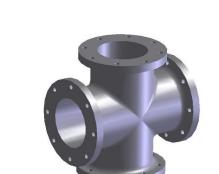
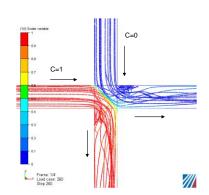
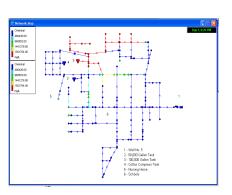


Cincinnati, OH, October 11, 2007

# A New Model for Solute Mixing in Pipe Junctions: Implementation of the Bulk Mixing Model in EPANET







### Clifford K. Ho and Siri Sahib S. Khalsa\*

Sandia National Laboratories Albuquerque, NM

\*Student at the University of Virginia

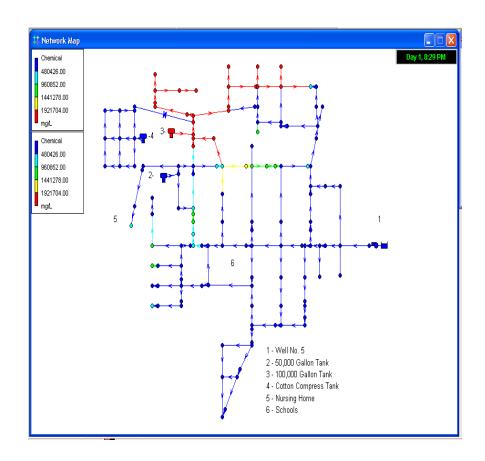


# Overview

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

# **Background - Motivation**

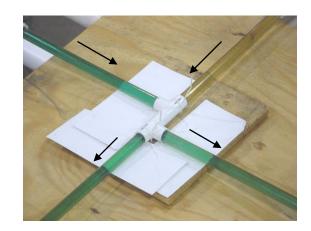
- Contaminant transport in water-distribution pipe networks is a growing concern
  - Mixing in junctions
  - Important for
    - Risk assessments
    - Vulnerability assessments
    - Inverse modeling (contaminant source detection, monitoring)





# **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)





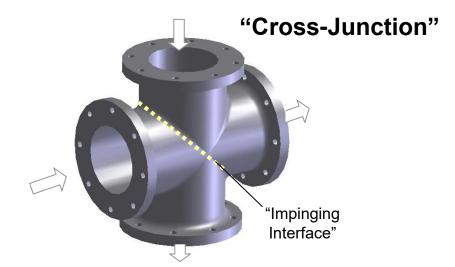
from Orear et al. (2005)

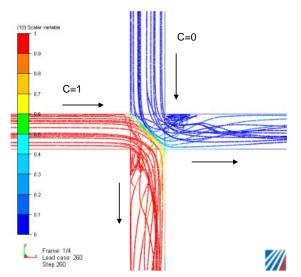




# **Objectives**

- 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







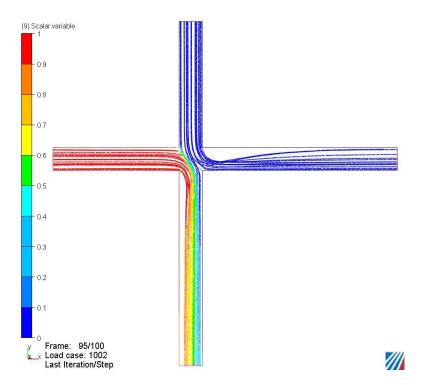
# **Overview**

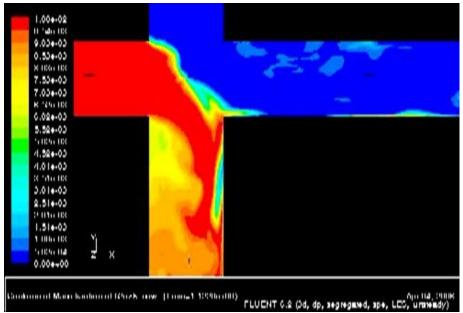
- Background
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# **Mixing in Pipe Junctions**

 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)

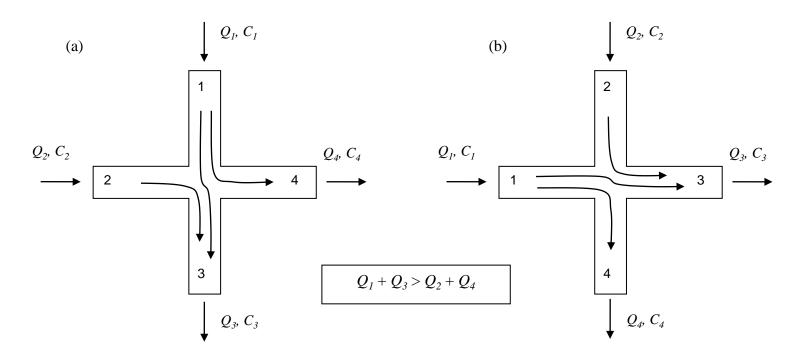




# **Bulk Mixing Model**

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

Honors conservation of momentum in the flow streams



$$C_3 = \frac{Q_2 C_2 + (Q_1 - Q_4) C_1}{Q_2} \qquad C_4 = C_1$$





# **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 ≤ s ≤ 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)



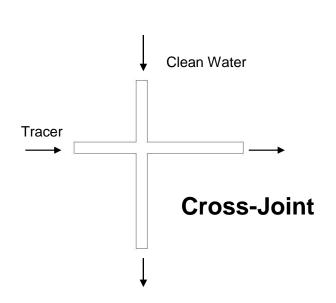
# **Overview**

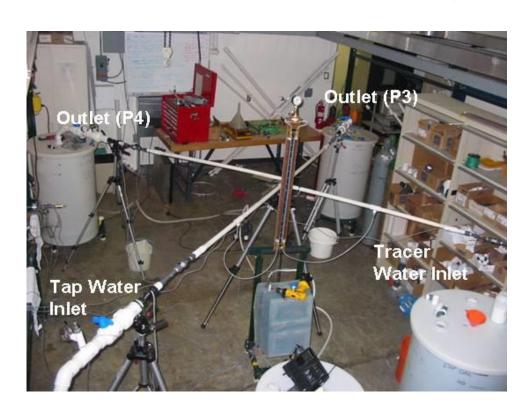
- Background
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# **Single-Joint Tests**

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



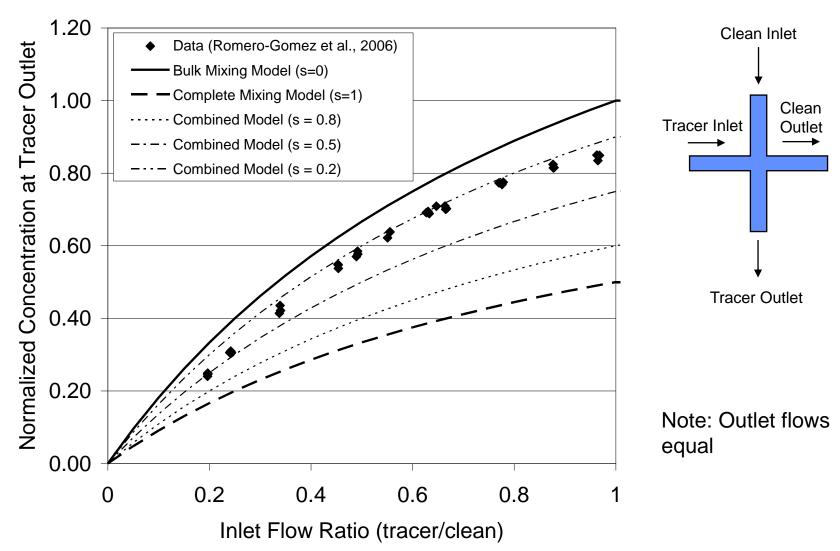


- Tracer consists of NaCl solution
- Tracer monitored continuously by electrical conductivity sensors
- Flow rate in each pipe was controlled
- Pipe diameters: 0.5", 1", 2"



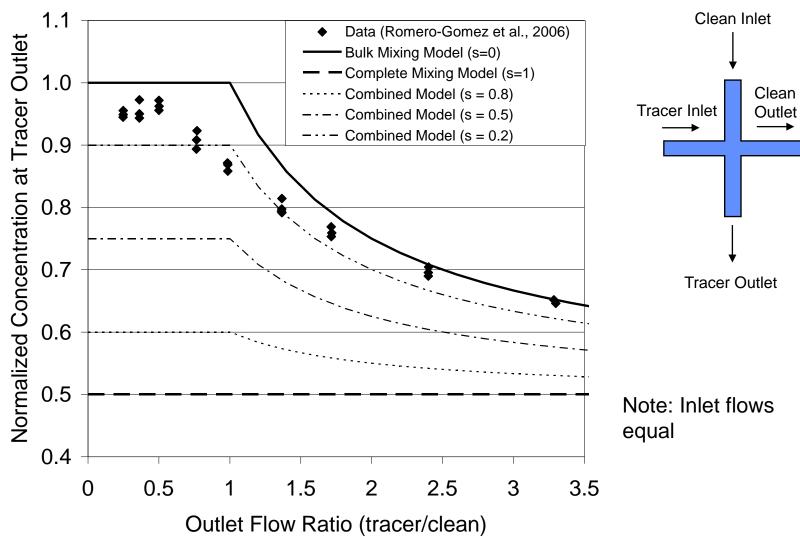
# **Single Cross-Joint Tests**

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



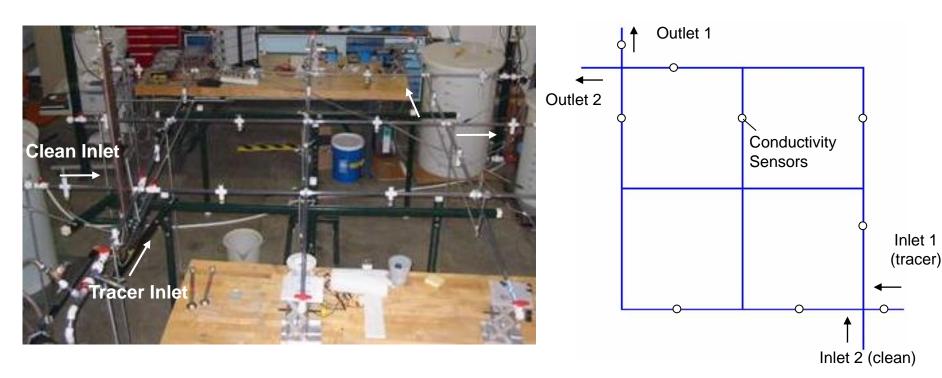
# **Single Cross-Joint Tests**

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



## **Multi-Joint Tests**

### (3x3 Small-Scale Network, Orear et al., 2005)

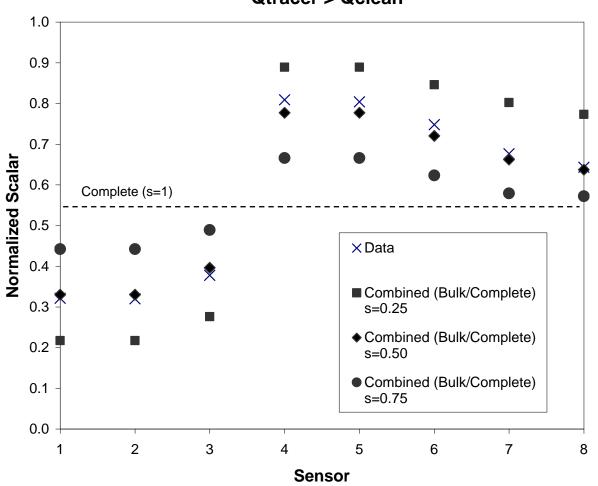


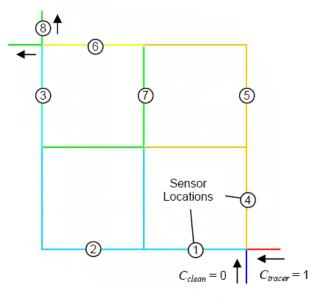
- 3x3 array of cross joints with 3-foot pipe lengths
- Flow rates at inlets and outlets controlled
- Pipe diameter: 0.5"



# **3x3 Network Tests**

#### **Qtracer > Qclean**

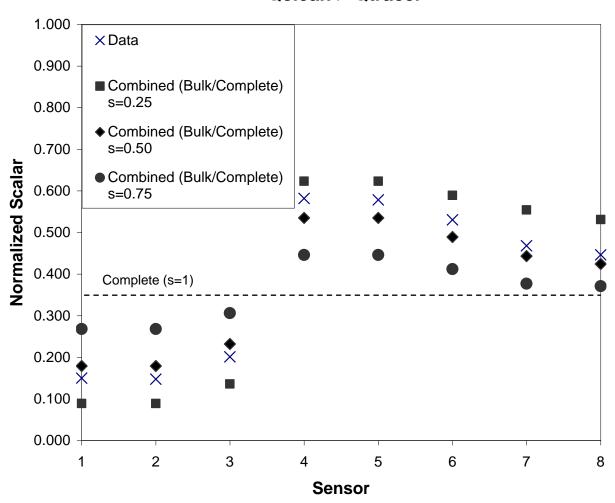


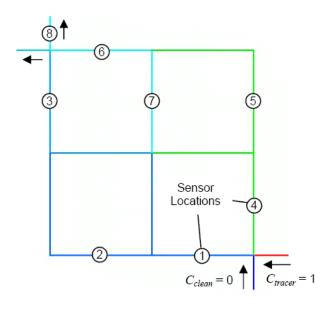




## **3x3 Network Tests**

#### **Qclean > Qtracer**









# **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)
    - $s \sim 0.2 0.5$  (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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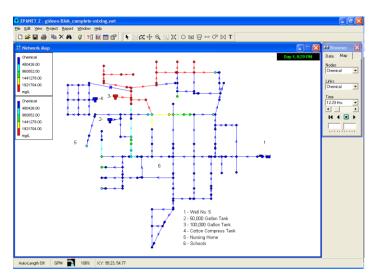




### **EPANET-BAM Features**

(Bulk Advective Mixing)

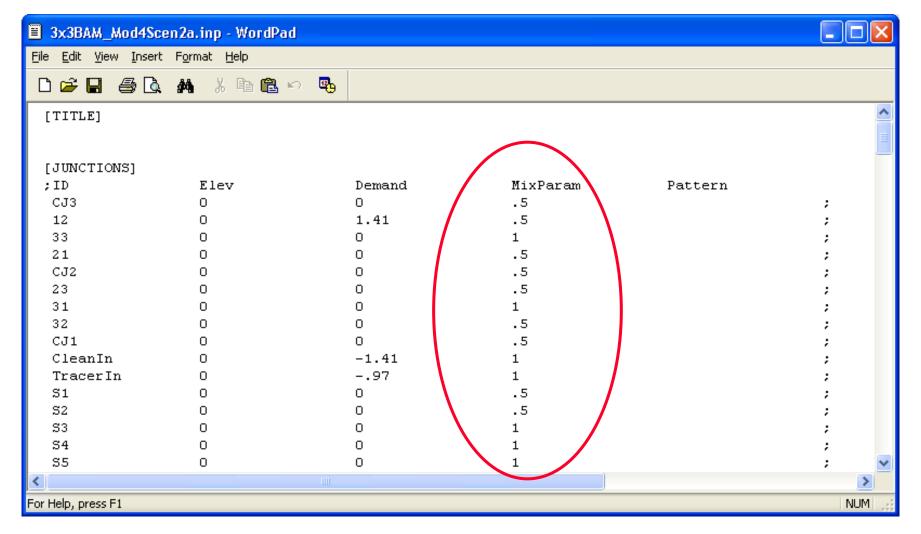
- Fully compatible with EPANET 2.0
  - New versions of 'Epanet2w.exe' and 'epanet2.dll'
  - GUI fully compatible
  - Mixing parameter can be adjusted at each junction
    - "Valid" cross junctions are analyzed with bulk-mixing model



Junction 140		2
Property	Value	
*Junction ID	140	
X-Coordinate	40.00	
Y-Coordinate	65.00	
Description		
Tag		
*Elevation	271	
Base Demand	1.819	
Mixing Parameter	0.5	
Demand Pattern	301	
Demand Categories	1	
Emitter Coeff.		
Initial Quality		
Source Quality		
Actual Demand	#N/A	
Total Head	#N/A	
Pressure	#N/A	
Quality	#N/A	



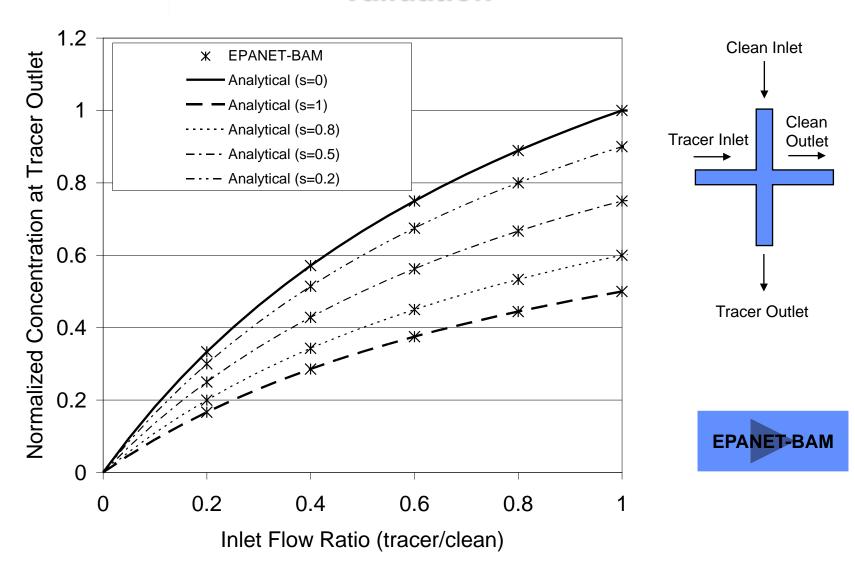
# Mixing Parameter Stored in Input File





# **EPANET-BAM**

### **Validation**





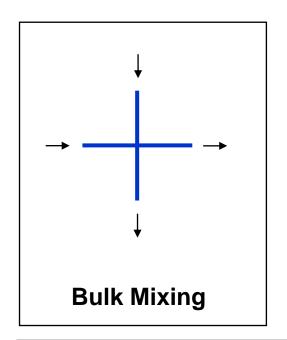
# **EPANET-BAM Applications**

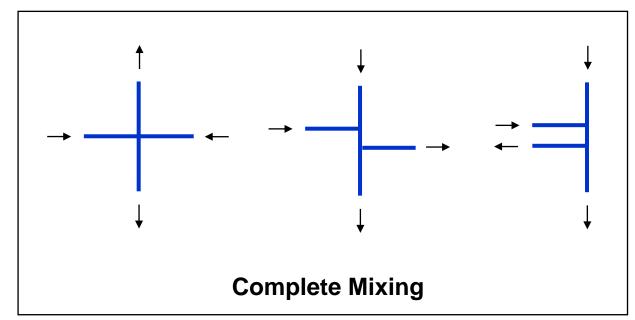
- Hydraulic and water quality simulations with incomplete mixing at junctions (bulk mixing, s < 1)</li>
  - Steady and transient
  - Bounding calculations for risk assessments
    - s=0, s=1
- Integration with PEST (Parameter ESTimation Software; <u>www.sspa.com/pest/</u>)
  - Calibration of mixing parameter at one or more junctions based on available concentration data
  - Contaminant source detection with sparse data





- 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



# Overview

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



## **EPANET-BAM Demonstrations**

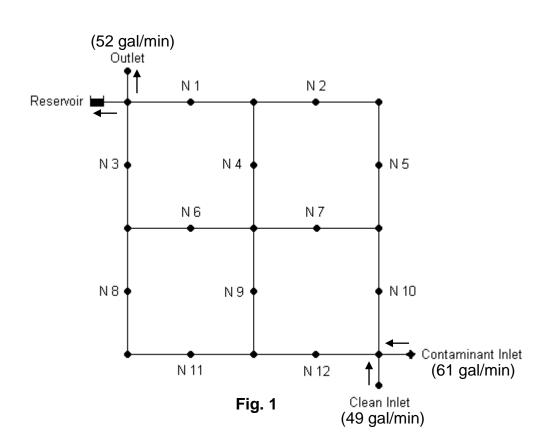
- Exercise 1: Steady contamination
- Exercise 2: Transient contamination
- Exercise 3: Source Detection
- Exercise 4: Gideon Network



# **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



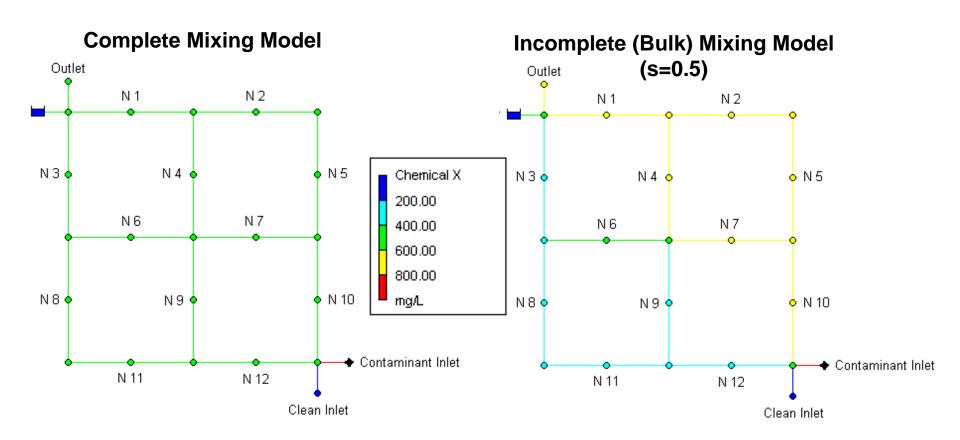
Note: simulated network is an up-scaled replica of a smaller network tested in the laboratory





# **Exercise 1**

### **Predicted Concentration Distributions**

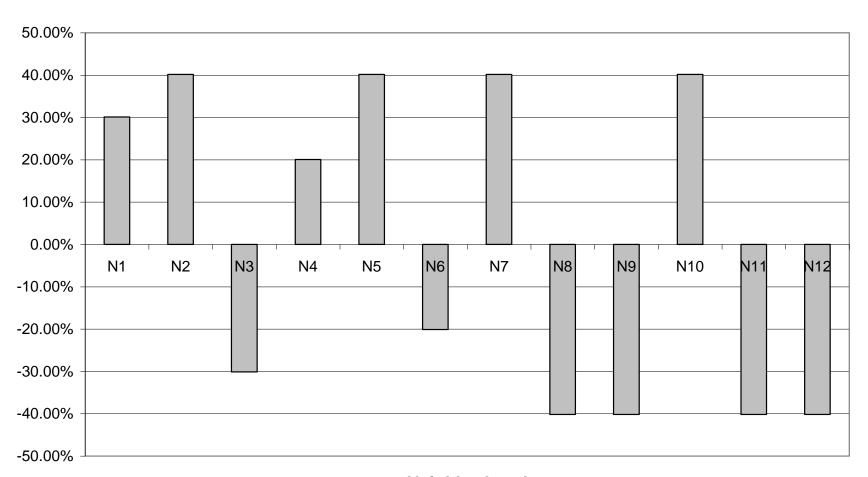






### **Concentration Differences**

### Neighborhood Concentration Differences between Bulk (s=0.5) Mixing Model and Complete Mixing Model

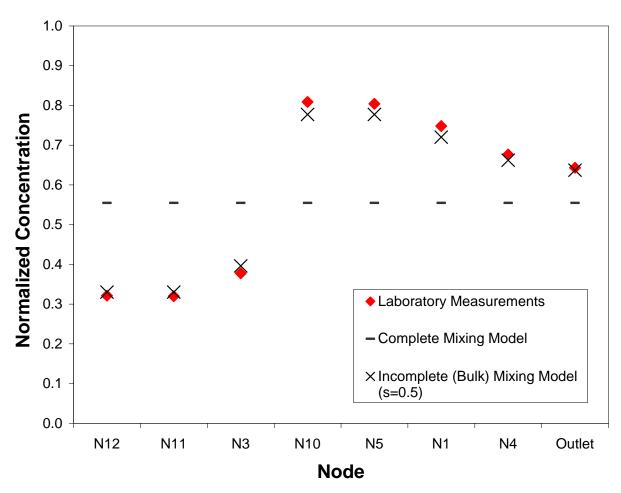


Neighborhood



# **Exercise 1**Comparison to Laboratory Experiments

#### **Concentrations at Selected Nodes**



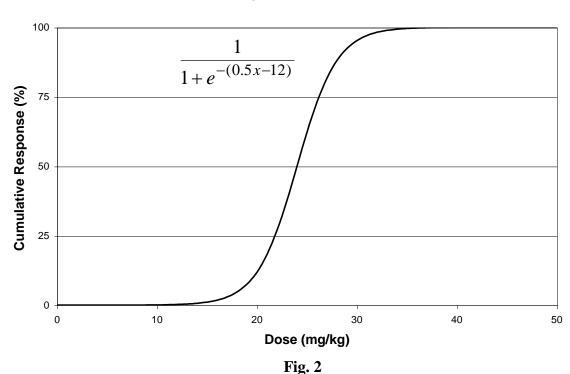




# Exercise 1 Risk Assessment

- 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

#### **Lethal Dose Response Curve - Chemical X**



# **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

<b>Predicted Death</b>	60
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	266
Toll:	366



# **EPANET-BAM Demonstrations**

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

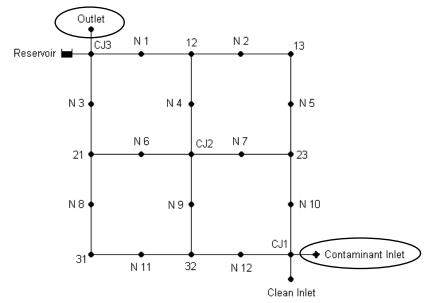


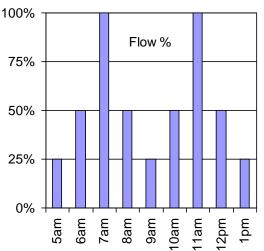
# **Exercise 2**

### **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

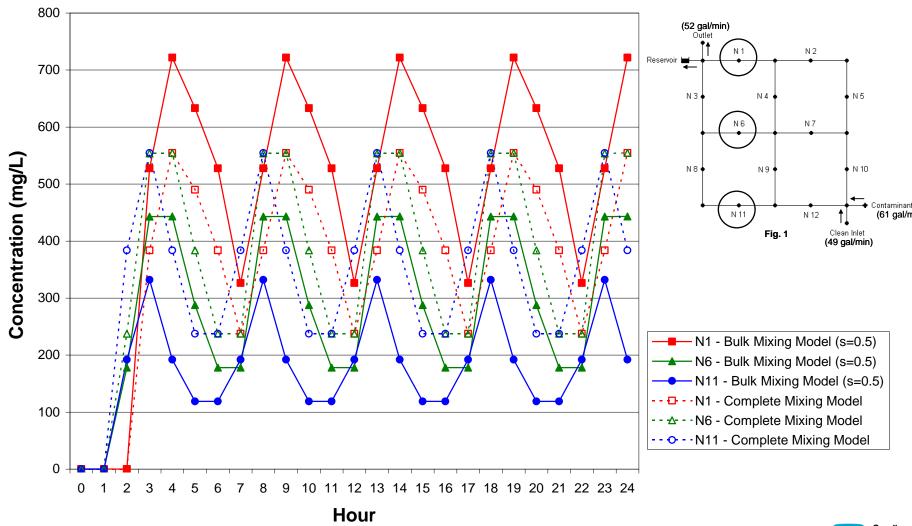






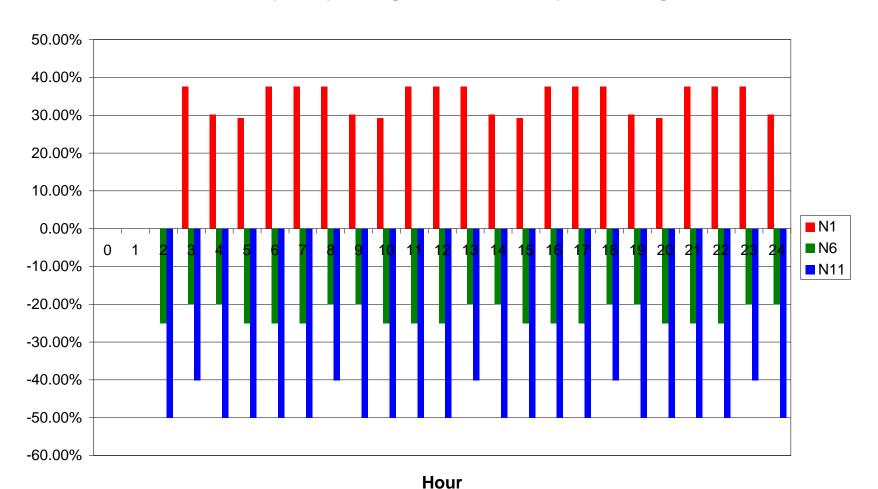
## **Exercise 2**

### **Transient Concentrations at N1, N6, and N11**



### **Concentration Differences**

# Transient Neighborhood Concentration Differences between Bulk (s=0.5) Mixing Model and Complete Mixing Model





### **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



### **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	0
Toll / 12 hours:	

Predicted Death Toll	36
/ 12 hours:	



# **EPANET-BAM Demonstrations**

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





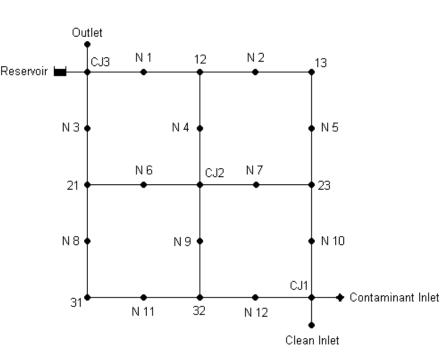
# **Exercise 3**Source Detection

- 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



### **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

Ou	itlet					
voir 🛏 🛶	слз	N 1	12	N 2	13	
N 3 •	•		N 4		• N €	5
21 •		N 6	CJ2	N 7	23	
N 8 •			N 9 <b>•</b>		N ·	10
31		N 11	32	N 12	CJ1	◆ Contaminant Inlet
					Clean Inle	t

Complete Mixing Model					
Node	Source Conc.				
ID	(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		



## **EPANET-BAM Demonstrations**

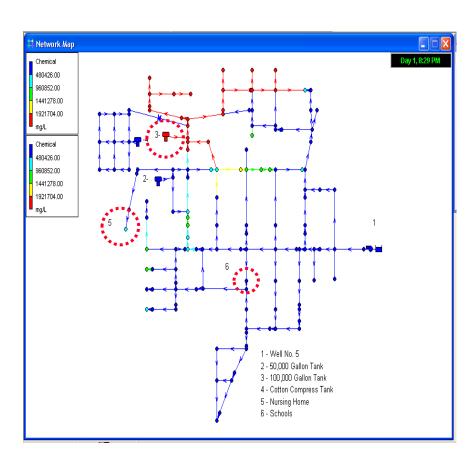
- Exercise 1: Steady contamination
- Exercise 2: Transient contamination
- Exercise 3: Source Detection
- Exercise 4: Gideon Network





# Exercise 4 Gideon Network

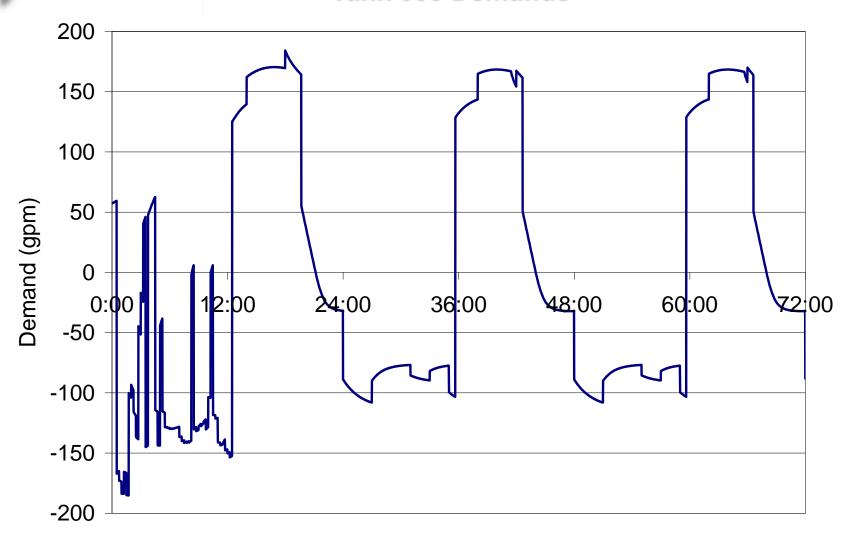
- Municipal water network in Gideon, MO (1993, pop. 1100)
  - Bird feces in "Tank 300" was believed to be source of Salmonella contamination
  - Due to reports of bad taste and smell, city decided to flush network through hydrants, releasing contaminated water from tank



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



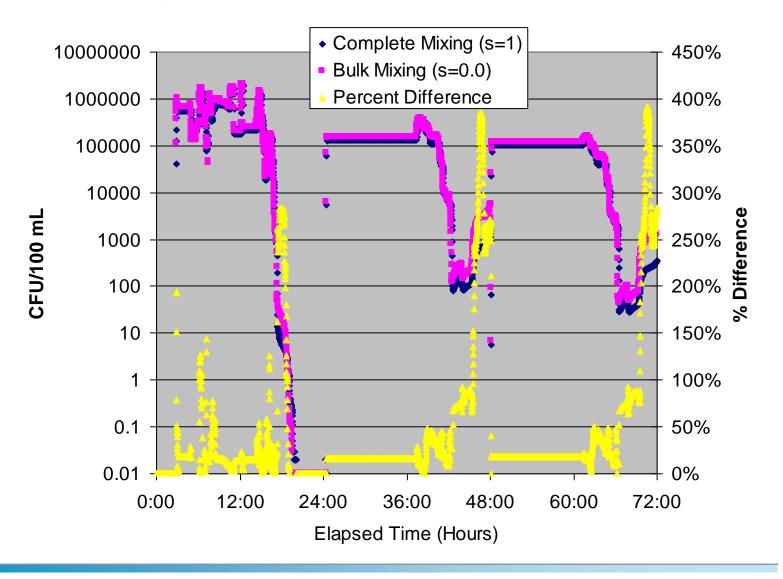
"Tank 300 Demands"



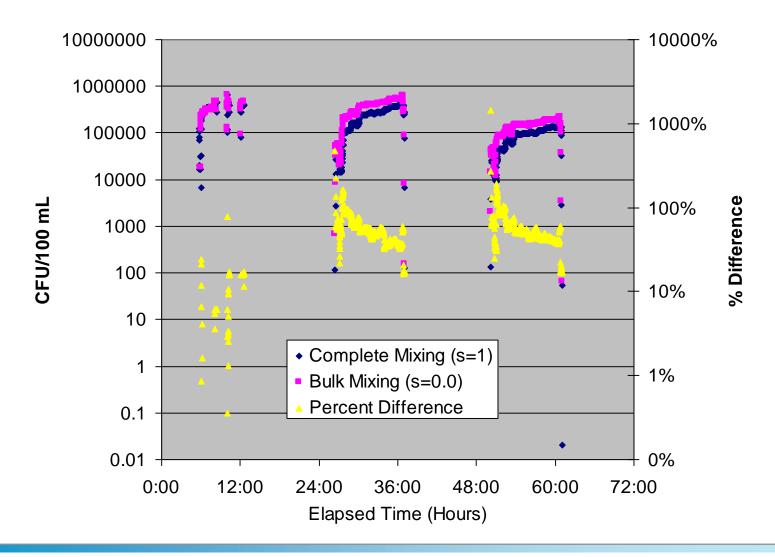
Time (hours:min)



### **Model Comparisons – Junction 185 (Nursing Home)**



# **Exercise 4**Model Comparisons – Junction 41 (Schools)



# **Summary and Next Steps**



# **Summary**

- 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 ≤ s ≤ 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?





# **Acknowledgments**

### Modeling

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

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Lee O'Rear, Jr. (SNL), Jerome Wright (SNL),
 Malynda Aragon (SNL), Sean McKenna (SNL), Ryan
 Austin (U. Arizona), Chris Choi (U. Arizona)

### Management

Ray Finley (SNL), Amy Sun (SNL)

