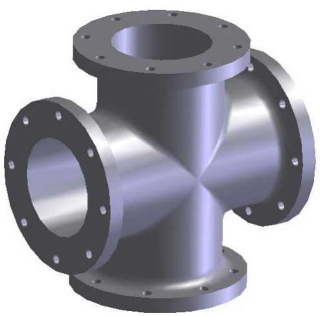
Presentation to EPA

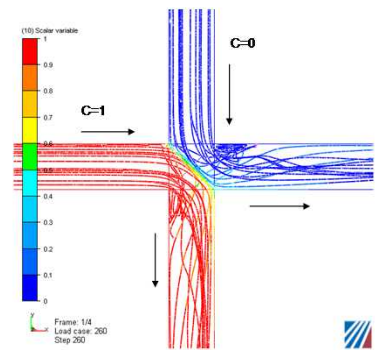
SAND2007-6646P

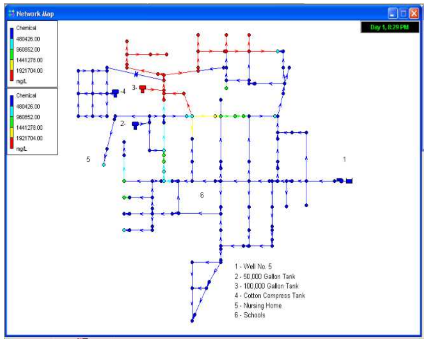
Cincinnati, OH, October 11, 2007

A New Model for Solute Mixing in Pipe Junctions:

Implementation of the Bulk Mixing Model in EPANET







Clifford K. Ho and Siri S. Khalsa*
Sandia National Laboratories
Albuquerque, NM

*Student at the University of Virginia

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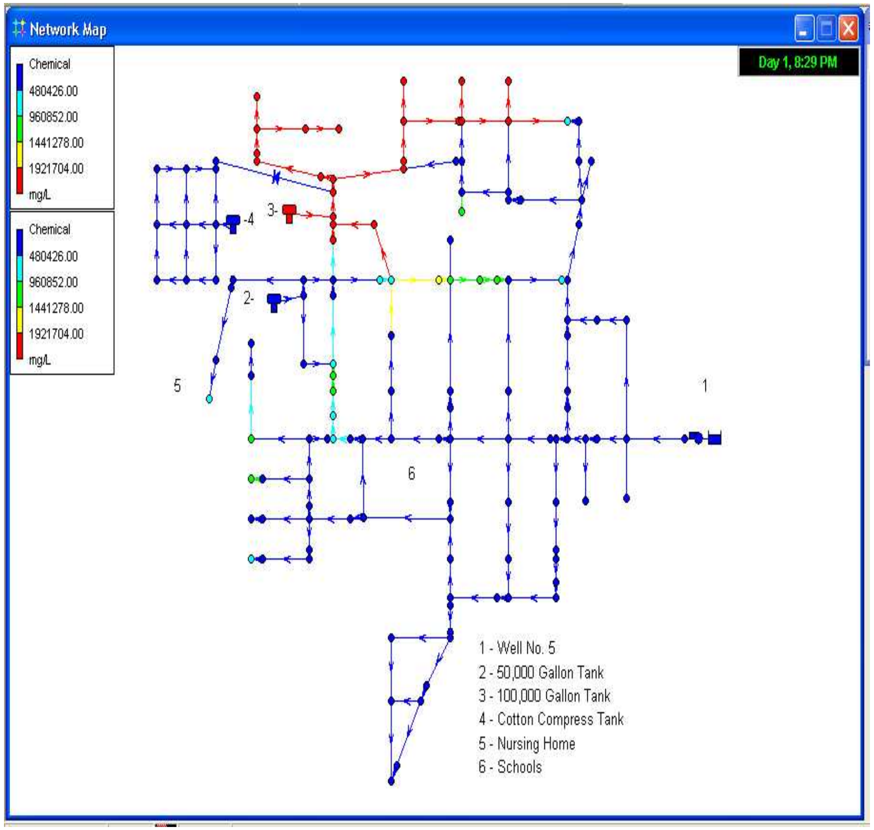
Overview

- Background
- Introduction to Bulk Mixing Model
- Comparisons with Experiments
- Implementation in EPANET
- EPANET-BAM Demonstrations

Background - Motivation

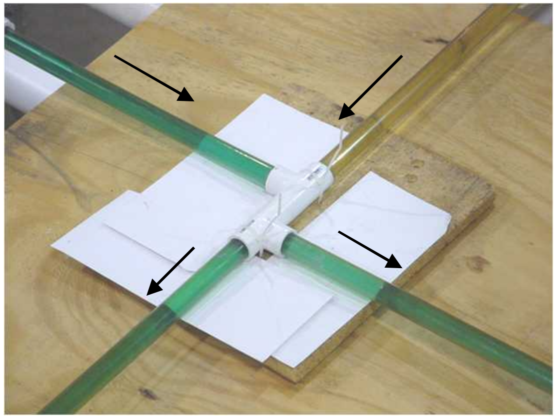
- **Contaminant transport in water-distribution pipe networks is a growing concern**
  - **Mixing in junctions**
  - **Important for**
    - **Risk assessments**
    - **Vulnerability assessments**
    - **Inverse modeling (contaminant source detection, monitoring)**

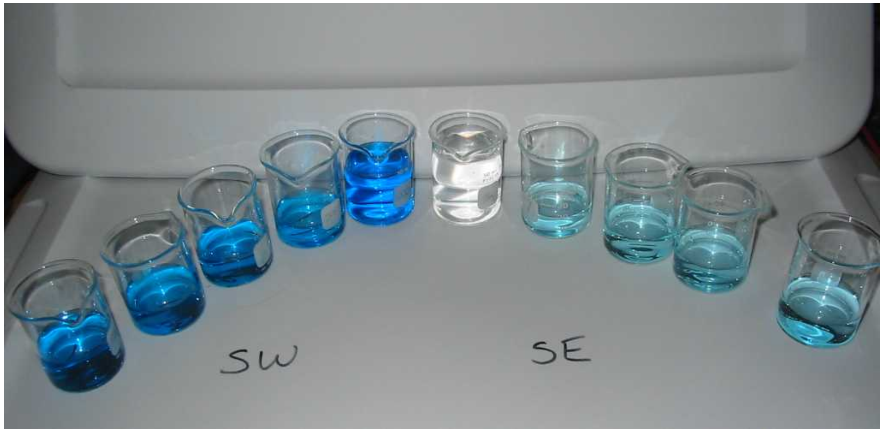


Background – Problem Statement

- **Many water-distribution network models (e.g., EPANET) assume complete mixing at junctions**

- **Previous studies have shown incomplete mixing in pipe junctions (experimental and computational)**
  - **van Bloemen Waanders et al. (2005)**
  - **O'rear et al. (2005)**
  - **Ho et al. (2006)**
  - **Romero-Gomez et al. (2006)**
  - **Webb and van Bloemen Waanders (2006)**
  - **McKenna et al. (2007)**





from Orear et al. (2005)

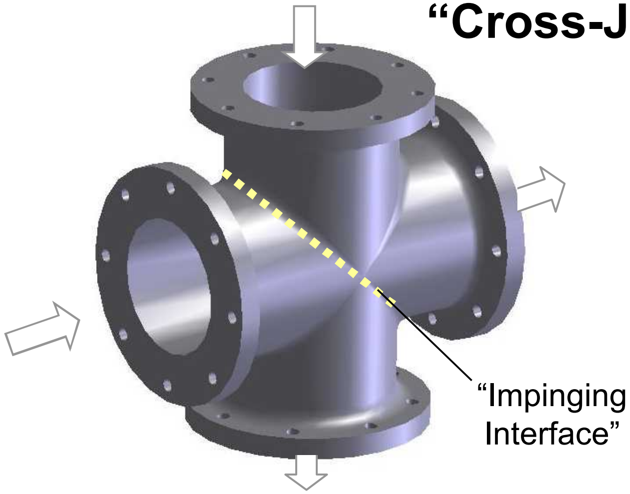
Objectives

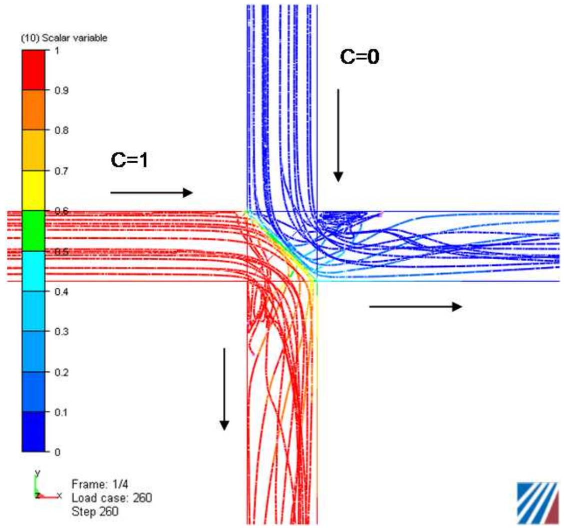
- **Conduct physical and numerical simulations of contaminant transport in pipe junctions**

- **Understand impact of parameters and processes on mixing behavior**
  - **Different flow rates**
  - **Effective mass transfer at impinging interface**

- **Develop improved mixing models and incorporate into EPANET**

“Cross-Junction”





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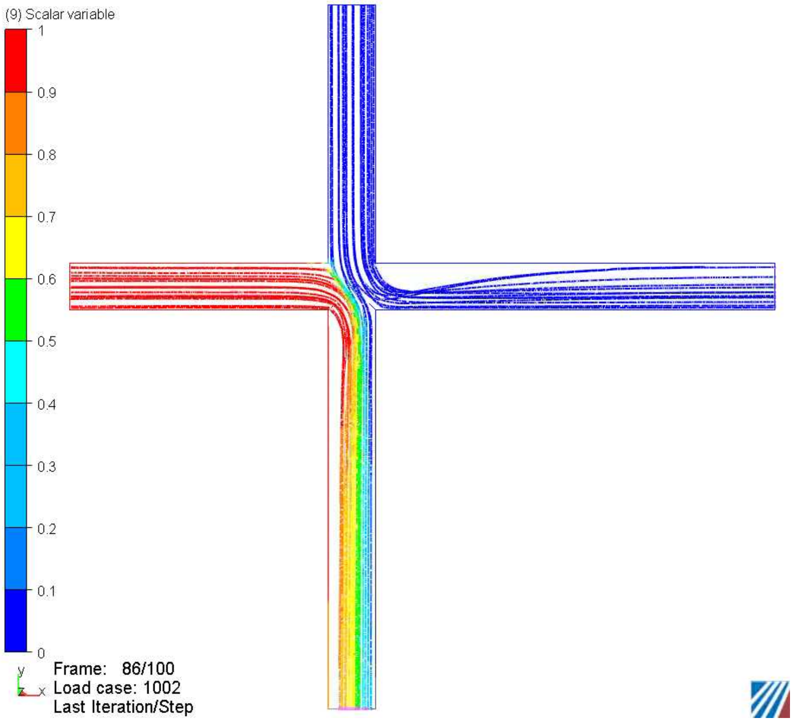
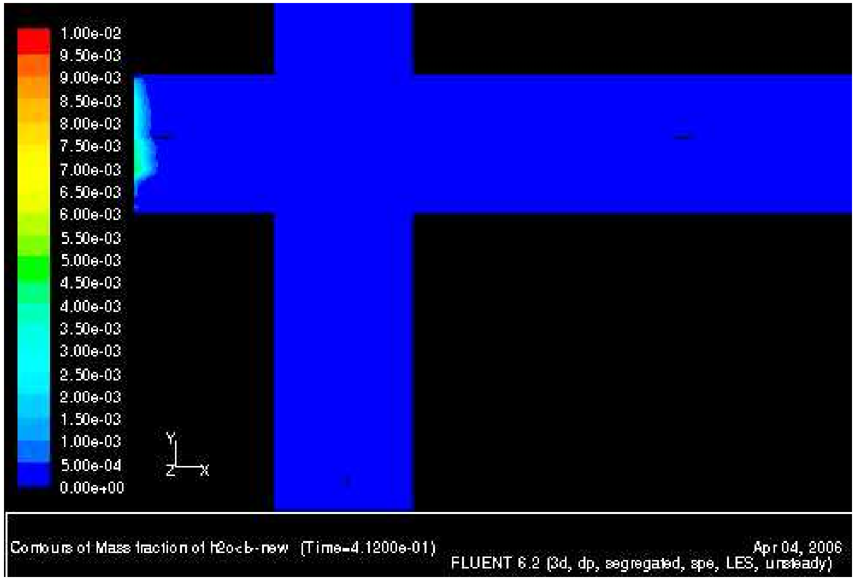
Mixing in Pipe Junctions

- **Bulk advective mixing caused by different flow rates**
- **Turbulent mixing caused by instabilities at the impinging interface**



(Ho et al., 2006)

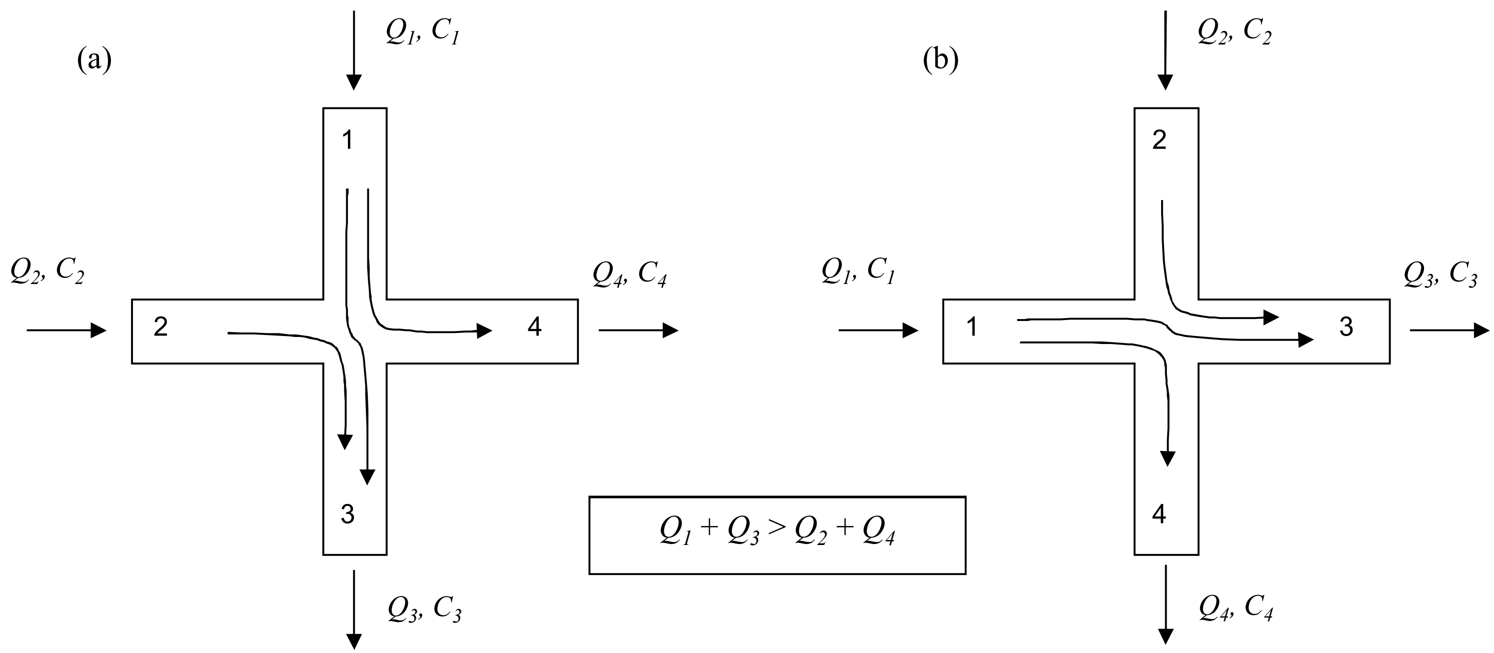


(Webb and von Bloemen Waanders, 2006)

Bulk Mixing Model

(Ho, 2007, J. Hydraulic Engr. in review)

- **Honors conservation of momentum in the flow streams**



$$C_3 = \frac{Q_2 C_2 + \left(Q_1 - Q_4\right) C_1}{Q_3}$$

$$C_4 = C_1$$

Bulk Mixing Model

- **Neglects mixing from turbulent instabilities**
- **Provides lower bound to the amount of mixing that can occur in junctions**
- **Complements the complete-mixing model in EPANET, which provides an upper bound to the amount of mixing that can occur in junctions**
- **A scaling (mixing) parameter, $0 \leq s \leq 1$, can be used to combine the results of the bulk-mixing and complete-mixing models for more accurate estimation**
  - $C_{combined} = C_{bulk} + s\,(C_{complete} - C_{bulk})$
    - **s = 0 (bulk mixing model)**
    - **s = 1 (complete mixing model)**

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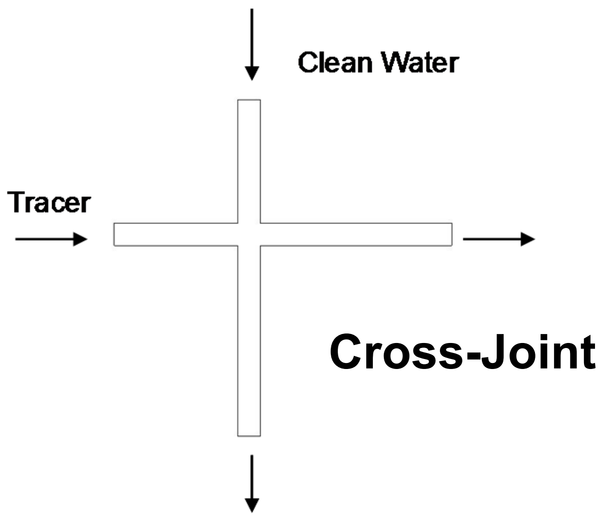
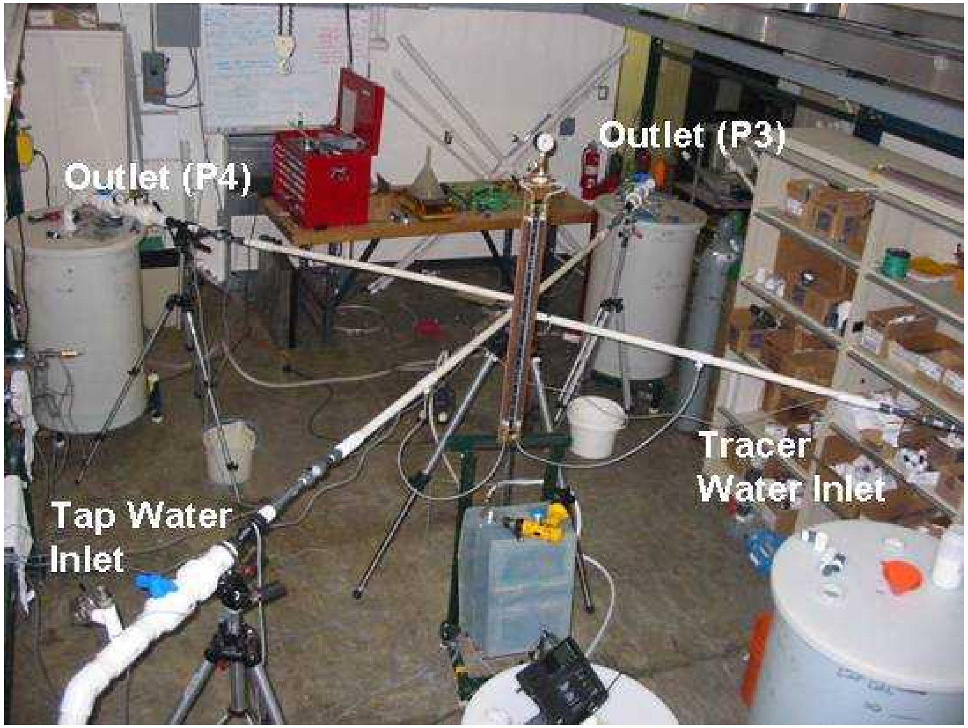
Single-Joint Tests

(Orear et al., 2005, Romero et al., 2006, McKenna et al., 2007)

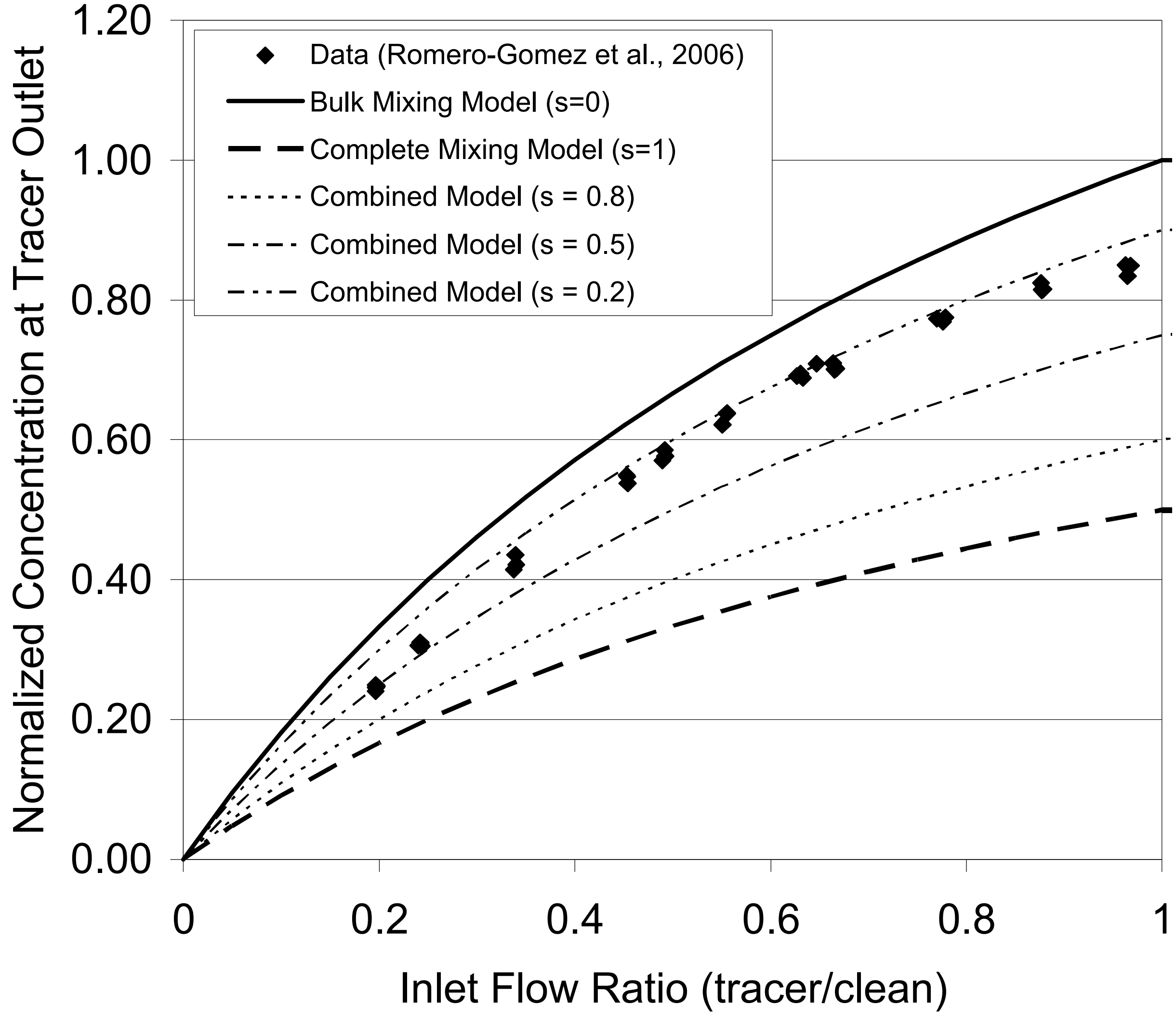


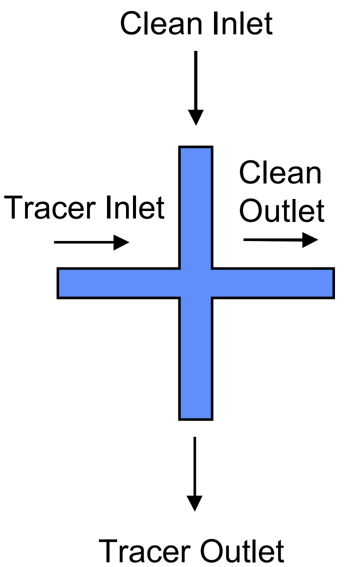


- Tracer consists of NaCl solution
- Tracer monitored continuously by electrical conductivity sensors
- Flow rate in each pipe was controlled
- Pipe diameters: 0.5”, 1”, 2”

Single Cross-Joint Tests

(Ho, 2007, J. Hydraulic Engr. in review)

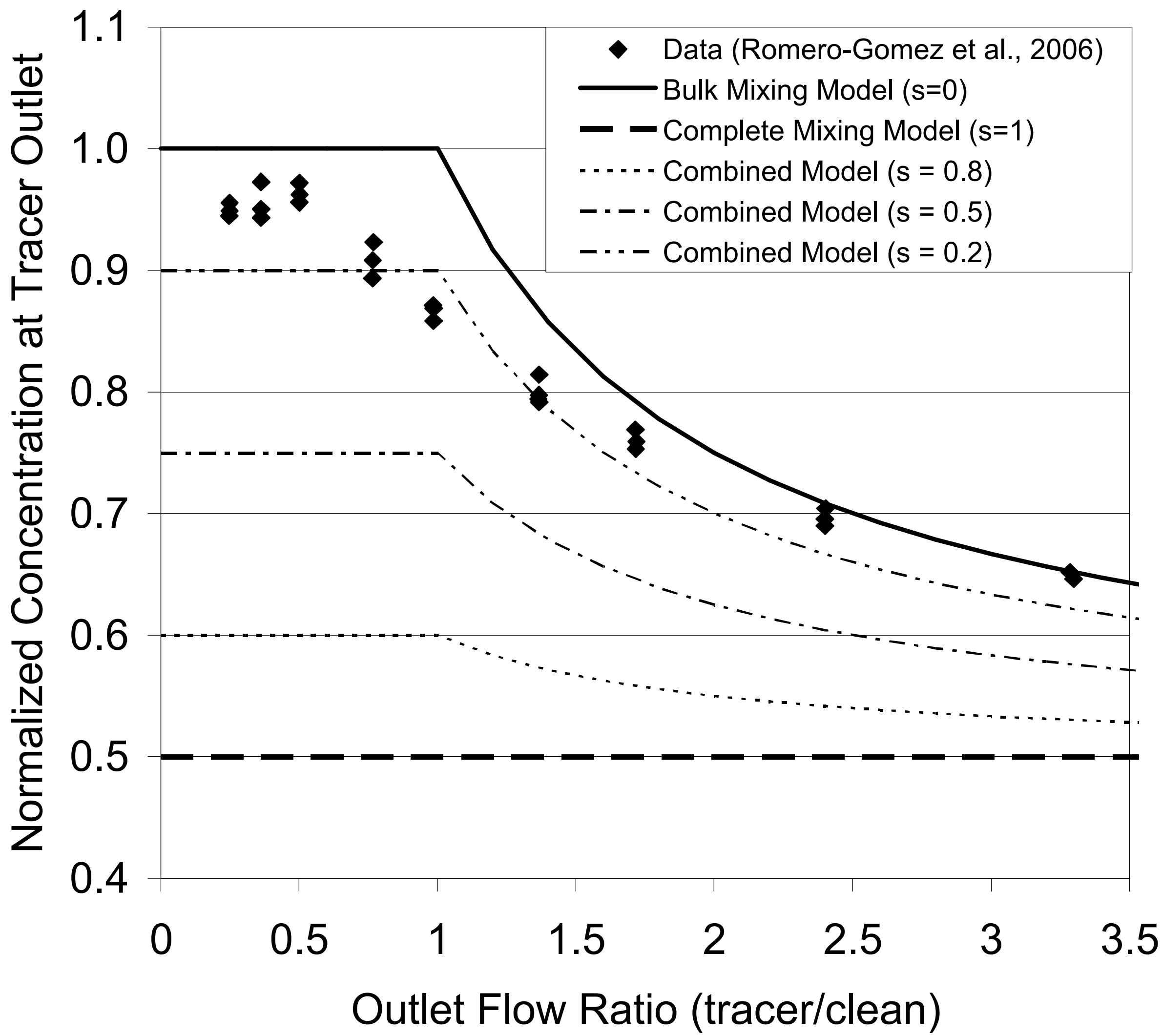


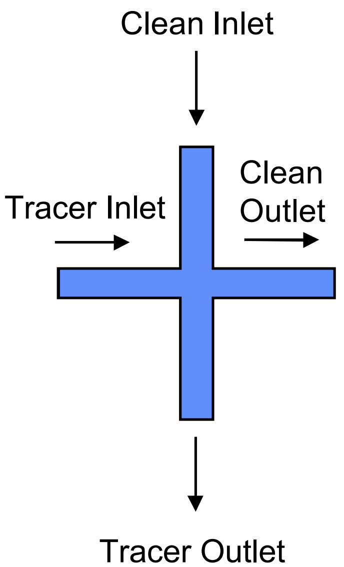


Note: Outlet flows equal

Single Cross-Joint Tests

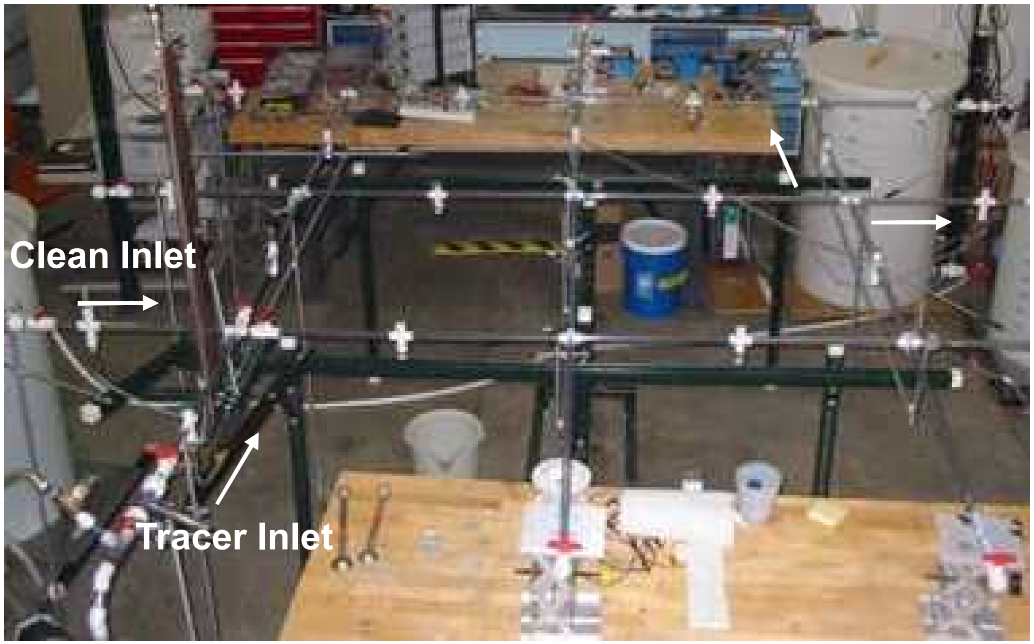
(Ho, 2007, J. Hydraulic Engr. in review)

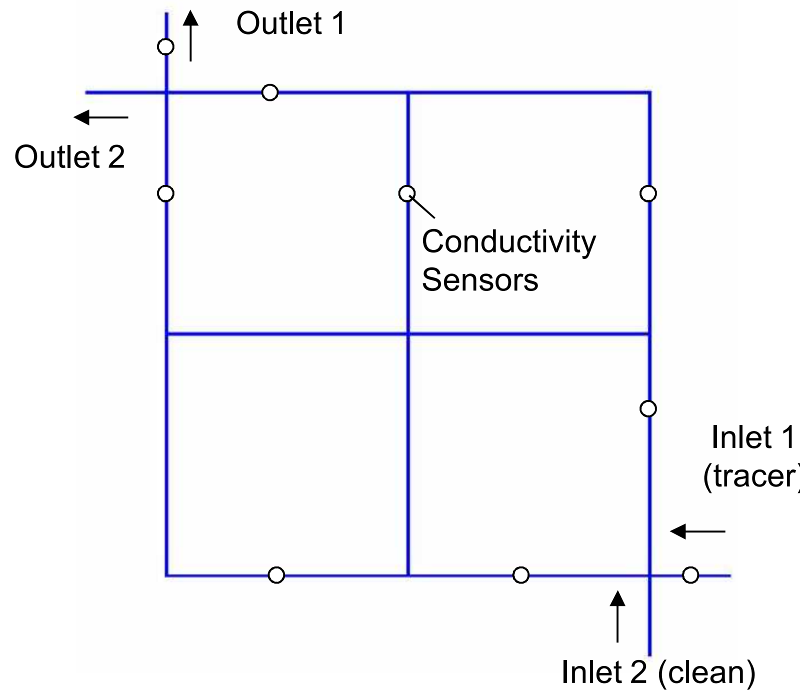




Note: Inlet flows equal

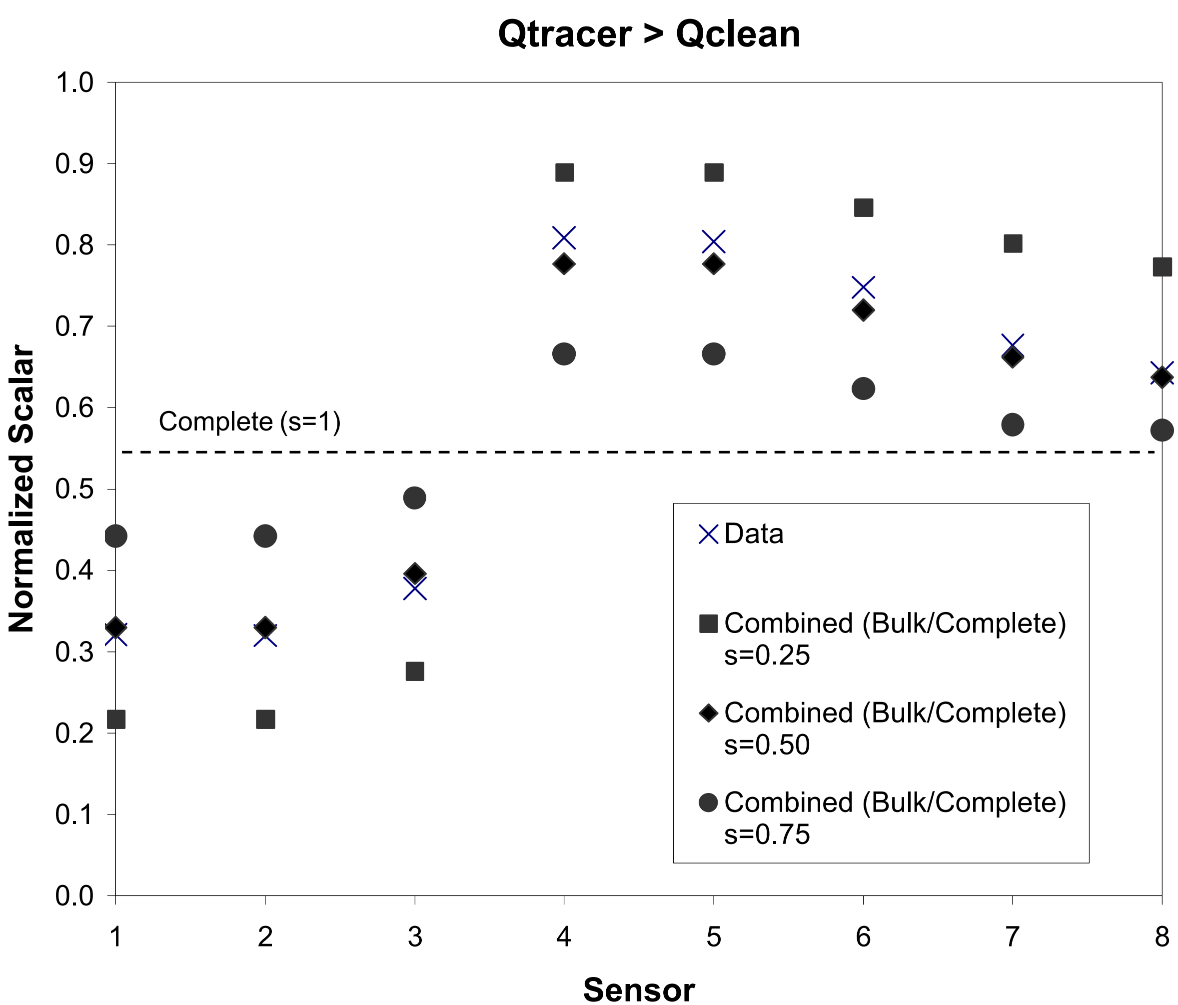
Multi-Joint Tests
(3x3 Small-Scale Network, Orear et al., 2005)

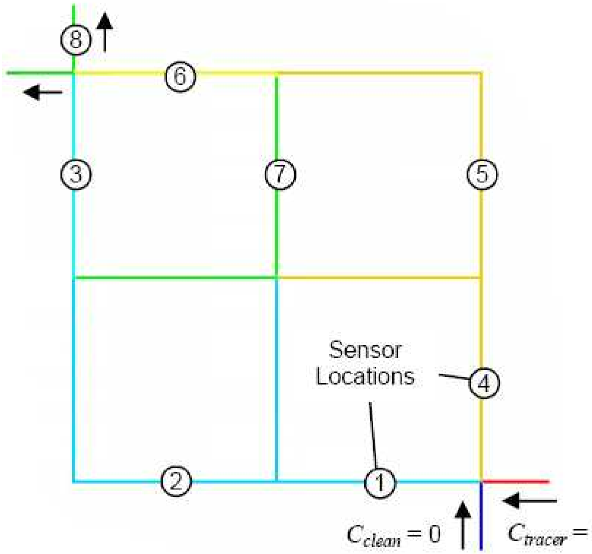




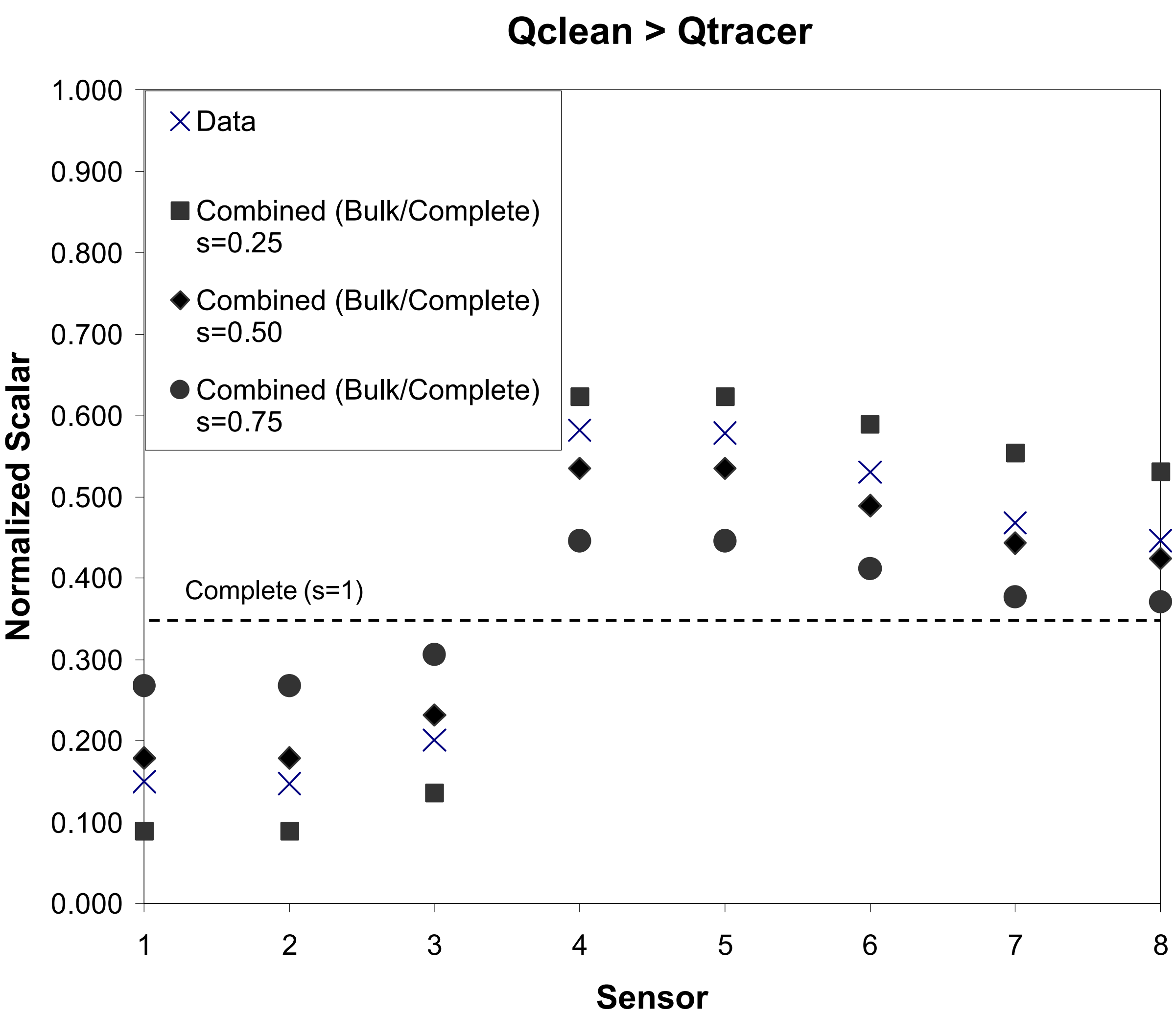
- **3x3 array of cross joints with 3-foot pipe lengths**
- **Flow rates at inlets and outlets controlled**
- **Pipe diameter: 0.5"**

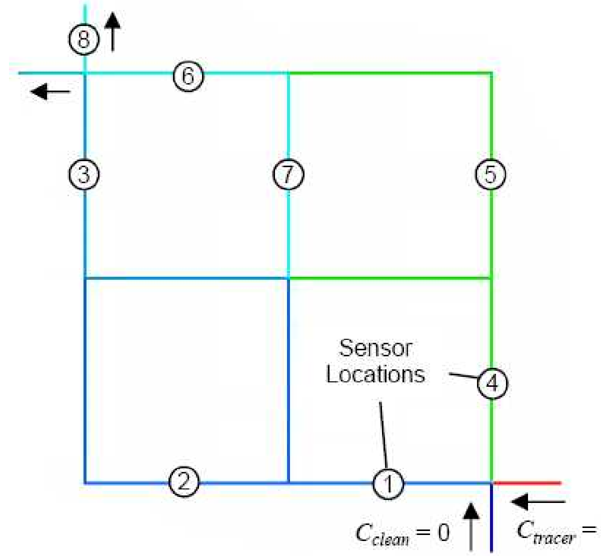
3x3 Network Tests





3x3 Network Tests





Experimental Findings

- **Mixing Parameter, s**
  - **0 ≤ s ≤ 1 (bulk mixing ↔ complete mixing) bounds data**
  - **Dependence on junction geometry and fitting**
    - **Flush vs. press fit (expansion in junction)**
    - **s ~ 0.2 – 0.5 (for most flow ratios)**
  - **Network results**
    - **3x3 network**
    - **Diamond (converging) network**
    - **s ~ 0.4 – 0.5 (for most boundary conditions and flow rates)**

Diamond converging network with 7 sequential cross junctions
(SNL - M. Aragon, J. Wright, S. McKenna)

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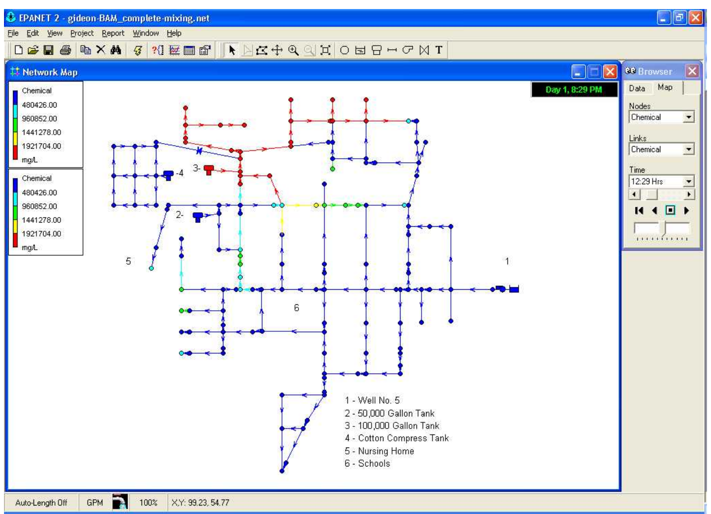
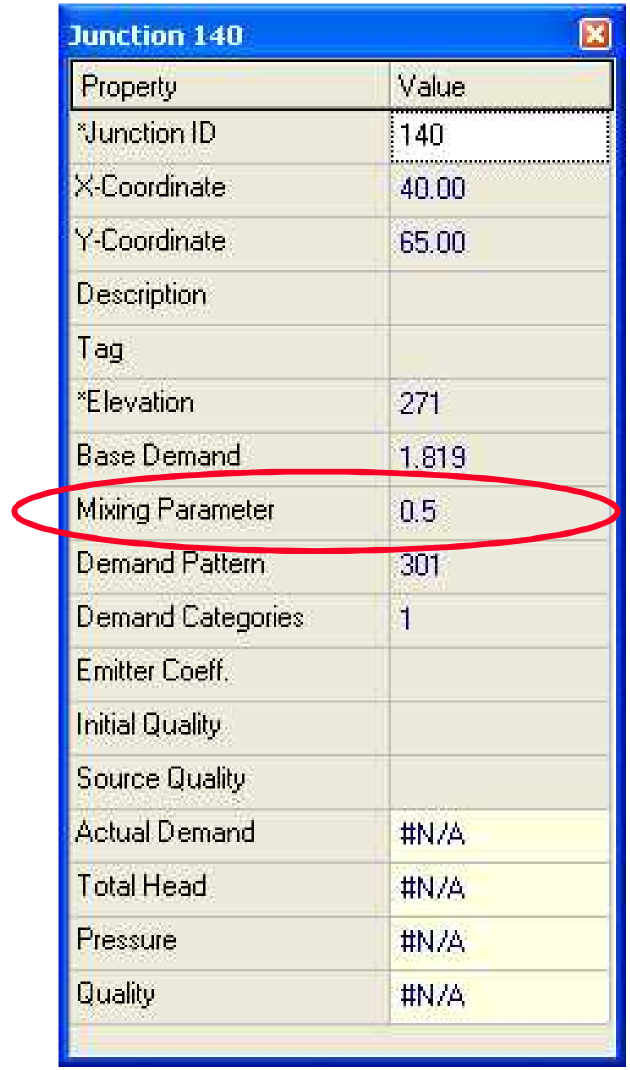
EPANET-BAM Features
(Bulk Advective Mixing)

- **Fully compatible with EPANET 2.0**
  - New versions of ‘Epanet2w.exe’ and ‘epanet2.dll’
  - GUI fully compatible
  - Mixing parameter can be adjusted at each junction
    - “Valid” cross junctions are analyzed with bulk-mixing model





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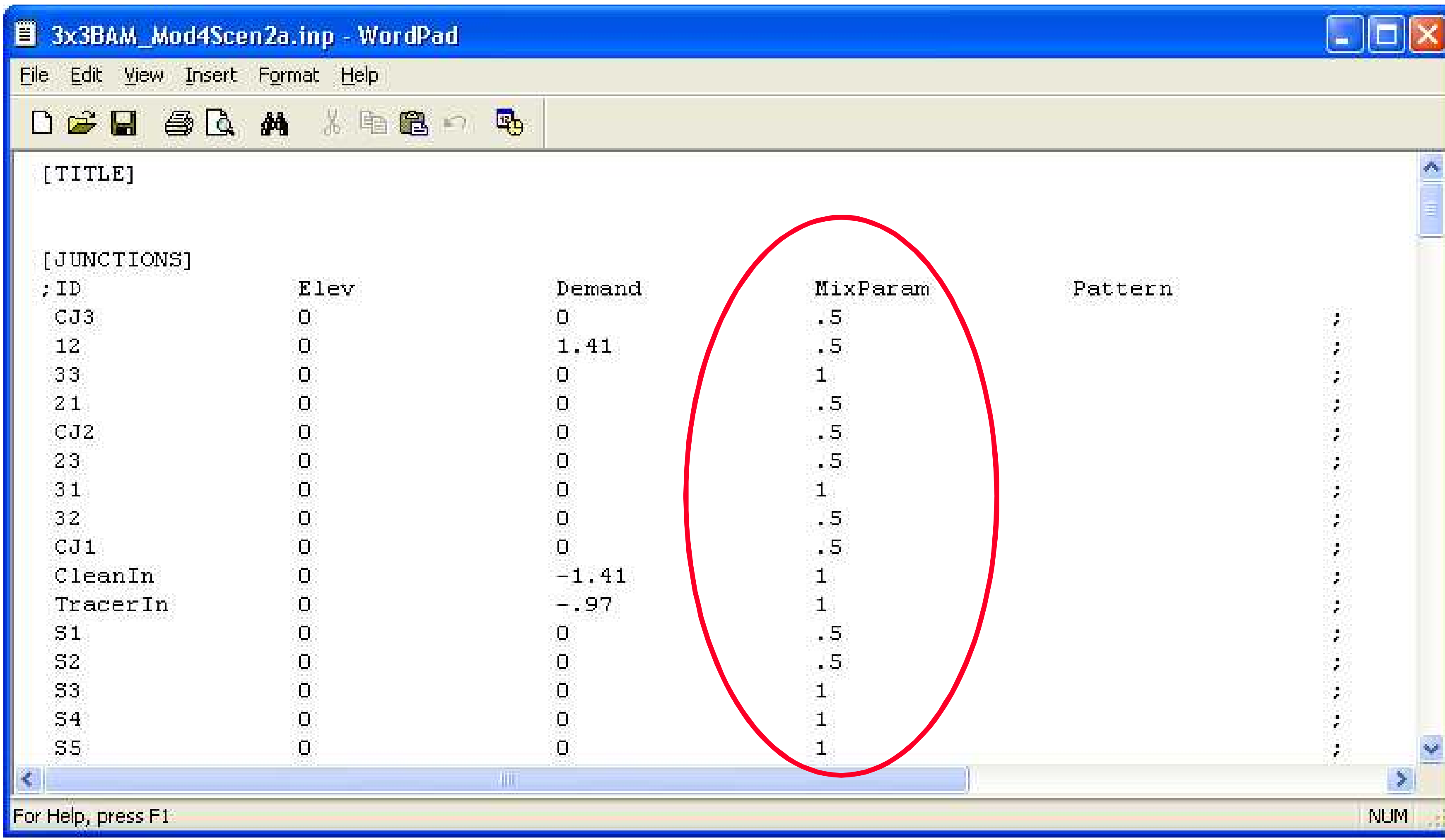
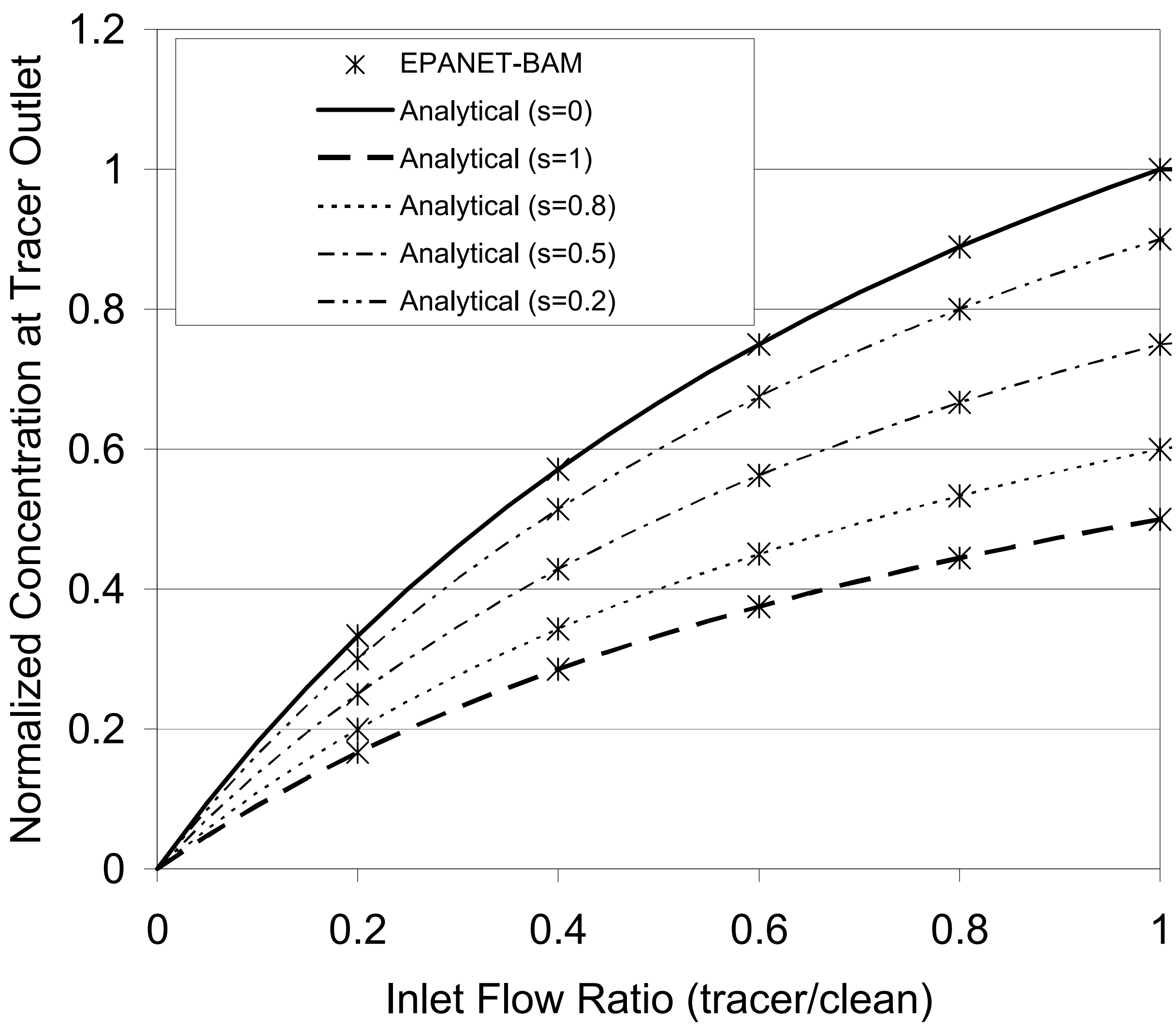
Mixing Parameter Stored in Input File

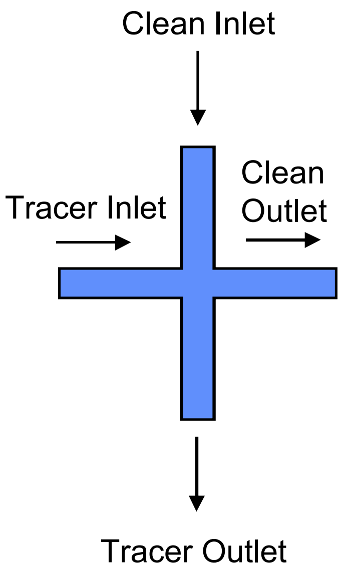



```
[TITLE]


[JUNCTIONS]
;ID          Elev        Demand      MixParam    Pattern
 CJ3         0           0           .5                      ;
 12          0           1.41        .5                      ;
 33          0           0           1                       ;
 21          0           0           .5                      ;
 CJ2         0           0           .5                      ;
 23          0           0           .5                      ;
 31          0           0           1                       ;
 32          0           0           .5                      ;
 CJ1         0           0           .5                      ;
 CleanIn     0           -1.41       1                       ;
 TracerIn    0           -.97        1                       ;
 S1          0           0           .5                      ;
 S2          0           0           .5                      ;
 S3          0           0           1                       ;
 S4          0           0           1                       ;
 S5          0           0           1                       ;
```

EPANET-BAM
Validation





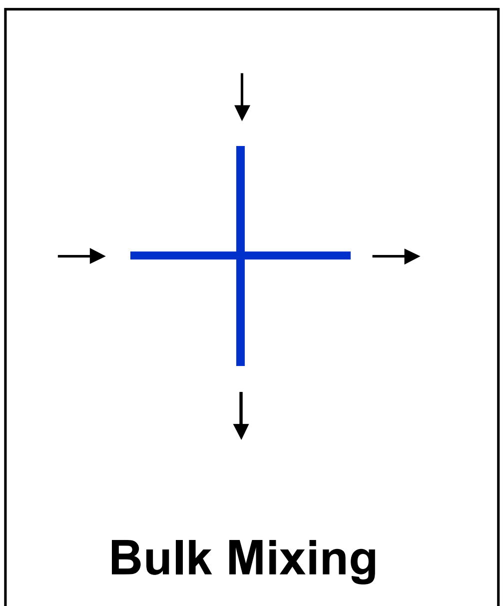
EPANET-BAM Applications

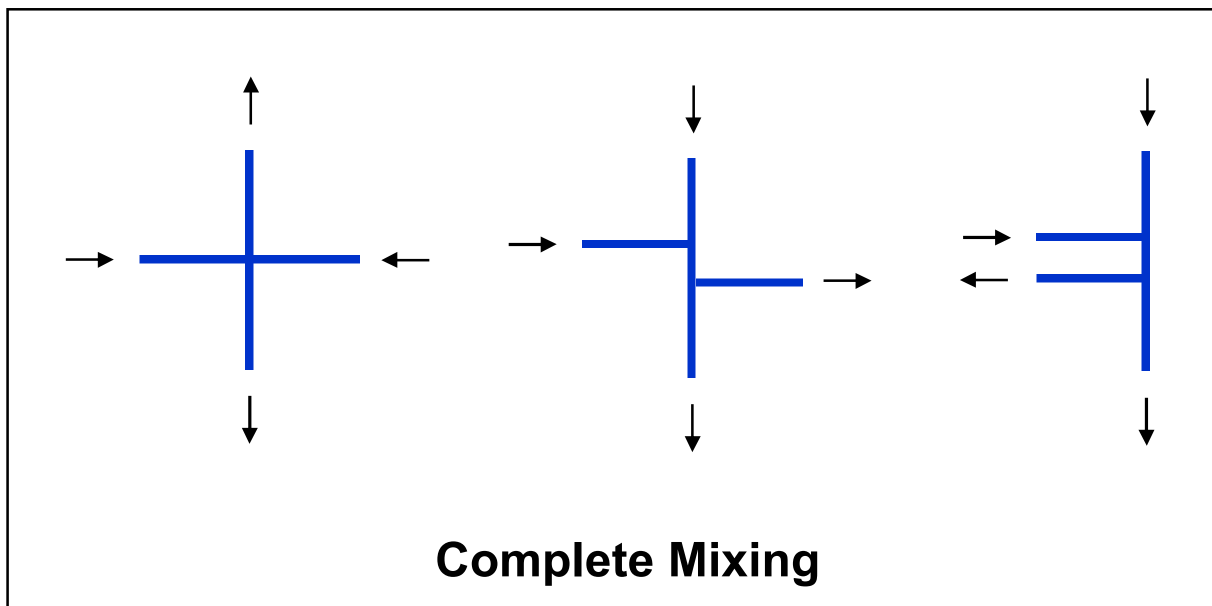
- Hydraulic and water quality simulations with incomplete mixing at junctions (bulk mixing, s < 1)
  - Steady and transient
  - Bounding calculations for risk assessments
    - s=0, s=1

- Integration with PEST (Parameter ESTimation Software; www.sspa.com/pest/)
  - Calibration of mixing parameter at one or more junctions based on available concentration data
  - Contaminant source detection with sparse data

Implementation Issues

- Only cross junctions with adjacent inlets (and outlets) are currently analyzed for bulk mixing
  - All other junction configurations are assumed to yield complete mixing





Alternative Implementation of Incomplete Mixing in EPANET

- Can use regressions based on empirical or numerical data to correlate incomplete mixing with different flow rates at each junction
  - Collaboration with U. Arizona (Prof. Chris Choi)
  - Romero et al. (2006, WDSA), Austin et al. (2007, J. Water Resources Planning & Management)
    - Requires lots of data
    - Assumes simulated junctions are identical to those used to derive regressions
      - Corrosion products, different geometries, etc. may change mixing behavior

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EPANET-BAM Demonstrations

- Exercise 1: Steady contamination
- Exercise 2: Transient contamination
- Exercise 3: Source Detection
- Exercise 4: Gideon Network

Exercise 1

Steady-State Contamination Scenario

- **1000 mg/L of Chemical X enters the network through *Contaminant Inlet***
- **Predict the concentration of Chemical X at each neighborhood after the contaminant has spread completely throughout the network, assuming:**
  - **Complete mixing in cross junctions**
  - **Incomplete mixing (mixing parameter = 0.5) in cross junctions**
- **Compare these predictions to laboratory measurements**

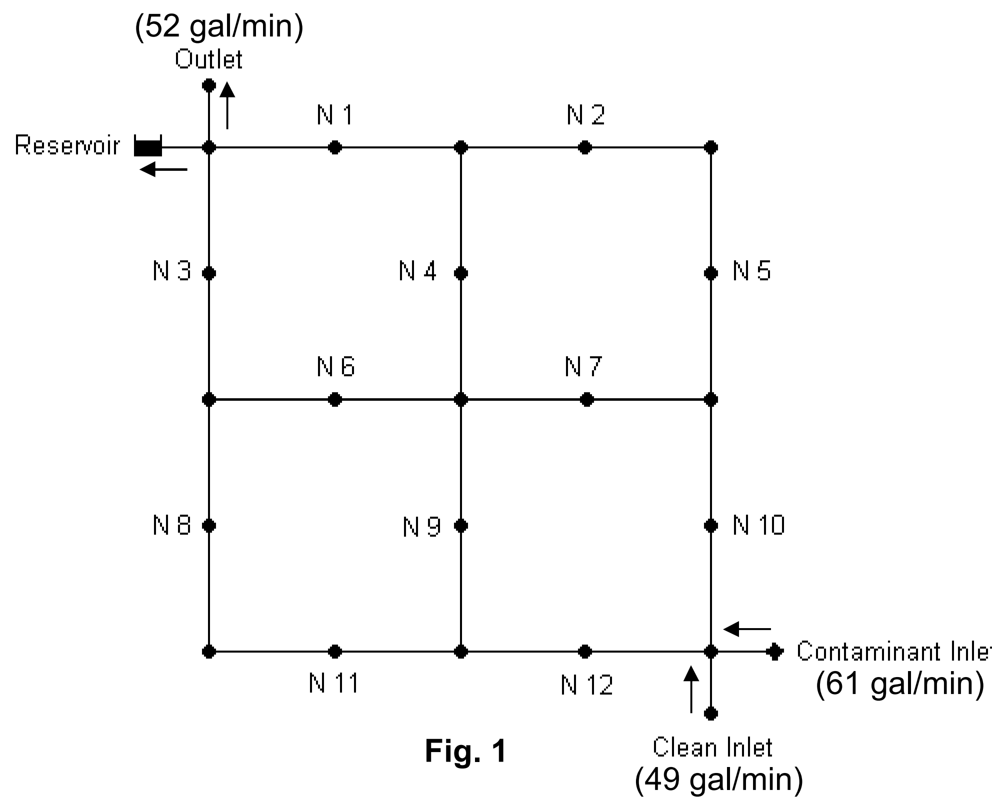


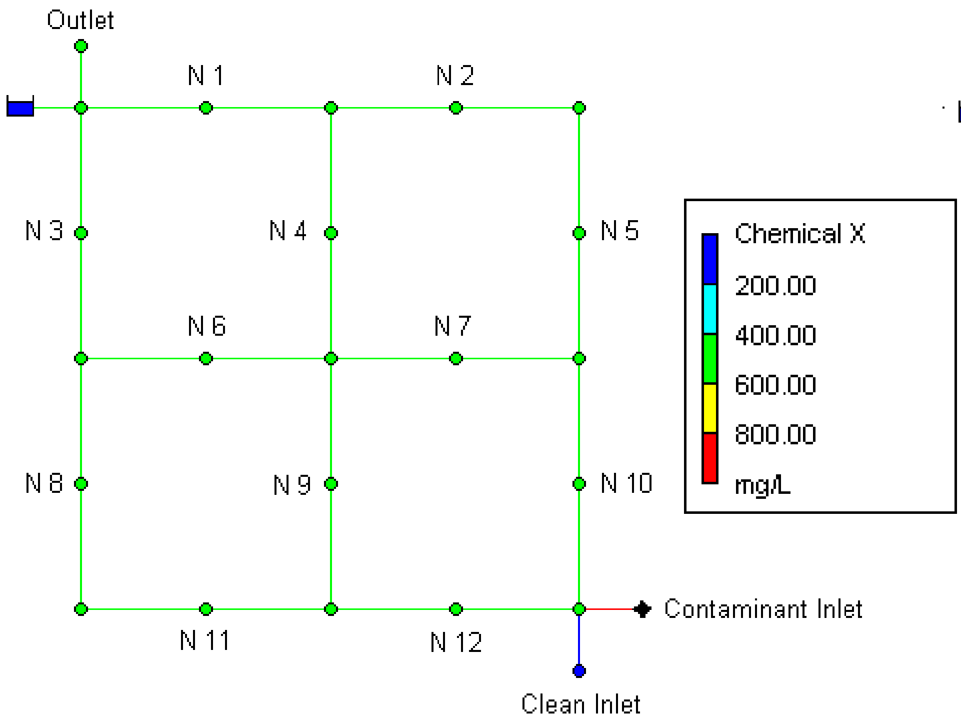
Fig. 1

Note: simulated network is an up-scaled replica of a smaller network tested in the laboratory

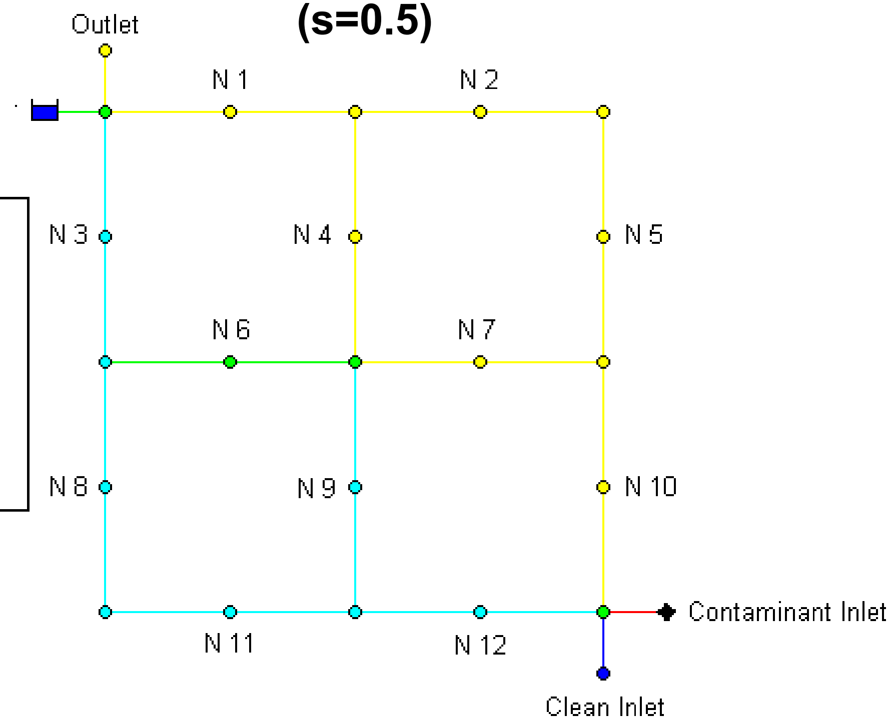
Exercise 1

Predicted Concentration Distributions

Complete Mixing Model



Incomplete (Bulk) Mixing Model (s=0.5)



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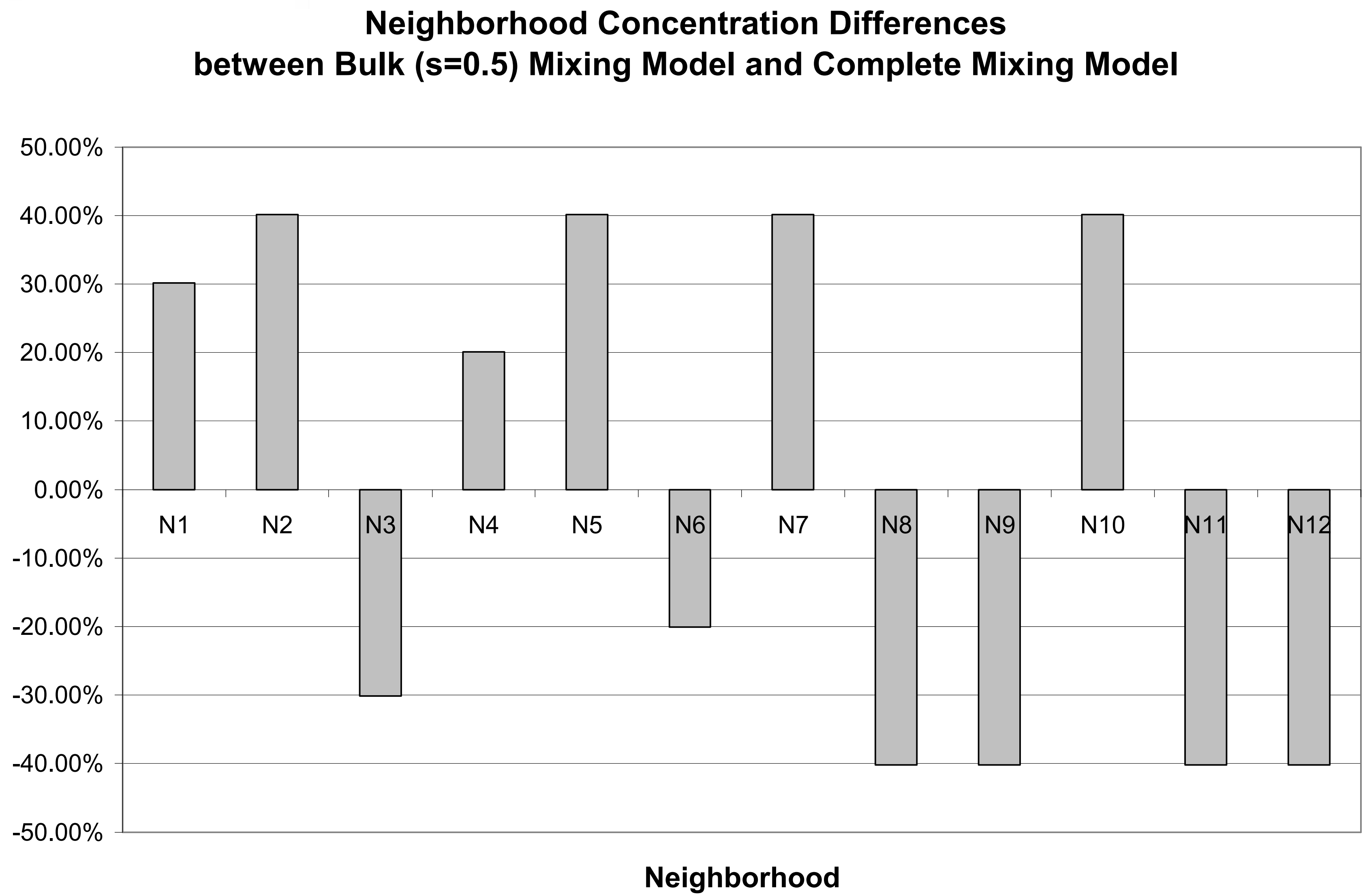
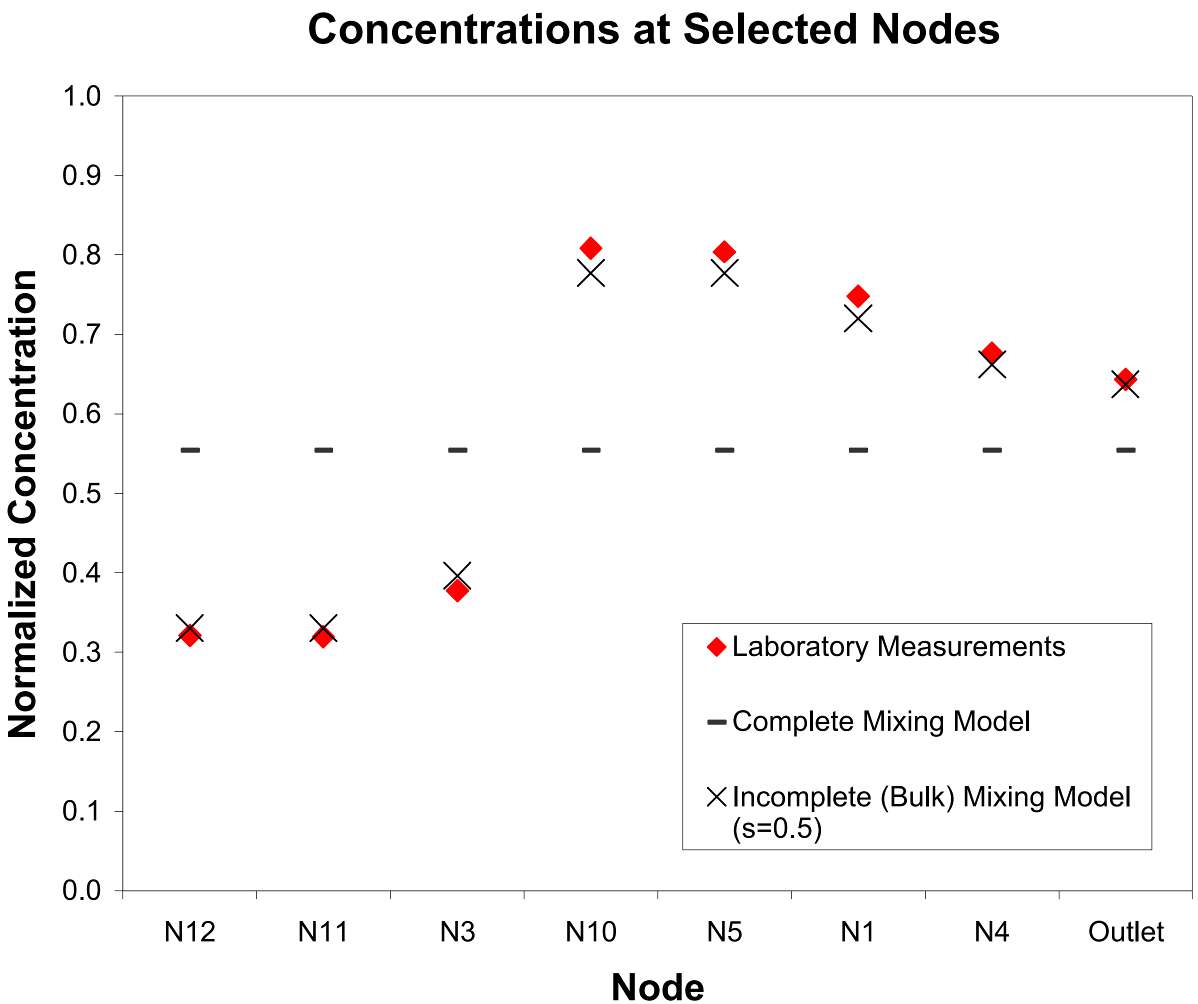
Exercise 1

Concentration Differences



Exercise 1

Comparison to Laboratory Experiments



Exercise 1

Risk Assessment

- **Each neighborhood is populated by 100 people, each of whom weighs 60kg**
- **Assume each person consumes 2L of water per day**
- **The lethal dose response curve of Chemical X is shown in Fig 2**
- **Predict the number of deaths that will occur in each neighborhood after one day, assuming:**
  - **Complete mixing in cross junctions**
  - **Incomplete (bulk) mixing (mixing parameter = 0.5) in cross junctions**

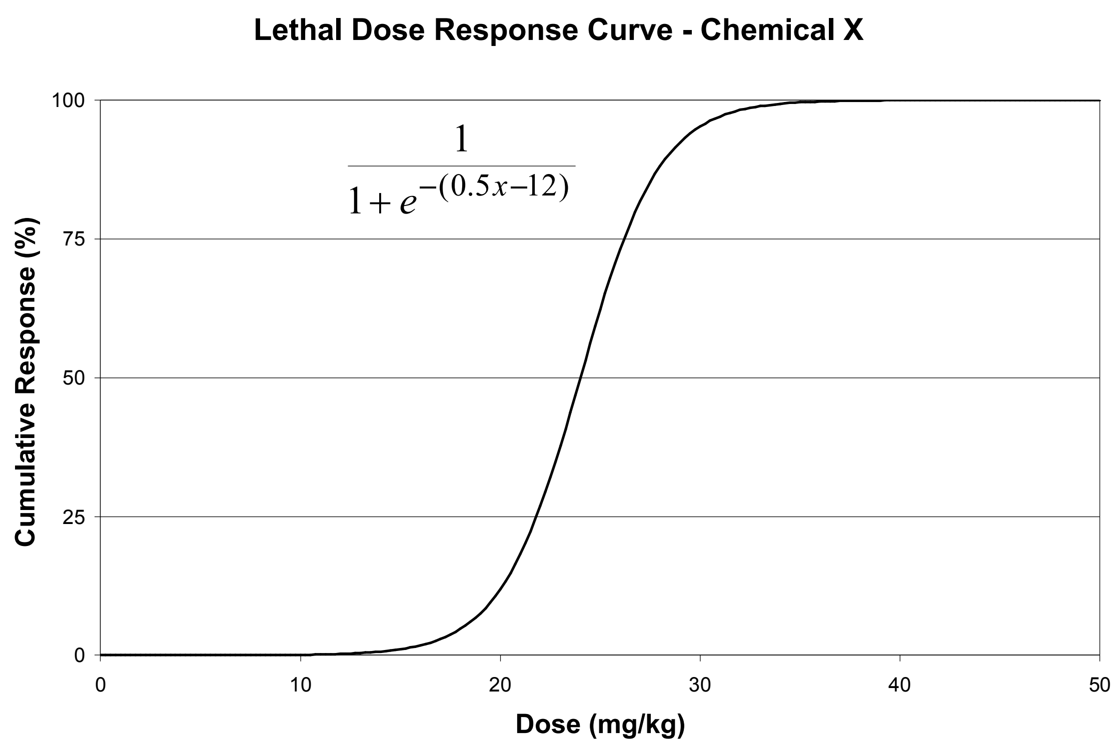


Fig. 2

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Exercise 1

Risk Assessment: Complete Mixing

Neighborhood	Concentration (mg/L)	Mass of X Ingested per Person per Day (mg)	Dose (mg/kg)	Predicted Mortality (%)	**Predicted Deaths**
N1	554.55	1109.10	18.49	5.97%	**5**
N2	554.55	1109.10	18.49	5.97%	**5**
N3	554.55	1109.10	18.49	5.97%	**5**
N4	554.55	1109.10	18.49	5.97%	**5**
N5	554.55	1109.10	18.49	5.97%	**5**
N6	554.55	1109.10	18.49	5.97%	**5**
N7	554.55	1109.10	18.49	5.97%	**5**
N8	554.55	1109.10	18.49	5.97%	**5**
N9	554.55	1109.10	18.49	5.97%	**5**
N10	554.55	1109.10	18.49	5.97%	**5**
N11	554.55	1109.10	18.49	5.97%	**5**
N12	554.55	1109.10	18.49	5.97%	**5**

Predicted Death Toll:	**60**

Exercise 1

Risk Assessment: Incomplete Mixing (s=0.5)

Neighborhood	Concentration (mg/L)	Mass of X Ingested per Person per Day (mg)	Dose (mg/kg)	Predicted Mortality (%)	**Predicted Deaths**
N1	721.59	1443.18	24.05	50.66%	**50**
N2	777.27	1554.54	25.91	72.20%	**72**
N3	387.50	775.00	12.92	0.39%	**0**
N4	665.91	1331.82	22.20	28.87%	**28**
N5	777.27	1554.54	25.91	72.20%	**72**
N6	443.18	886.36	14.77	0.98%	**0**
N7	777.27	1554.54	25.91	72.20%	**72**
N8	331.82	663.64	11.06	0.15%	**0**
N9	331.82	663.64	11.06	0.15%	**0**
N10	777.27	1554.54	25.91	72.20%	**72**
N11	331.82	663.64	11.06	0.15%	**0**
N12	331.82	663.64	11.06	0.15%	**0**

Predicted Death Toll:	**366**

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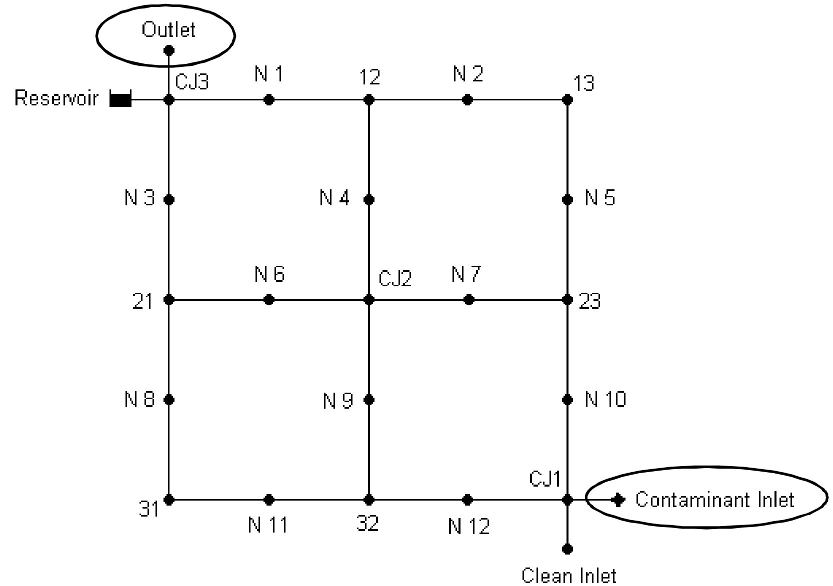
EPANET-BAM Demonstrations

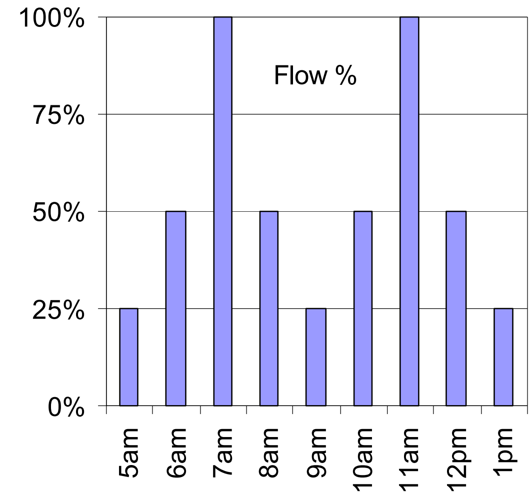
- **Exercise 1: Steady contamination**
- **Exercise 2: Transient contamination**
- **Exercise 3: Source Detection**
- **Exercise 4: Gideon Network**

Exercise 2

Transient Contamination

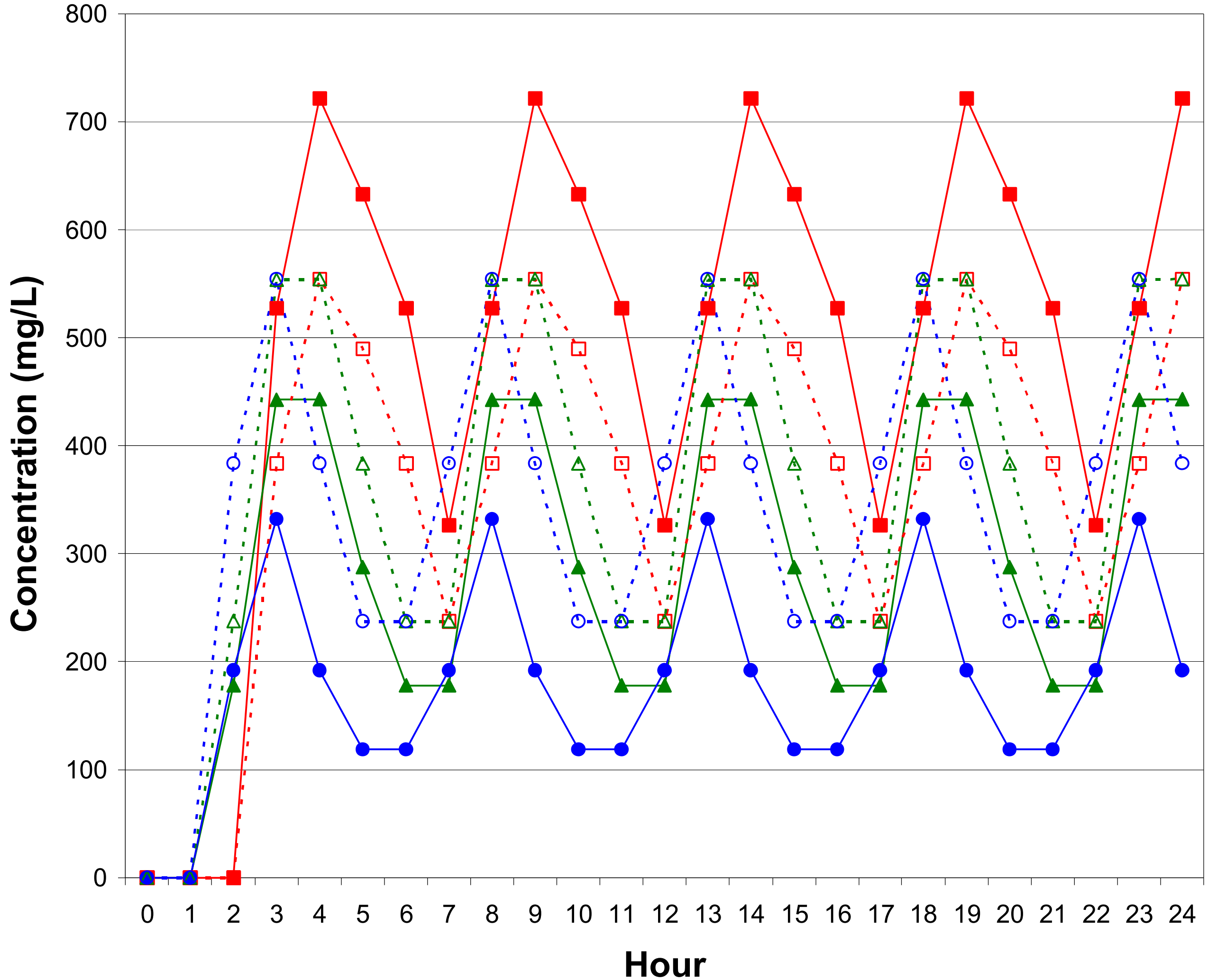
- Consider the water distribution network subdomain of Exercise 1
- In order to account for fluctuating demands throughout the day, the city adjusts the flow rates through the *Outlet* and the *Contaminant Inlet* every hour
  - Assume the flow adjustment pattern repeats itself
- Assume the contamination of *Contaminant Inlet* occurs at 5 am. Predict the concentration of Chemical X at neighborhoods N1, N6, and N11 at every hour over the 24 hours following the contamination event, assuming:
  - Complete mixing in cross junctions
  - Incomplete (bulk) mixing (mixing parameter = 0.5) in cross junctions





Exercise 2

Transient Concentrations at N1, N6, and N11



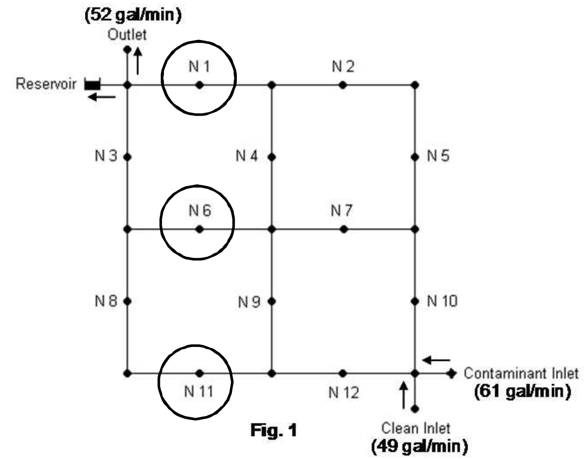
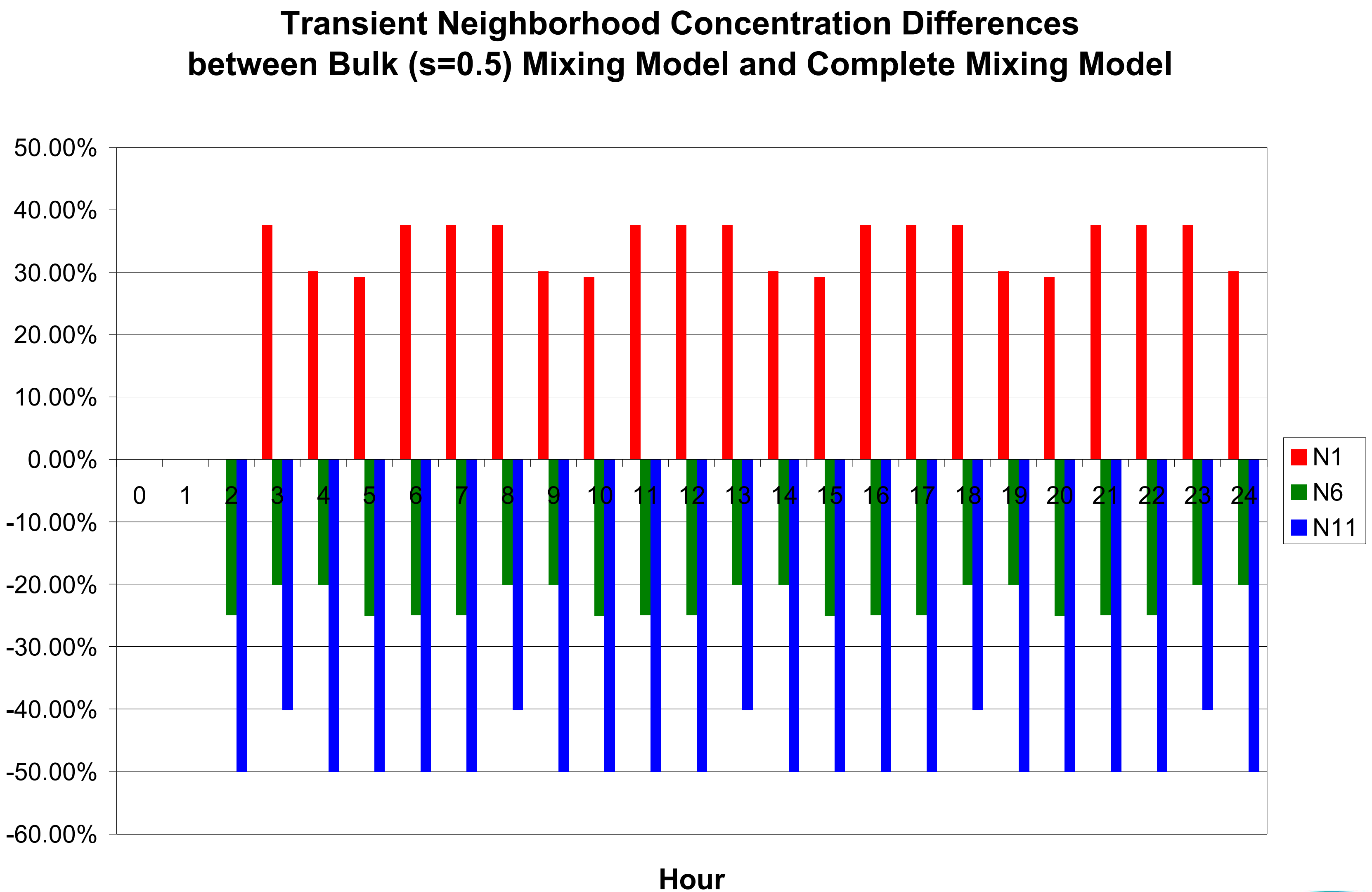


Fig. 1

Exercise 2

Concentration Differences



Exercise 2

Transient Risk Assessment

- **As in Exercise 1, assume each neighborhood is populated by 100 people, each of whom weighs 60kg**
- **Assume each person consumes 1/6 L of water per hour (2 L in 12 hours) and that a dose of Chemical X accumulates over 12 hours**
- **Predict the number of deaths that will occur in each neighborhood due to ingestion of contaminated water from 8 am to 8 pm, assuming:**
  - **Complete mixing in cross junctions**
  - **Incomplete (bulk) mixing (mixing parameter = 0.5) in cross junctions**

Exercise 2

Transient Risk Assessment Results

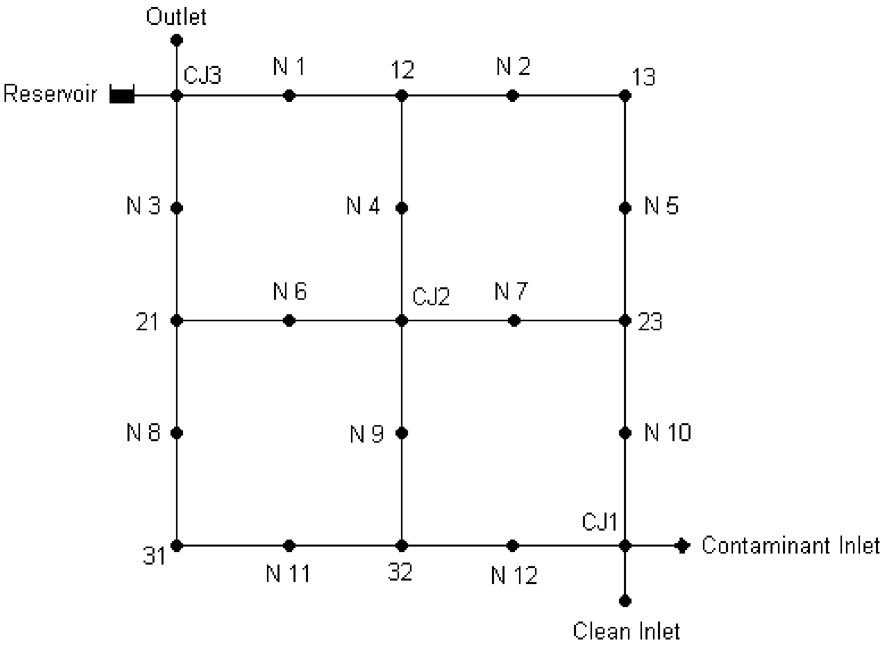
	Complete Mixing			Incomplete (Bulk) Mixing (s=0.5)		
Neighborhood	Dose per person (mg/kg)	Predicted Mortality (%)	Predicted Deaths	Dose per person (mg/kg)	Predicted Mortality (%)	Predicted Deaths
N1	13.99	0.67%	**0**	18.67	6.51%	**6**
N2	14.00	0.67%	**0**	20.10	12.45%	**12**
N3	13.99	0.67%	**0**	9.17	0.06%	**0**
N4	14.00	0.67%	**0**	17.05	3.01%	**3**
N5	12.59	0.33%	**0**	18.43	5.80%	**5**
N6	14.00	0.67%	**0**	10.96	0.15%	**0**
N7	12.59	0.33%	**0**	18.43	5.80%	**5**
N8	14.00	0.67%	**0**	7.91	0.03%	**0**
N9	12.59	0.33%	**0**	6.75	0.02%	**0**
N10	12.59	0.33%	**0**	18.43	5.80%	**5**
N11	12.59	0.33%	**0**	6.75	0.02%	**0**
N12	12.59	0.33%	**0**	6.75	0.02%	**0**

Predicted Death Toll / 12 hours:	**0**

Predicted Death Toll / 12 hours:	**36**

Exercise 3
Source Detection

- Consider the steady-state water distribution network subdomain of Exercise 1. After the contaminant spreads completely throughout the network, residents report that the municipal water has a strange taste and smell.
- In response to the complaints, city officials take two water samples, one from N1 and the other from N11, for analysis. Chemical X is detected in the following concentrations*:
  - N1: 747.92 mg/L
  - N11: 319.73 mg/L
- Determine the source node and the source concentration, assuming:
  - Complete mixing in cross junctions
  - Incomplete (bulk) mixing (mixing parameter = 0.5) in cross junctions



*Concentrations correspond to laboratory measurements from a down-scaled replica of the simulated network

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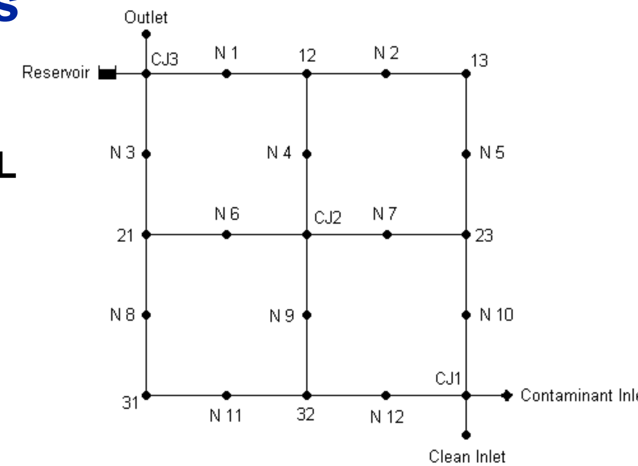
Exercise 3

Source Detection Results



- **Each node in the network was simulated as a potential source and optimized for a source concentration in the range 0-2000mg/L using EPANET-BAM and PEST**
  - **The nodes are listed in increasing order of the objective function, "phi" (the sum of squared weighted residuals)**
  - **Only the first 10 nodes on these lists are listed in the tables below**
  - **Recall that the actual source was at "TracerIn" at 1000 mg/L**

Complete Mixing Model		
Node ID	**Source Conc. (mg/L)**	**Phi**
CJ1	*533.83*	*91673*
CleanIn	*1198.39*	*91673*
TracerIn	*962.64*	*91673*
12	747.92	102230
13	1495.84	102230
CJ2	1495.84	102230
23	997.23	102230
N1	747.92	102230
N2	1495.84	102230
N4	1495.84	102230

Incomplete (Bulk) Mixing Model (s=0.5)		
Node ID	**Source Conc. (mg/L)**	**Phi**
TracerIn	*1023.77*	*483*
CJ1	533.83	91673
12	747.92	102230
13	1495.84	102230
CJ2	1495.84	102230
23	854.77	102230
N1	747.92	102230
N2	1495.84	102230
N4	1495.84	102230
N5	1495.84	102230

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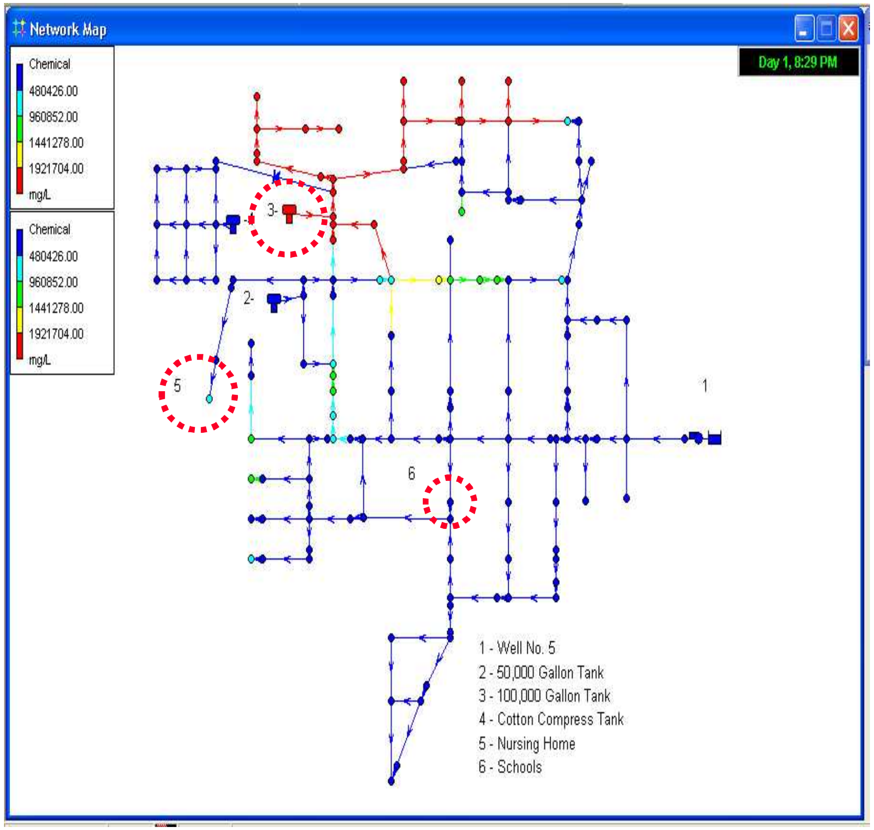
Exercise 4
Gideon Network

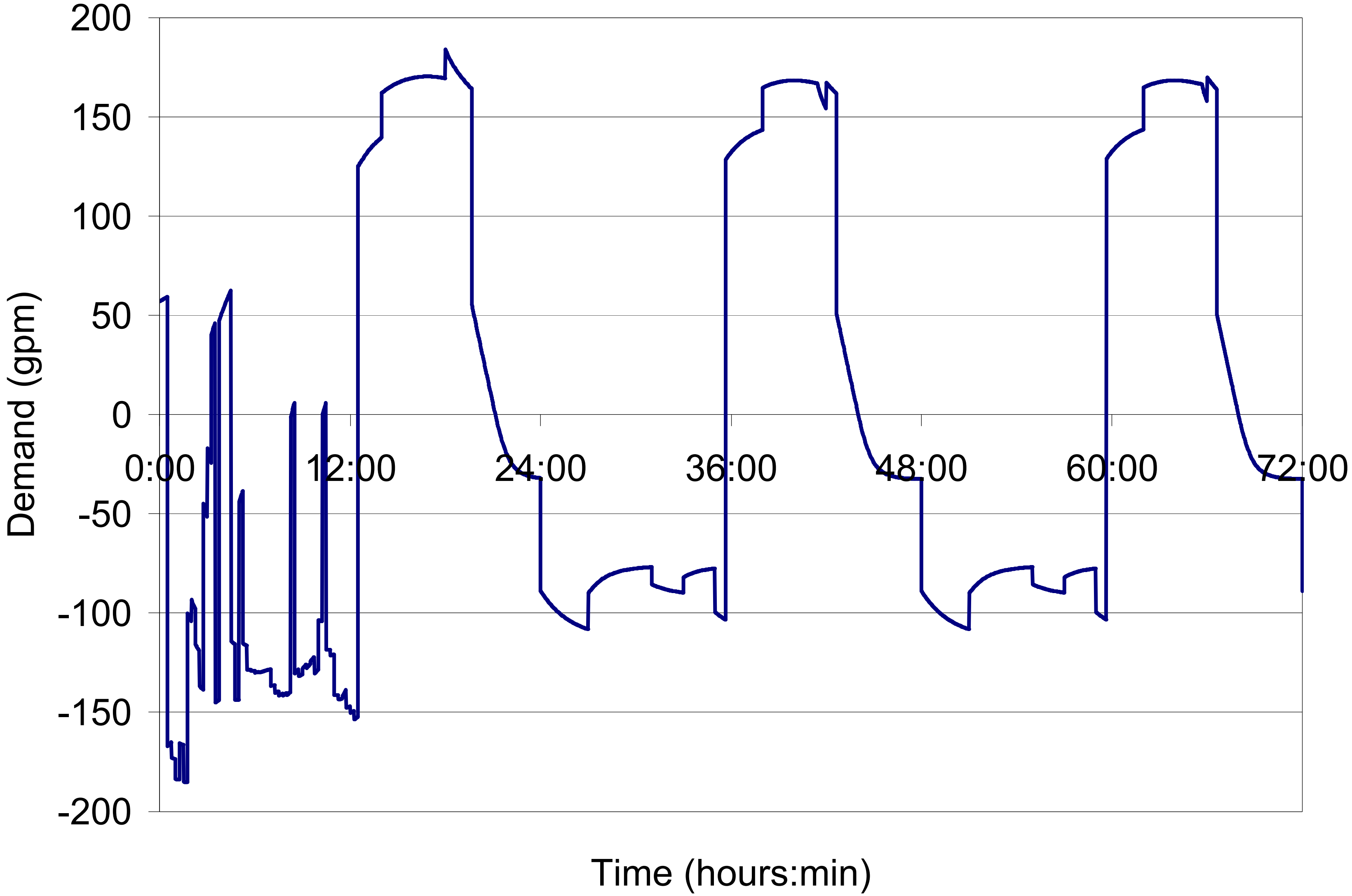
- **Municipal water network in Gideon, MO (1993, pop. 1100)**
  - **Bird feces in "Tank 300" was believed to be source of *Salmonella* contamination**
  - **Due to reports of bad taste and smell, city decided to flush network through hydrants, releasing contaminated water from tank**



(courtesy of L. Chandrasekaran, R. Herrick, R. Clark)

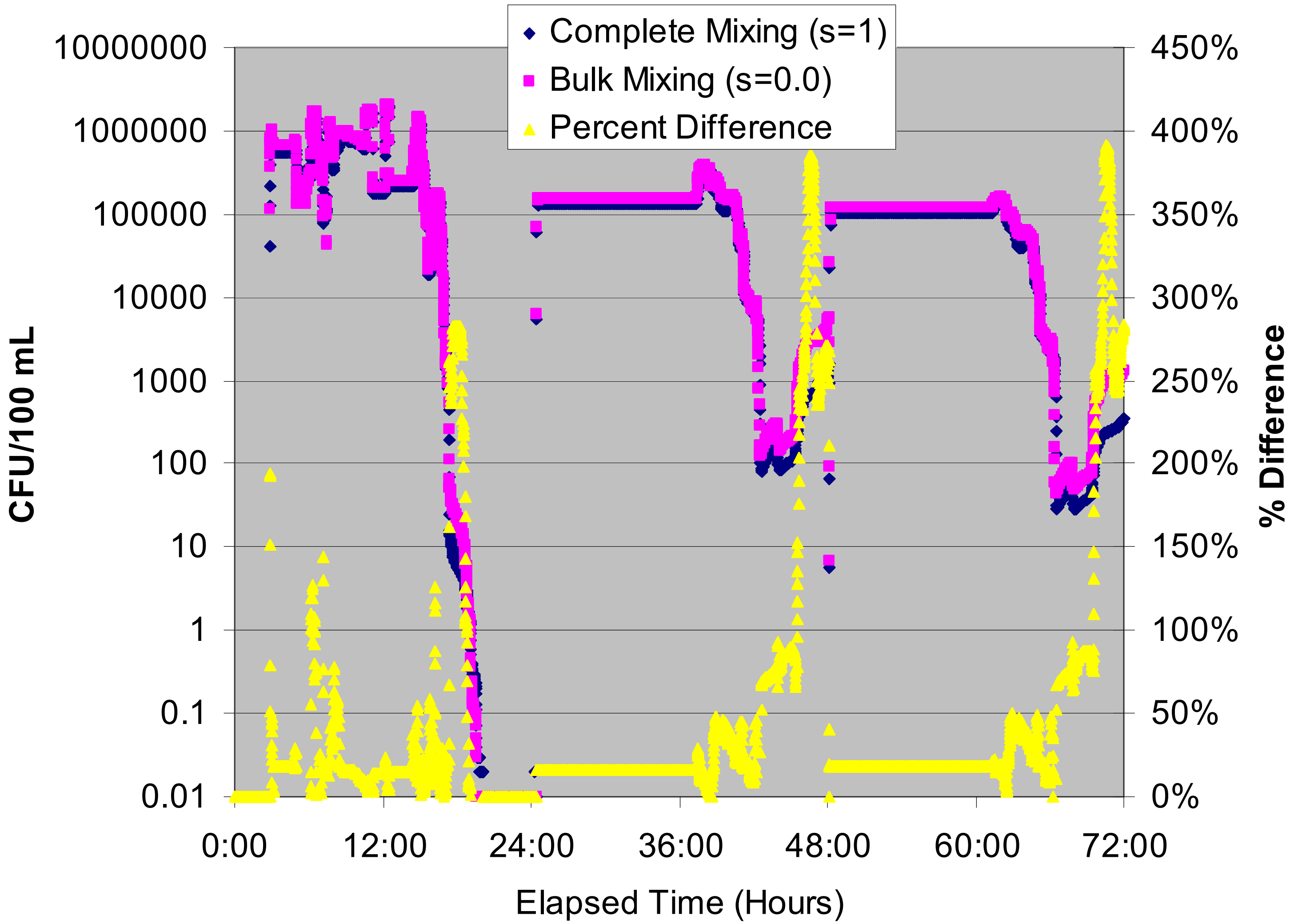
Exercise 4

"Tank 300 Demands"



Exercise 4

Model Comparisons – Junction 185 (Nursing Home)



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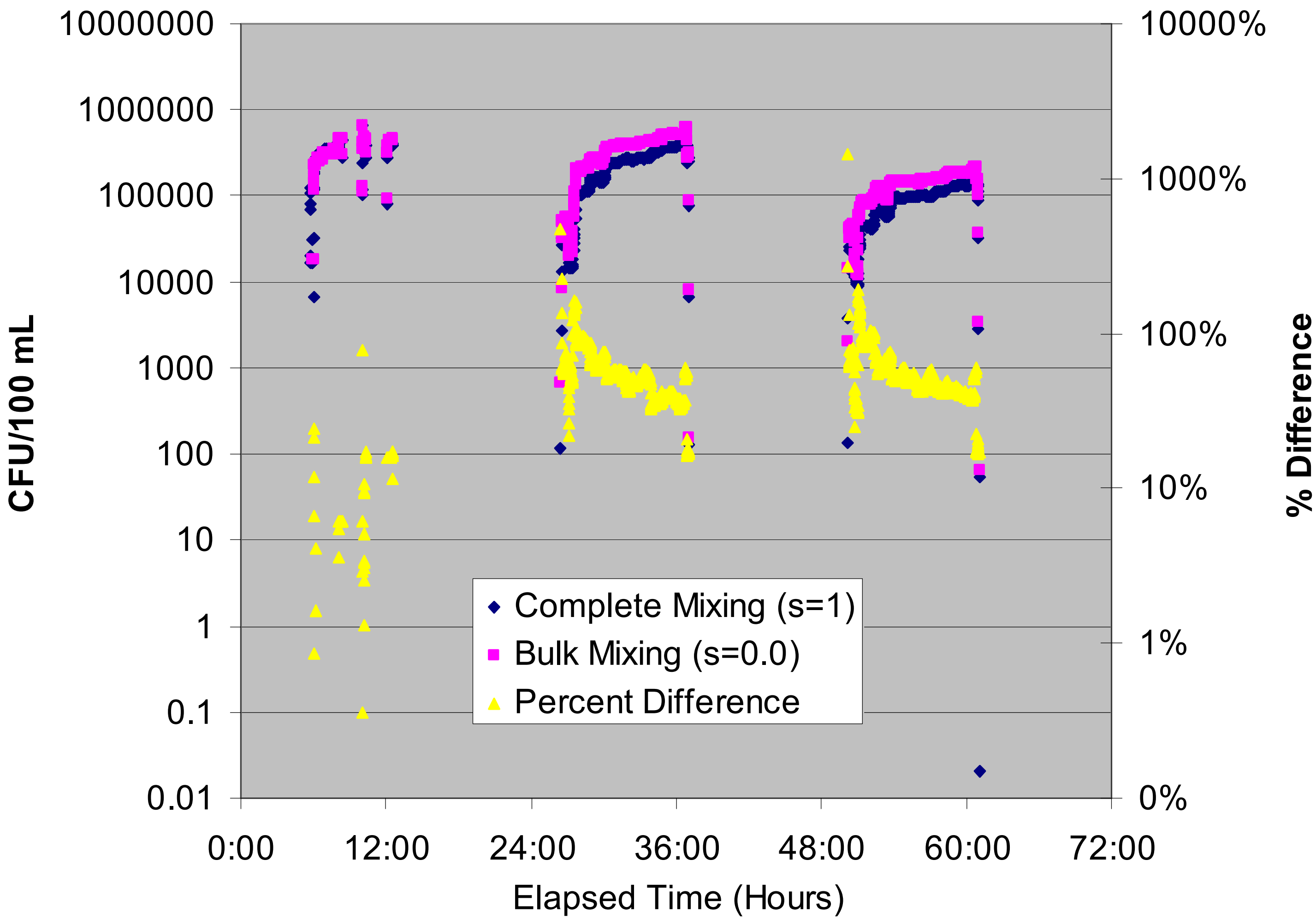
Exercise 4

Model Comparisons – Junction 41 (Schools)



Summary and Next Steps

Summary and Next Steps

- Bulk Advective Mixing (BAM) Model
  - Allows incomplete mixing at pipe junctions
    - Provides lower bound
  - Complements existing complete-mixing model for bounding calculations

- EPANET-BAM implements new model
  - Mixing parameter ($0 \le s \le 1$) can be applied to any junction
    - Values of s ~ 0.2-0.5 yielded good matches to data
  - All EPANET features functional with new model
  - Integration with PEST allows calibration and optimization (e.g., source detection)

Next Steps

- Use EPANET-BAM to guide development of network experiments
  - Compare results with storage and transients
  - Demonstrate capability to calibrate and/or optimize parameters (e.g., source detection, monitoring)
- Develop bulk mixing models for other junction configurations
- Incorporate BAM into EPANET-MSX?
- Release EPANET-BAM?

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  - Steve Webb (SNL), Bart Van Bloemen Waanders (SNL), Glen Hammond (SNL), Pedro Romero (U. Arizona), Chris Choi (U. Arizona)
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