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# Adding Multispecies Water Quality Reactions to Resilience Modeling Tools



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# Why do we need multispecies modeling?

**Contaminants of Concern are usually reactive**

- Lead (widespread; e.g., *Flint MI*)
- Arsenic (nationwide; AZ, NM, NV, UT specifically)
- Bacteria (worldwide; e.g., *e coli.*)

**Challenges of multispecies modeling**

- Parameters from lab do not always reflect system
- Slow, computationally expensive
- Manual intervention

# WNTR / EPANET-MSX Integration

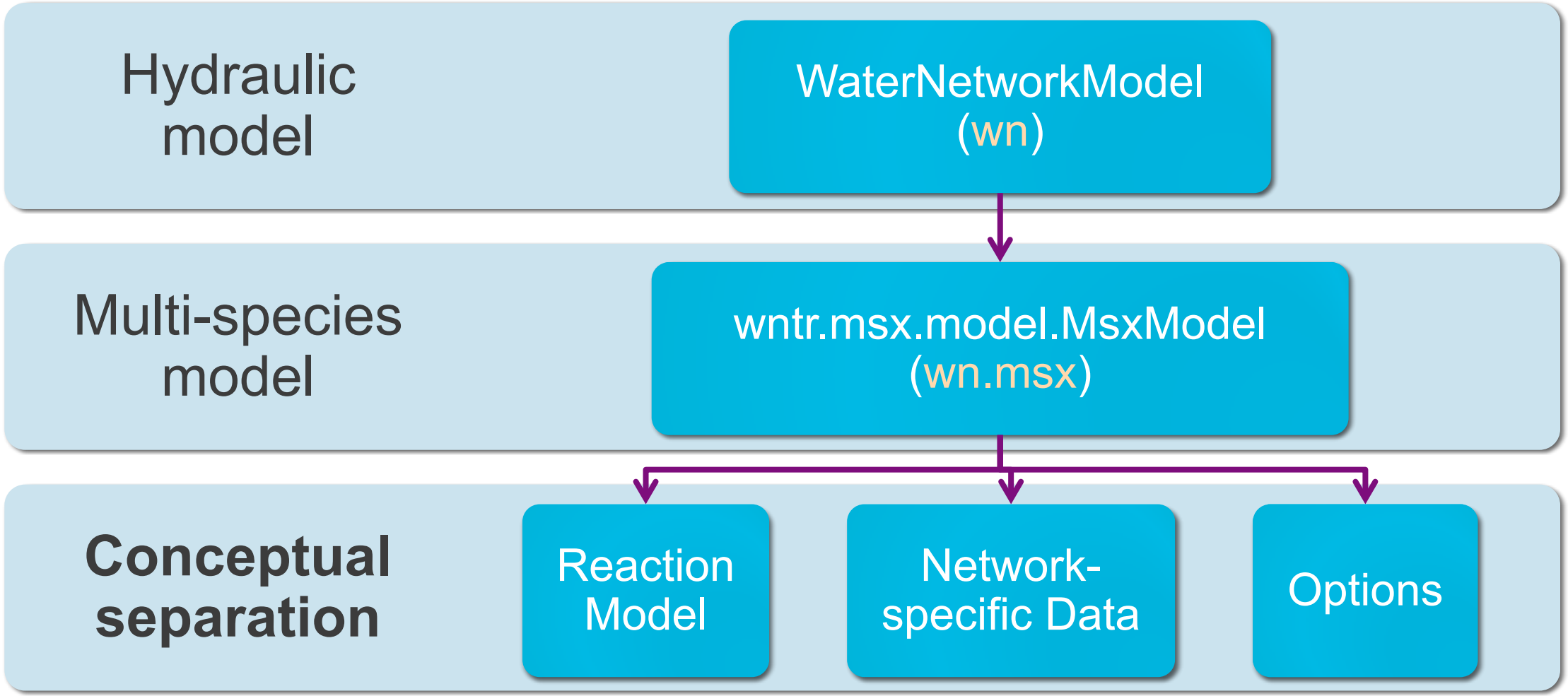
# WNTR + EPANET-MSX

## Requirements

- Read/write EPANET-MSX input files
- Similar style to WNTR
- Library of reactions
- Result-object integration
  - Direct use with existing metrics
- Well-defined JSON format / schema

```
[SPECIES]
  BULK AS3   UG              ;Dissolved arsenite
  BULK AS5   UG              ;Dissolved arsenate
  BULK AStot UG              ;Total dissolved arsenic
  WALL AS5s  UG              ;Adsorbed arsenate
  BULK NH2CL MG              ;Monochloramine

[COEFFICIENTS]
  CONSTANT Ka   10.0         ;Arsenite oxidation rate coefficient
  CONSTANT Kb   0.1          ;Monochloramine decay rate coefficien
  CONSTANT K1   5.0          ;Arsenate adsorption coefficient
  CONSTANT K2   1.0          ;Arsenate desorption coefficient
  CONSTANT Smax 50           ;Arsenate adsorption saturation limit

[TERMS]
  Ks       K1/K2             ;Equil. adsorption coeff.

[PIPES]
  ;Arsenite oxidation
  RATE    AS3    -Ka*AS3*NH2CL
  ;Arsenate production
  RATE    AS5    Ka*AS3*NH2CL - Av*(K1*(Smax-AS5s)*AS5 - K2*AS5s)
  ;Monochloramine decay
  RATE    NH2CL  -Kb*NH2CL
  ;Arsenate adsorption
  EQUIL   AS5s   Ks*Smax*AS5/(1+Ks*AS5) - AS5s
  ;Total bulk arsenic
  FORMULA AStot  AS3 + AS5

[TANKS]
  RATE    AS3    -Ka*AS3*NH2CL
  RATE    AS5    Ka*AS3*NH2CL
  RATE    NH2CL  -Kb*NH2CL
  FORMULA AStot  AS3 + AS5
```

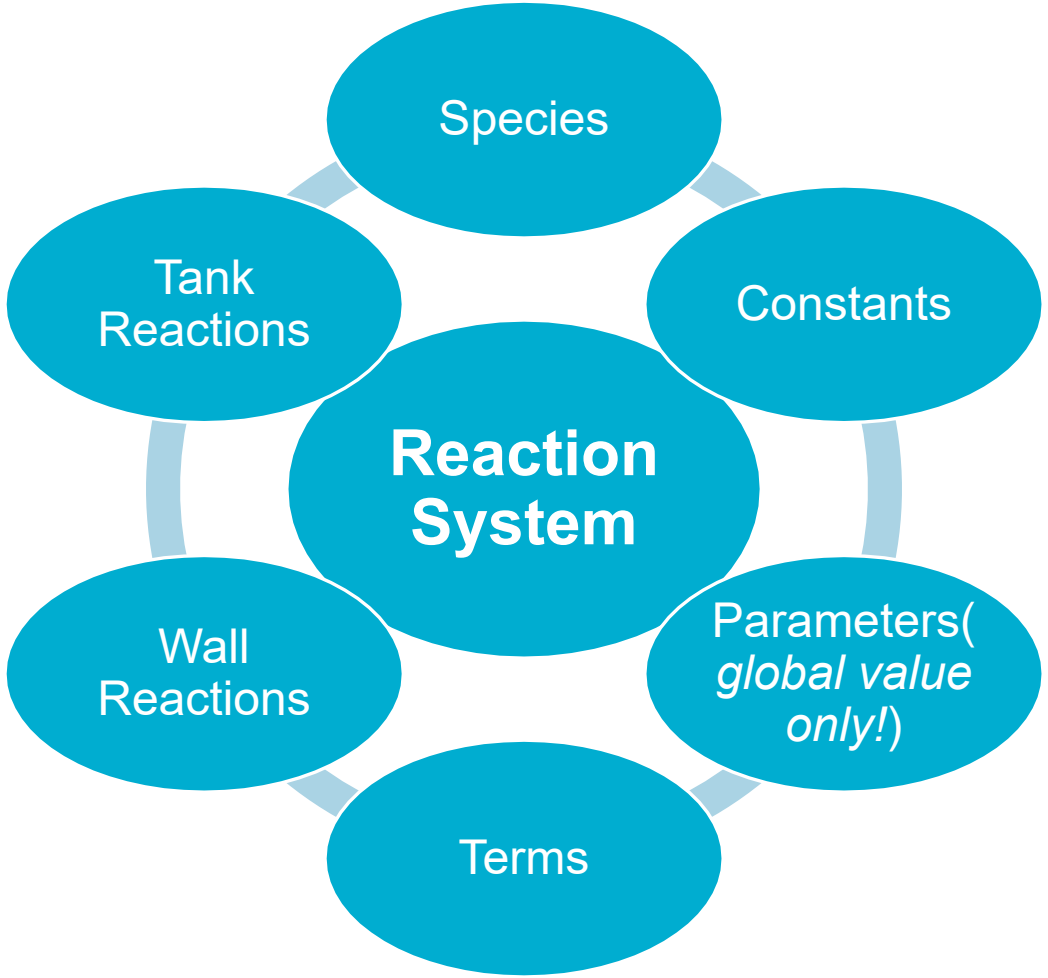
# WNTR + EPANET-MSX integration structure



# wntr.msx.model.MsxReactionSystem

## Differences from EPANET-MSX

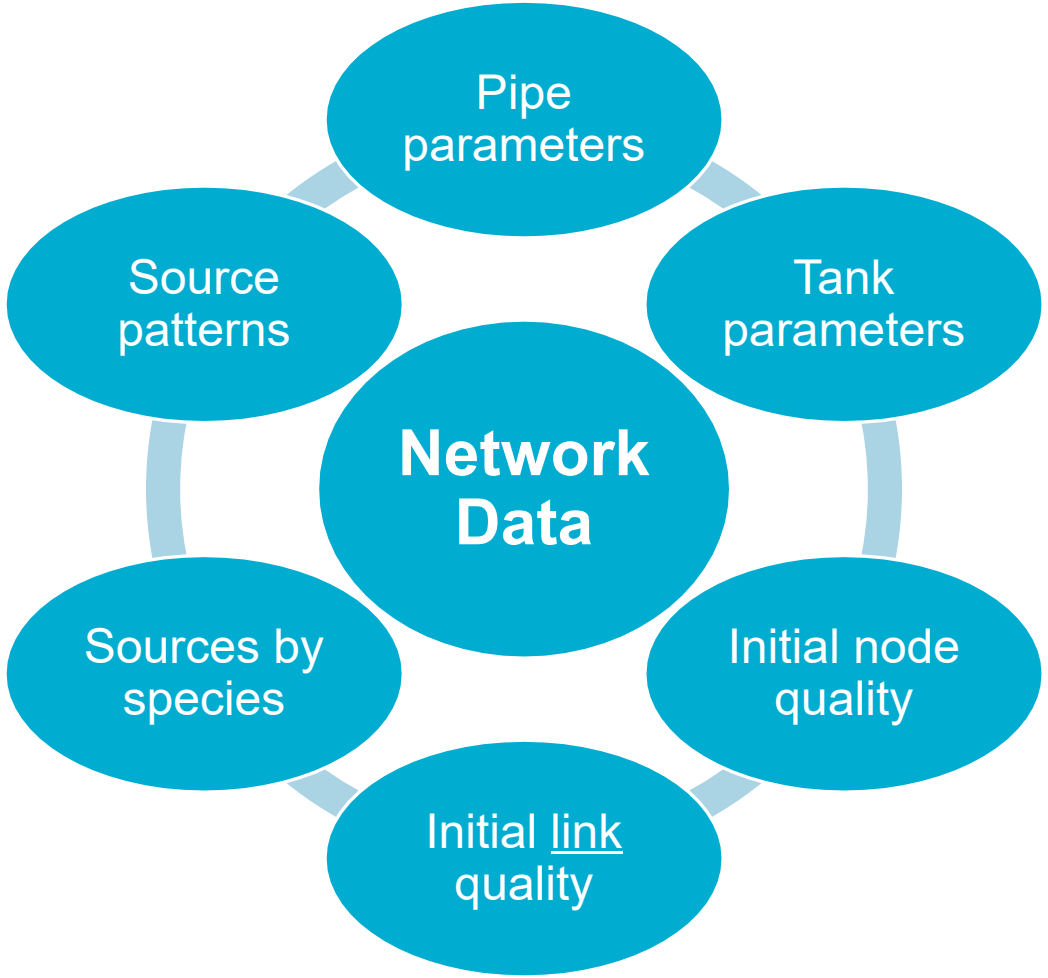
- Diffusivity assigned on species objects
- Coefficients can carry units
- ReactionSystem object checks names immediately
- **NO NETWORK-SPECIFIC INFORMATION IN THIS SECTION**



# wntr.msx.model.MsxNetworkData

## Differences from EPANET-MSX

- Per-tank and per-pipe attributes in dictionaries
- **ONLY NETWORK INFORMATION IN THIS SECTION**

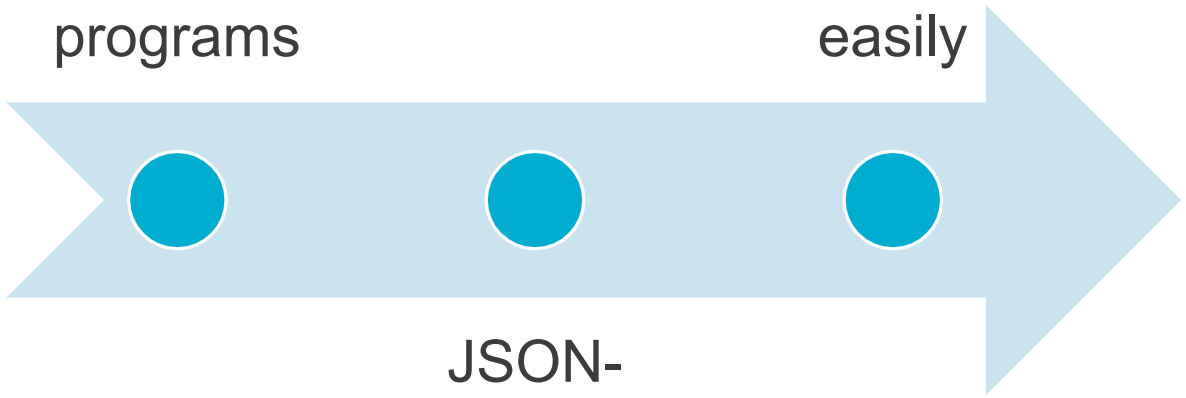


# JSON based data files

Easily passed between programs

Can be extended easily

JSON-schema provides validation



```
"title": "Arsenic Oxidation/Adsorption Example",
"description": "This example models monochloramine oxidati
wall adsoption/desorption, as given in section 3 of the E
"references": [
    "Shang, F., Rossman, L. A., and Uber, J.G. (2023). EP
    S. Environmental Protection Agency, Cincinnati, OH. E
],
"reaction_system": {
    "species": [ ···
    ],
    "constants": [ ···
    ],
    "parameters": [],
    "terms": [ ···
    ],
    "pipe_reactions": [
        { ···
        },
        {
            "species_name": "AS5",
            "expression_type": "rate",
            "expression": "Ka*AS3*NH2CL - Av*(K1*(Smax-AS
            "note": "Arsenate production less adsorption"
        },
        { ···
        },
        { ···
        },
        { ···
        }
    ],
    "tank_reactions": [ ···
    ]
}
```

# Reaction libraries

- Any reaction model can be used in a library
- “network_data” should be removed
  - No initial quality
  - No parameter values
  - No sources
- WNTR has a basic library of reactions from the EPANET-MSX user guide
- Users can specify own library directory to use

- Once loaded, a library must be adapted to your network
  1. Set global initial quality
  2. Set parameters for individual pipes or tanks
  3. Set initial quality for non-global values
  4. Create sources, if necessary

# Example

# Model initialization

```
import wntr
wn = wntr.network.WaterNetworkModel('../networks/Net3.inp')
wn.options.quality.parameter = 'NONE'
```

[2] ✓ 3.5s Python

```
wn.add_msx_model()
wn.msx.title = 'Multisource Chlorine Decay'
wn.msx.references.append("""(2023) Shang F, L Rossman, and J Uber.
"EPANET-MSX 2.0 User Manual". EPA/600/R-22/199""")
wn.msx.options.area_units = 'FT2'
wn.msx.options.rate_units = 'DAY'
wn.msx.options.timestep = 300
```

[3] ✓ 0.0s Python

# Add the reaction system

```
T1 = wn.msx.add_species('T1','bulk',units='MG', note='Source 1 Tracer')
Cl2 = wn.msx.add_species('CL2','bulk', units='MG', note='Free Chlorine')
pprint(repr(Cl2))
```

[4] ✓ 0.0s Python

```
("Species(name='CL2', species_type=<SpeciesType.BULK: 1>, units='MG', "
 "atol=None, rtol=None, note='Free Chlorine')")
```

```
k1 = wn.msx.add_constant('k1', 1.3, units='1/day')
k2 = wn.msx.add_constant('k2', 17.7, units='1/day')
pprint(repr(k2))
```

[5] ✓ 0.0s Python

```
"Constant(name='k2', value=17.7, units='1/day')"
```

```
rxn_T1 = wn.msx.add_reaction('T1', 'pipe', 'rate', '0')
rxn_Cl2 = wn.msx.add_reaction('CL2', 'pipe', 'rate', '-(k1*T1 + k2*(1-T1))*CL2')
pprint(repr(rxn_Cl2))
```

[6] ✓ 0.0s Python

```
("Reaction(species_name='CL2', expression_type=<ExpressionType.RATE: 2>, "
 "expression='-(k1*T1 + k2*(1-T1))*CL2')")
```

# Add the network-specific data

```
from wntr.msx.elements import InitialQuality
net_data = wn.msx.network_data
net_data.initial_quality['T1'] = InitialQuality(
    node_values={'River': 1.0}
)
net_data.initial_quality['CL2'] = InitialQuality(
    node_values={'River':1.2, 'Lake':1.2}
)
pprint(net_data.initial_quality)
```

[7] ✓ 0.0s Python

```
{'CL2': InitialQuality(global_value=0.0, node_values=<2 entries>, link_values=<0 entri
 'T1': InitialQuality(global_value=0.0, node_values=<1 entries>, link_values=<0 entrie
```

# Run the simulation

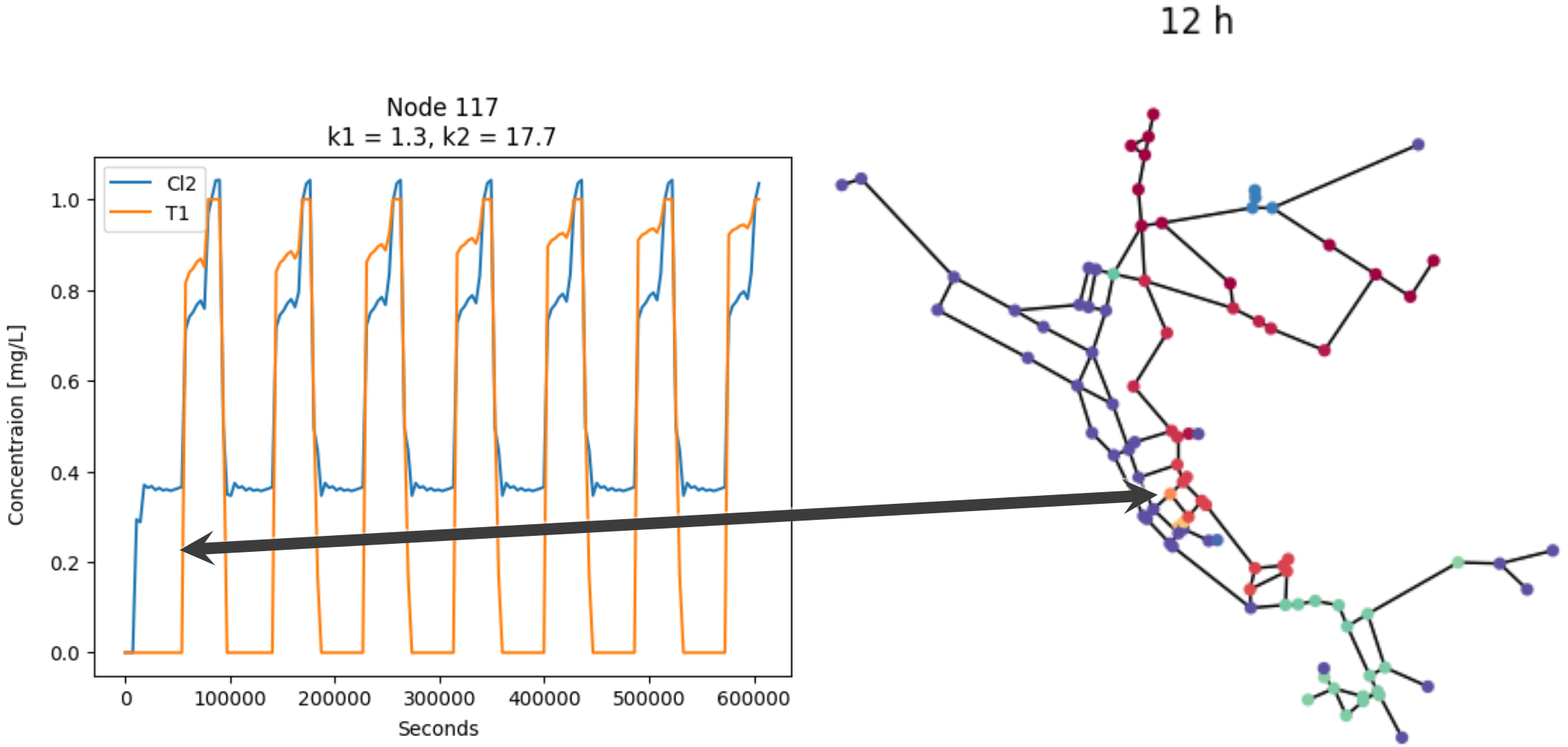
```
[8]  ✓ 1.5s                                                    Python

sim = wntr.sim.EpanetSimulator(wn)
res = sim.run_sim()
pprint('Node results: ' + ', '.join([k for k in res.node.keys()]))
pprint('Link results: ' + ', '.join([k for k in res.link.keys()]))
```

```
... 'Node results: demand, head, pressure, quality, T1, CL2'
('Link results: quality, flowrate, velocity, headloss, status, setting, '
 'friction_factor, reaction_rate, T1, CL2')
```

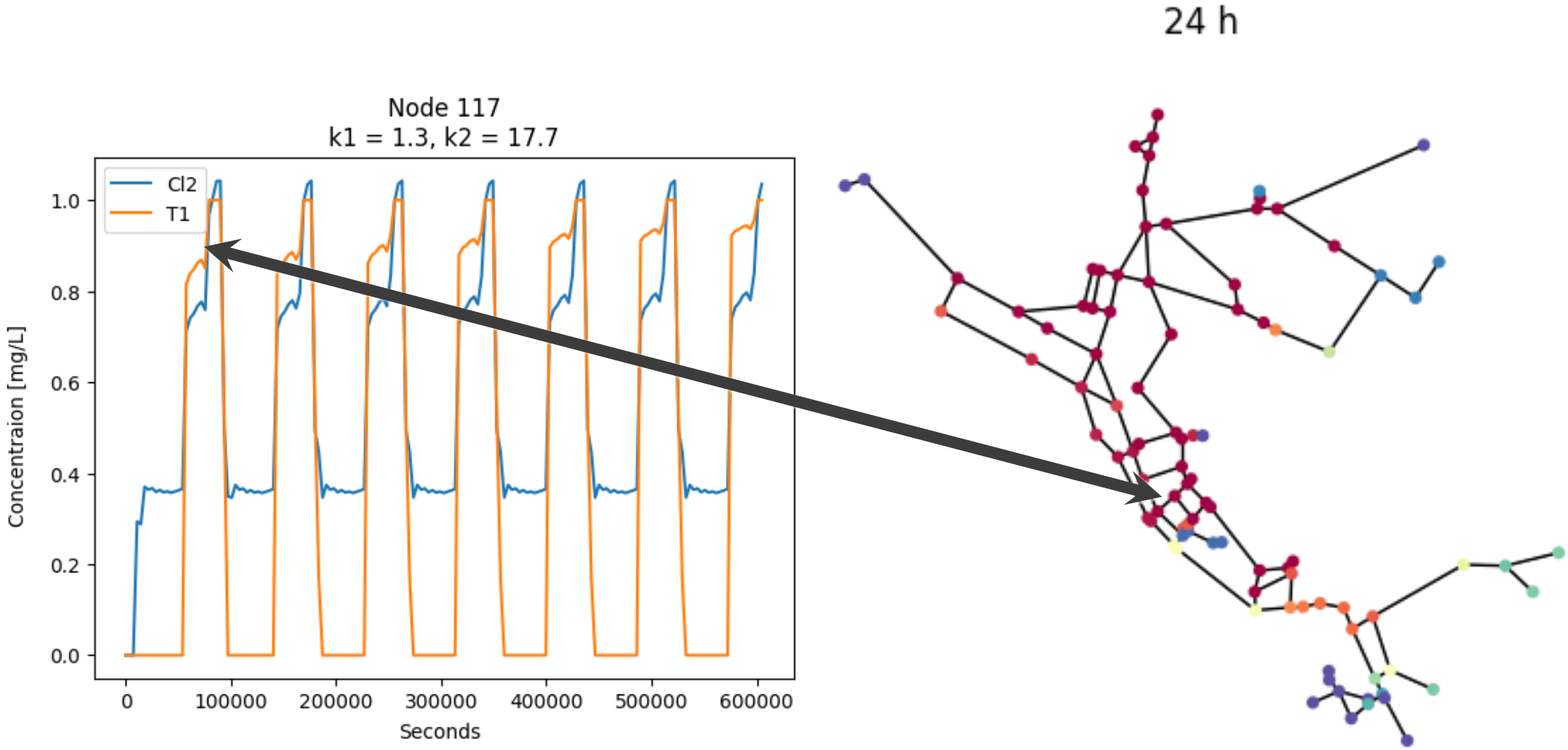
EPANET quality parameter is saved as the “quality” key in the WNTR results object

MSX species quality values are saved using their name as the key in the results object

# Simulation results, hour 12



# Simulation results, hour 24



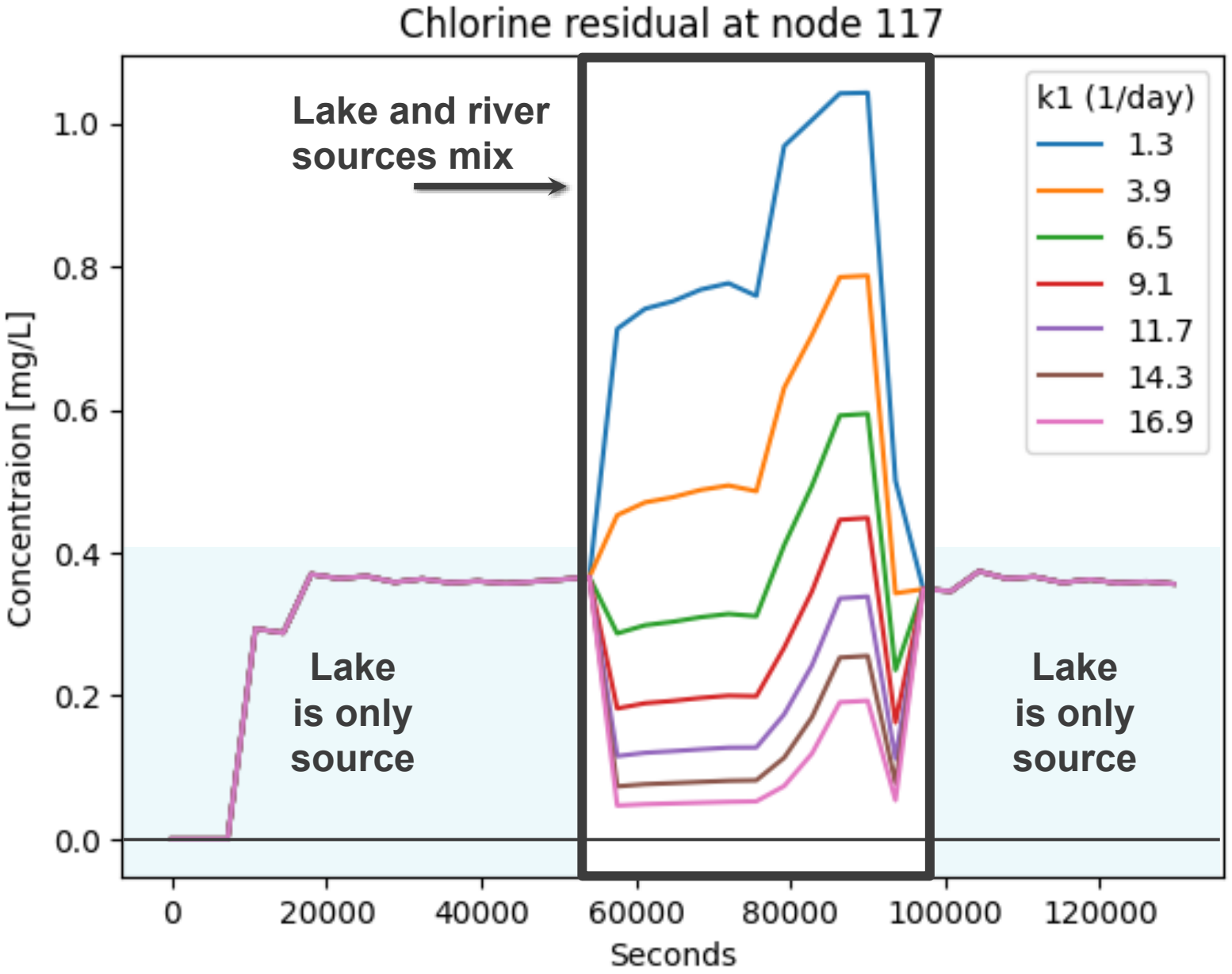
# Example parameter study

- Examine the effect of changes in the river decay coefficient, $k_1$, on chlorine residuals in the network
- Vary $k_1$ from 1.3 to 16.9 day $^{-1}$

```
d_k1 = dict()
k1 = wn.msx.reaction_system.constants['k1']
for i in range(7):
    # Increase the reaction rate
    newk = 1.3 + i*2.6
    k1.value = newk
    resk = sim.run_sim()
    d_k1[newk] = resk
```

[10] ✓ 9.9s Python

# Example parameter study results



# Conclusions

# Summary

1. Multispecies water quality using EPANET-MSX coupled with WNTR
2. Library of reaction models built-in, and user customizable and extensible
3. Resilience and impact metrics from WNTR can be used directly on MSX data

# References and resources

WNTR Source Code, Issue Tracker

- https://github.com/USEPA/WNTR

WNTR Documentation

- https://usepa.github.io/WNTR

EPANET-MSX Source, Issue Tracker, Docs

- https://github.com/USEPA/EPANETMSX
- Shang, F, L Rossman, J Uber. 2023. *"EPANET-MSX 2.0 User Manual"*. U.S. Environmental Protection Agency, Cincinnati OH. EPA/600/R-22/199.

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- https://www.sandia.gov/
- https://sandialabs.github.io/

U.S. EPA, Office of Research & Development

- https://www.epa.gov/emergency-response-research/water-modeling-tools-decision-support