET 2.0: **https://www.epa.gov/water-research/epanet**
- EPANET 2.2: https://github.com/OpenWaterAnalytics/EPANET/releases/tag/v2.2

Analysis and research tools

- Anaconda (Python for scientists): https://www.anaconda.com/distribution/
- WNTR (water network tool for resilience): **https://github.com/USEPA/WNTR**
- Pecos (event detection): https://github.com/sandialabs/pecos

Other community resources (EPANET and SWMM)

- Open Water Analytics: http://wateranalytics.org/

This is not exhaustive, nor is it an endorsement or lack thereof for

References

Primary source

Hart, David, J. Santiago Rodriguez, Jonathan Burkhardt, Brian Borchers, Laird, Regan Murray, Katherine Klise, Terranna Haxton. "Quantifying hydraulic and water quality uncertainty to inform sampling of drinking water distribution systems." *Journal of water resources planning and management* (J WRPM)145, no. 1 (2019): 04018084.

Related sources

Bargiela, A. and Hainsworth, G. D. "Pressure and flow uncertainty in water systems." J WRPM, 115(2), 212-229.

Davis, M. J. and Janke, R. (2011). in potential impacts associated with contamination events in water distribution systems." J WRPM, 137(1), 1-9.

Davis, M. J., Janke, R., and Magnuson, (2014). "A framework for estimating the adverse health effects of contamination events in water distribution systems its application." Risk Analysis, 34(3), 513.

De Sanctis, A., Shang, F., and Uber, J. "Real-time identification of possible contamination sources using network backtracking methods?' J WRPM, 444-453.

Klise, K. A., Bynum, M., Moriarty, D., and Murray, R. (2016). "Water network tool for resilience (WNTR) user manual, version 0.1." Report No. EPA/600/R-17/264, U.S. Environmental Protection Agency.

Lansey, K. E. and Basnet, C. (1991). "Parameter estimation for water distribution networks." J WRPM, 117(1), 126-144.

Mann, A. V., McKenna, S. A., Hart, W. E., Laird, C. D. (2012). "Real-time inversion large-scale water networks using measurements!' Computers & Chemical Engineering, 37,143-151.

Sanz, G. and Pérez, R. (2014). "Demand Pattern Calibration in Water Networks." Procedia Engineering, 70,1495-1504.

Seth, A., Klise, K. A., Siirola, J. D., Haxton, and Laird, C. D. (2016). "Testing contamination source identification methods for water distribution Journal of Water Resources591 Planning and Management, 142(4), 04016001.

U.S. EPA (2010). "Assessing potential impacts associated with contamination events in water distribution systems: A sensitivity analysis!' Report No. EPA/600/R-10/061, U.S. Environmental Protection Agency, Washington, DC.

Wagner, D. E., Neupauer, R. M., and Cichowitz, C. (2015). "Adjoint-based probabilistic source characterization in water-distribution systems with flows and imperfect sensors!' J WRPM, 141(9), 04015003.

Yang, X. and Boccelli, D. L. (2013). "Simulation Study to Evaluate Temporal Aggregation and Variability of Water Demands on Distribution System Hydraulics and Transport." J WRPM, 140(8), 04014017.

Yang, X. and Boccelli, D. L. (2014). "Bayesian approach for real-time probabilistic contamination source identification." J WRPM, 140(8),