EPANET Multispecies Extension to Model Advection-Dispersion-Reaction within Water Distribution System

2022 World Environmental & Water Resources Congress
June 6-8, 2022

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Presentation Outline

- Water Quality Modeling in Distribution System: Lagrangian approach
- Multispecies Reaction with Dispersion
- Other EPANET-MSX updates
- Application Demo

Water Quality: Transport Equation

- General transport equation: Advection – Dispersion – Reaction (ADR)
  - Governing partial differential equation (PDE)

Advection **Dispersion** **Reaction**

$$\frac{\partial C_k}{\partial t} = -v\frac{\partial C_k}{\partial x} + D\frac{\partial^2 C_k}{\partial x} + f(C_1, C_2, \dots C_n)$$

  - Both hyperbolic and parabolic.

  - D is the effective dispersion coefficient in the longitudinal direction

Water Quality Modeling with EPANET-MSX

- Lagrangian Approach
- Time Driven
- Dispersion was ignored

$$\frac{\partial C_i}{\partial t} = -v\frac{\partial C_i}{\partial x} + D\frac{\partial^2 C_i}{\partial x^2} + f(C_1, C_2, \ldots C_n)$$

Shang, F., Uber, J. G. & Rossman, L. A. Modeling reaction and transport of multiple species in water distribution systems. Environ. Sci. Technol. ***42****(3), 808–814 (2008).*

Shang, F., J. G. Uber, AND L. Rossman. EPANET Multi-Species Extension Software and User's Manual. U.S. Environmental Protection Agency, Washington, DC, EPA/600/C-10/002, 2011.

EPANET-MSX Update

1. Developed an approach to add dispersion within EPANET-MSX
   - Fully Lagrangian
   - Operator Splitting
   - Dispersion as an option defined in the MSX input file
2. Implemented the topological WQ routing and provide mass balance report as in EPANET 2.2
3. Implemented OPENMP to parallelize the MSX solver

Lagrangian Approach

- Little numerical diffusion
- Easy to understand
- Simple to implement
- No fixed computation grid is required

Rossman, L. A. & Boulos, P. F., 1996. Numerical methods for modeling water quality in distribution system: A comparison. Journal of Water Resource Planning and Management, pp. 137-146.

Topological Routing in EPANET2.2

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + f(C)$$

- In EPANET 2.0, water quality routing is implemented in an arbitrary order (according to link/node indices). With large time step and small link volumes, mass balance error can be significant.

  Davis, M. J., Janke, R., and Taxon, T. N. 2018. "Mass imbalances in EPANET water-quality simulations", Drinking Water Engineering and Science, Vol. 11, pp. 25-47.

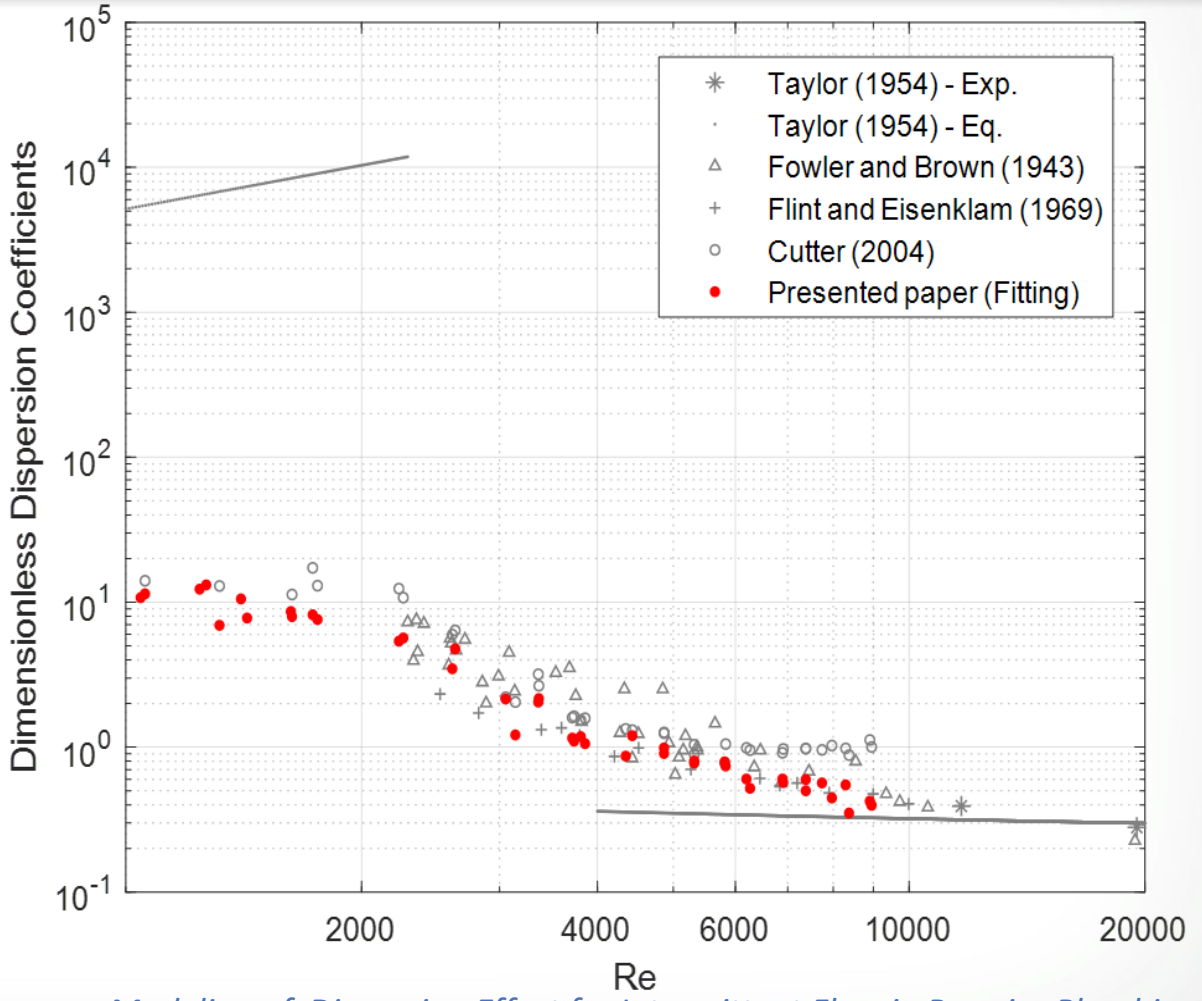
- In EPANET 2.2, nodes are sorted topologically whenever hydraulic conditions change and the water quality routing is from upstream nodes to downstream nodes. Therefore, there is no mass loss or creation during the WQ routing.

- Mass balance report is provided in EPANET 2.2.

- EPANET-MSX now implements the new Lagrangian Time Driven transport method as in EPANET 2.2 and provides mass balance report for all the RATE species.

Dispersion in Water Distribution System

- Dispersion can be reasonably ignored for most parts of a water distribution system.
- In dead end regions and premise plumbing systems, dispersion may play an important role in constituent transport.
- Relative importance of the dispersion depends on the Reynolds number.



Modeling of Dispersion Effect for Intermittent Flow in Premise Plumbing Systems. H. Woo, et al. WDSA/CCWI, Kingston, Canada, 2018.

Operator Splitting

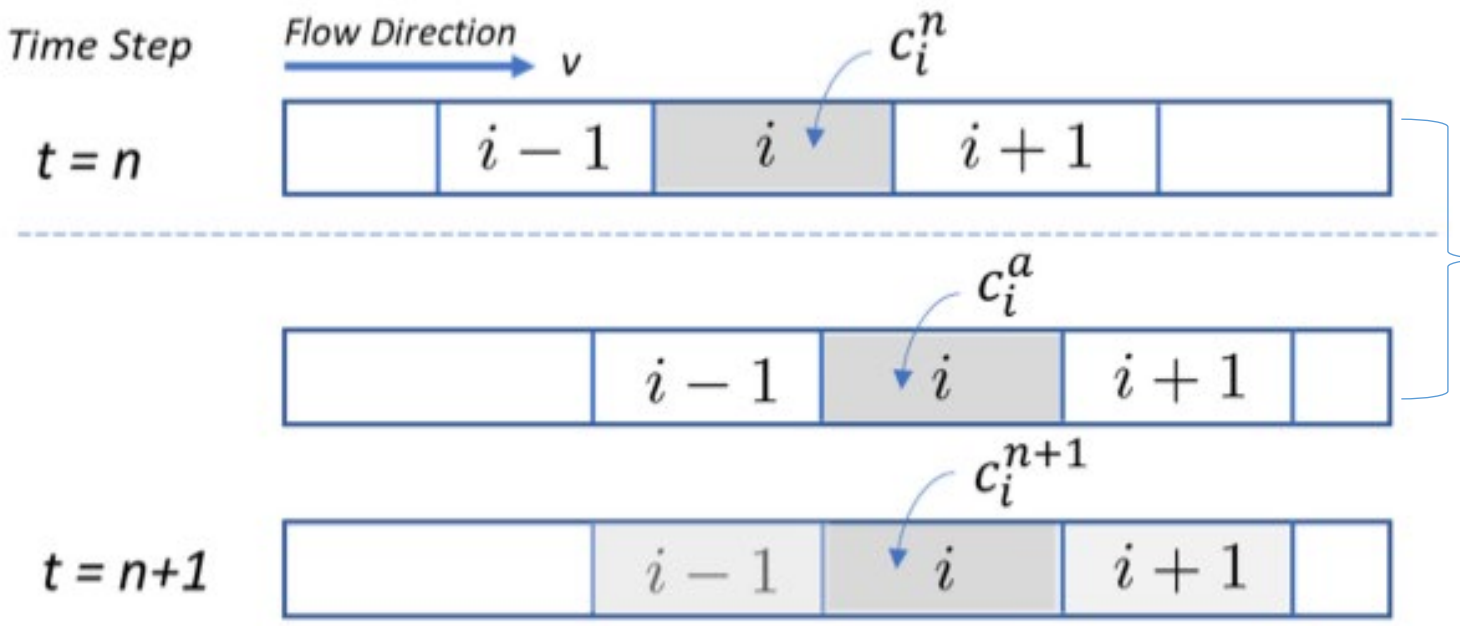
$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + f(C)$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x}$$

Advection and Reaction processes are solved first

Advection processes is solved next

Lagrangian Approach for MSX



EPANET/MSX

EPANET/MSX with Dispersion

Solving the Dispersion Equation

To solve the dispersion equation: $\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x}$

F. Shang, H. Woo, J. B. Burkhardt, and R. Murray, "Lagrangian method to model advection-dispersion-reaction transport in drinking water pipe networks," Journal of Water Resources Planning and Management, vol. 147, no. 9, p. 04021057, 2021.

- Segment centered discretization: same discretization as in EPANET, fixed computational grid is not needed.
- Linear relationship between internal segment concentration and junction concentrations is established for every pipe by solving tridiagonal matrices.
- Equal flux internal boundary conditions were applied to the network junctions.
- A ***symmetrical*** matrix is constructed for junction concentrations and EPANET's sparse matrix solver is used to calculate the concentration at junctions.

Parallelization

- For each time step, the differential algebraic equations (DAE) can be solved parallelly for the pipes.
- For each time step, the dispersion solver is also solved parallelly for the pipes.
- Solving dispersion process is much less expensive compared to solving a relatively complex DAE system.
- OPENMP is easy to implement within Visual C.
- Up to 60% computational time reduction is achieved in simulation studies.

Runtime Compilation: Not New in MSX

- In EPANET-MSX, most of the computational time is on solving the DAEs.
- The reaction kinetics are defined in an input file. The inputs are parsed, and expression trees are built and evaluated during runtime. The evaluation through expression tree is slow.
- If the reaction kinetics are hard coded, the simulation is much faster.
- EPANET-MSX has the option to compile the reaction equations using a C compiler that already resides on the user's system.
- This runtime compilation option is NOT new.
- What is new: the MSX application can now automatically find the installed C compiler and set up the environmental variables to run the compilation.

Application Demo – MSX Model

Table 5-1 Monochloramine decay model based on Vikesland et al. (2001) and Duirk et al. (2005).

	Reaction Stoichiometry	*Rate Coefficient/ Equilibrium Constant*[a]
R.1	$HOCl + NH_3 \rightarrow NH_2Cl + H_2O$	$k_1 = 1.5\times10^{10}\ M^{-1}h^{-1}$
R.2	$NH_2Cl + H_2O \rightarrow HOCl + NH_3$	$k_2 = 7.6\times10^{-2}\ h^{-1}$
R.3	$HOCl + NH_2Cl \rightarrow NHCl_2 + H_2O$	$k_3 = 1.0\times10^{6}\ M^{-1}h^{-1}$
R.4	$NHCl_2 + H_2O \rightarrow HOCl + NH_2Cl$	$k_4 = 2.3\times10^{-3}\ h^{-1}$
R.5	$NH_2Cl + NH_2Cl \rightarrow NHCl_2 + NH_3$	$k_5 = 2.5\times10^{7}\ [H^+] + 4.0\times10^{4}\ [H_2CO_3] + 800\ [HCO_3^-]\ M^{-2}h^{-1}$
R.6	$NHCl_2 + NH_3 \rightarrow NH_2Cl + NH_2Cl$	$k_6 = 2.2\times10^{8}\ M^{-2}h^{-1}$
R.7	$NHCl_2 + H_2O \rightarrow I$	$k_7 = 4.0\times10^{5}\ M^{-1}h^{-1}$
R.8	$I + NHCl_2 \rightarrow HOCl + products$	$k_8 = 1.0\times10^{8}\ M^{-1}h^{-1}$
R.9	$I + NH_2Cl \rightarrow products$	$k_9 = 3.0\times10^{7}\ M^{-1}h^{-1}$
R.10	$NH_2Cl + NHCl_2 \rightarrow products$	$k_{10} = 55.0\ M^{-1}h^{-1}$
R.11	$NH2Cl + S_1\times TOC \rightarrow products$[b]	$k_{11} = 3.0\times10^{4}\ M^{-1}h^{-1}$ $S_1 = 0.02$
R.12	$HOCl + S_2\times TOC \rightarrow products$[c]	$k_{12} = 6.5\times10^{5}\ M^{-1}h^{-1}$ $S_2 = 0.5$
E.1	$HOCl \leftrightarrow H^+ + OCl^-$	$pK_a = 7.5$
E.2	$NH_4^+ \leftrightarrow NH_3 + H^+$	$pK_a = 9.3$
E.3	$H_2CO_3 \leftrightarrow HCO_3^- + H^+$	$pK_a = 6.3$
E.4	$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$	$pK_a = 10.3$

Notes:

a. All rate coefficients and equilibrium constants are for 25 degrees C.
b. S_1 is the fast reactive fraction of TOC.
c. S_2 is the slow reactive fraction of TOC.

Application Demo – Input File

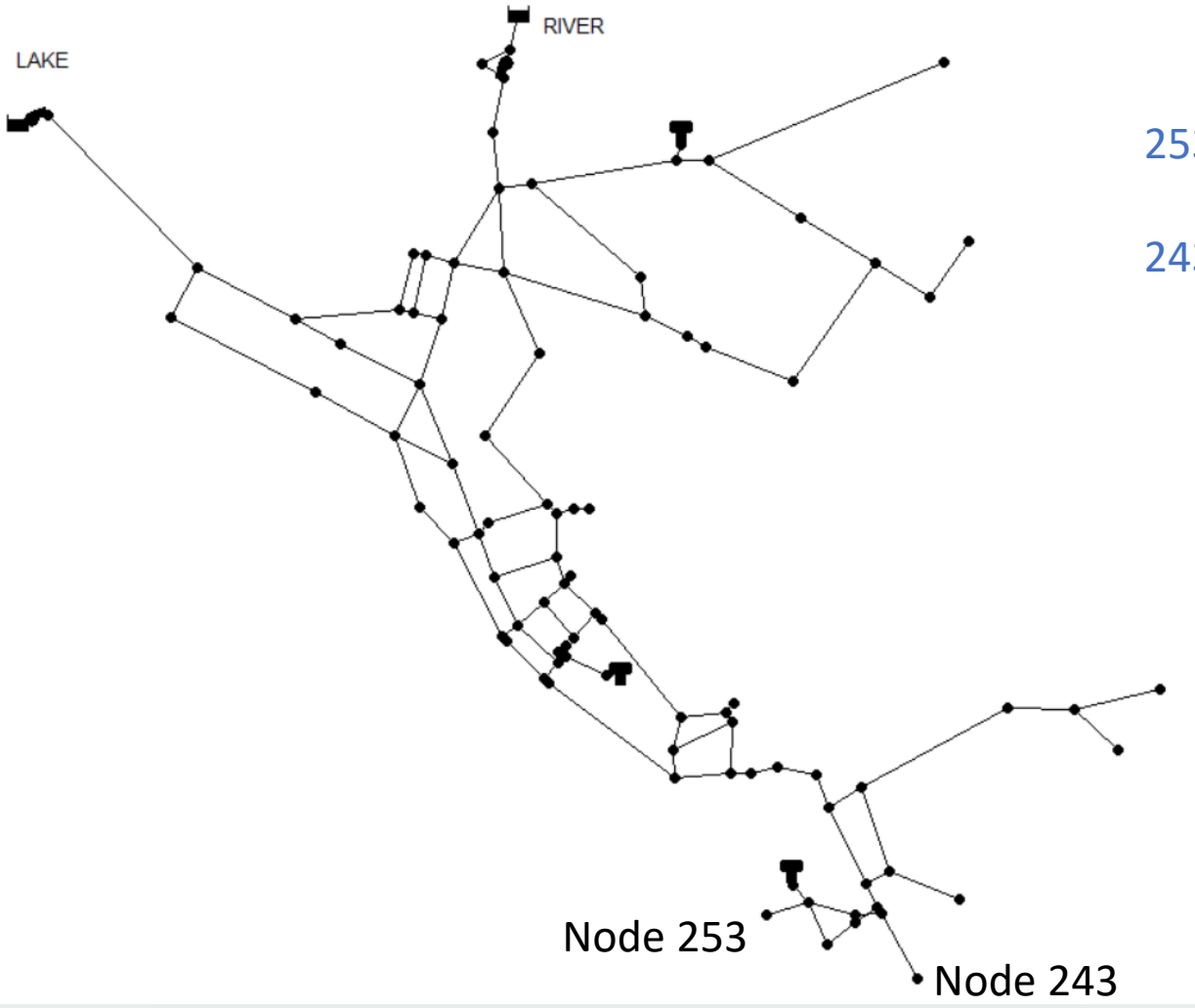
```
[TITLE]
NET3 Chloramine Decay Example

[OPTIONS]
AREA_UNITS  FT2
RATE_UNITS  HR
SOLVER      ROS2
COUPLING    NONE
TIMESTEP    60
RTOL        0.0001
ATOL        1.0e-8
COMPILER    VC
```

```
[DISPERSION]
HOCL 1.0
NH3 1.0
NH2CL 1.0
NHCL2 1.0
I 1.0
H 1.0
ALK 1.0
TOC 1.0
```

Relative diffusivity
Times of $1.2*10^{-9}$ m^2/s

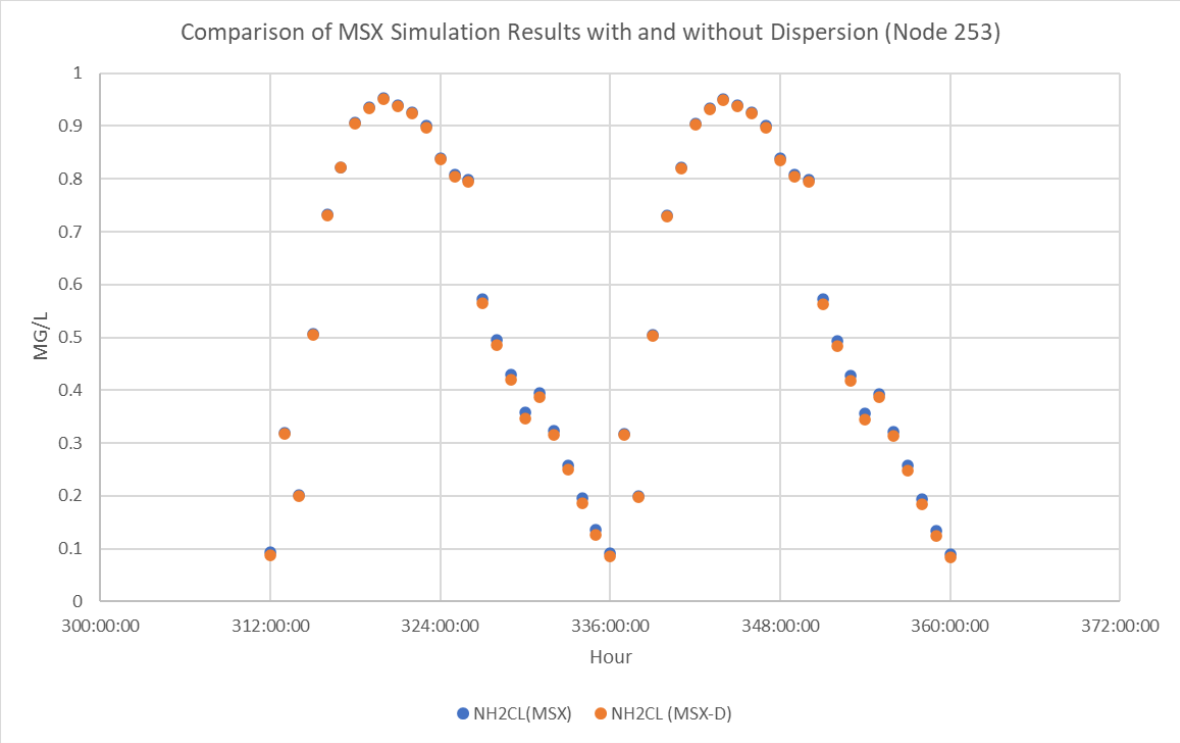
Application Demo - Network

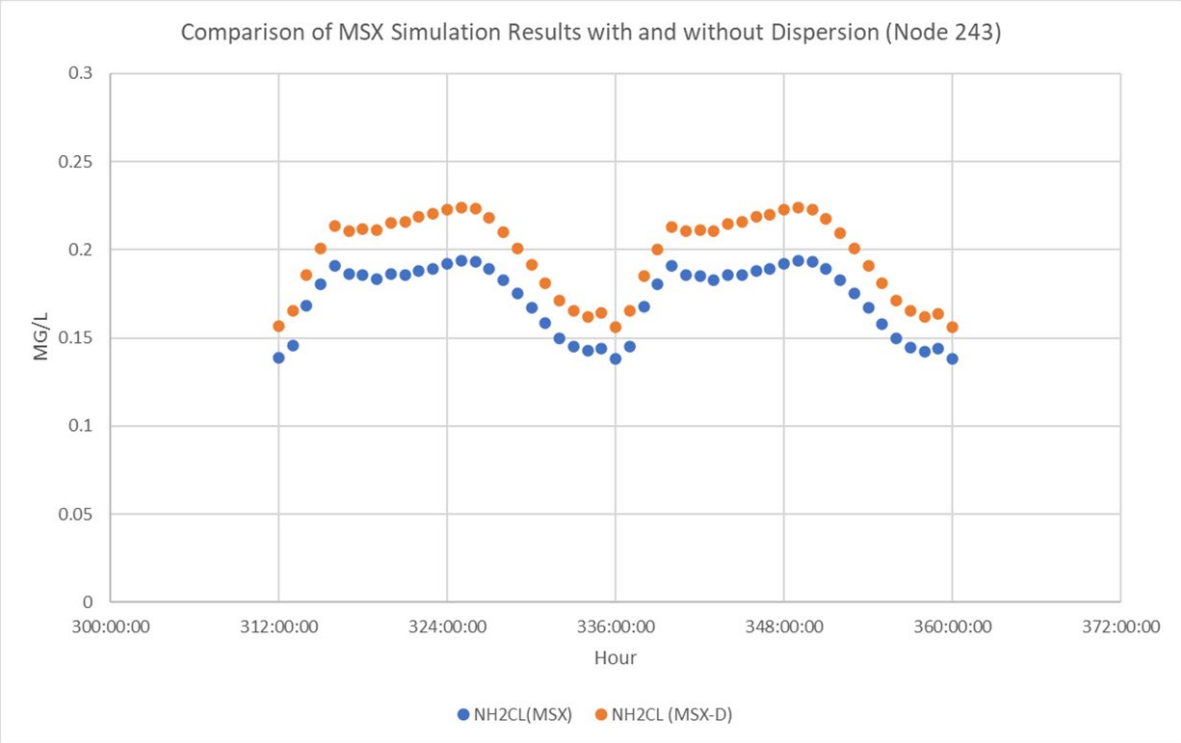


253 Base demand 54.5 GPM

243 Base demand 4.3 GPM

Application Demo – Results





Application Demo – Mass Balance

Water Quality Mass Balance: NH2CL (MMOL)

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Initial Mass:	0.00000e+00
Mass Inflow:	4.48429e+04
Mass Outflow:	2.89633e+04
Mass Reacted:	-1.53565e+04
Final Mass:	5.23105e+02
Mass Ratio:	1.00000

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Application Demo – Computational Cost

NET3 Chloramine Decay Example
WQ time step = 60 seconds

	OpenMP	Dispersion	Computational Time (s)
No	No	No	81
No	No	Yes	85
No	Yes	Yes	44
Yes	Yes	Yes	20

Conclusion

- Dispersion solver is added into the EPANET-MSX. It is an option to include the dispersion into the water quality modeling.
- OPENMP and Run time compilation can speed up the simulation significantly.
- Better mass balance through topological routing as in EPANET 2.2 and mass balance report is provided.
- The new EPANET-MSX with dispersion will be released in the fall.

Disclaimer

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Questions?

https://github.com/usepa/epanetmsx/tree/dev

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