

Overview of EPA Tools and Models

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US EPA Office of Research and Development Center for Environmental Solutions and Emergency Response

Springboarding Digital Water Symposium

October 11, 2023

Presentation Overview

- History & Background
- EPA's Drinking Water Models & Tools
- EPA's Stormwater & Water Reuse Models & Tools
- Looking to the Future

Disclaimer

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EPA Water Research Facility in Cincinnati



Drinking Water Infrastructure Tools



- Disinfection
- Treatment
- Treatability DB



- Drinking Water Distribution System Models & Tools
- EPANET
- EPANET-MSX
- Real-time
- Resilience



• PPM Tools

Drinking Water Disinfection Models

Web-based calculators

- Chloramine formation and decay <u>https://shiny.epa.gov/cfd/</u>
- Chlorine breakpoint curve <u>https://shiny.epa.gov/cbcs/</u>
- Chlorine and cyanuric acid chemistry <u>https://shiny.epa.gov/fccas/</u>
- Free chlorine estimator for dichlor/trichlor disinfection <u>https://shiny.epa.gov/fcedts</u>



Drinking Water Treatment Models

Environmental Technologies Design Option Tool (ETDOT)

- Suite of software for modeling a variety of treatment technologies by MTU.
- Includes models for adsorption, advanced oxidation, aeration, biofilters, PAC adsorption, ion exchange.

http://www.epa.gov/water-

research/environmental-technologies-design-

option-tool-etdot

Granular Activated Carbon Model

- Pore and Surface Diffusion Model (PSDM)
- Includes parameter estimation
- Ion Exchange Media
 - Supports gel-type, macroporous ion exchange resins & competition from divalent ions, such as sulfate



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Treatment Tools: Treatability Database

- Interactive searchable database
- 142 regulated and unregulated contaminants, including 37 PFAS
- 35 treatment processes commonly employed or known to be effective
- Referenced information gathered from thousands of literature sources

epa.gov/waterresearch/drinkingwater-treatabilitydatabase-tdb

Home About the TDB Contact Us Find Contaminant Find Treatment Process Help

Quick Links

Welcome to the Drinking Water Treatability Database

Premise Plumbing Models

- Premise Plumbing Modeling Tools (PPMtools)
- Leverages EPANET and WNTR
- Models real-world fixtures & usage patterns
- Generates and runs many scenarios
- Predicts water quality information over time
- Simulates flushing to remove contaminants
- Estimates exposure to contaminants
- Being validated through experiments
- https://github.com/USEPA/PPMtools

EWRI Premise Plumbing Modeling Workgroup Webinar Series



70del

Stormwater and Water Reuse Models and Tools



- SWMM
- Stormwater
 Calculator
- GI Toolkit



Models & Tools

- NEWR
- Microbial Risk Assessment

National Stormwater Calculator



- Distributed, Estimates annual rainwater and frequency of runoff
- Site specific
- Low impact development controls









https://www.epa.gov/water-research/national-stormwater-calculator

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Building Water Reuse Calculator

Non-Pota

- NEWR compares water reuse options within a single building
- Based on geography, end use, building specifications, and source water type
- Calculates costs as well as environmental benefits



NEWR - Non-potable Environmental and Economic Water Reuse Calculator:

			Show data entered				1	1		New Calculation
	ZIP Cod	e Data	Water Availability G & Demand	olobal Warming Potential	Total Energy Demand	Fossil Fuel Depletion	Water Consumption	Wate	r Scarcity	Cost (Net Presen Value)
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	January	0.00	0.0000	0.67			Electricity Rate ()	0.12	\$/kWh	
	February	0.00	0.0000	0.93		v	Vater Supply Rate 🛈	5.30	\$/1000 gall	ons
tal	March	0.00	0.0011	2.19						
	April	0.00	0.019	3.88	eGRID Su	bregion - MRO \	West ()			
	May	3.46	0.13	5.46		E	Electric Grid Reso	ource N	lix	≡
	June	4.25	0.85	5.96		Other	· Unknown: 0.2%			
	July	3.98	1.51	6.46		Geothermal: 0.0	%			
	August	3.98	1.22	5.42		Solar: 0.5%				
	September	2 00	0.68	4.05		Wind: 21.7%			\	
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EPA Water Modeling Workgroup

UPDATES & HIGHLIGHTS FROM THE WATER MODELING WORKGROUP

Who is WMW?

EPA's Water Modeling Workgroup (WMW) was formed by EPA Office of Water (OW), Office of Research and Development (ORD), and Regional Water Programs to address Agency-wide water quality modeling challenges.

Goals:

- Promote collaboration and communication between water quality modelers.
- Enable EPA to access modeling expertise for critical water quality projects and targeted consultations.
- Maintain and improve water quality models and resources.
- Provide training resources on water quality modeling and address emerging water quality modeling and research needs.

Final Peer Review for Nutrient-Related Modeling Expected This Year

The 1985 Second Edition of Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling is recognized as a trusted source for water quality modelers on kinetic formulations and associated rate constants and coefficients used in surface water quality modeling.

EPA Training Workshop

Exploring and Applying Surface Water Modeling Tools to Achieve Program Goals

For EPA, States, Tribes and Territories October 29, 2019 - November 1, 2019 EPA Region 6 HQ - Dallas, TX

This four-day workshop is for program staff from EPA, states, tribes, and territories who want to learn more about surface water quality modeling and how these tools can be used to support their program activities. The workshop will provide an opportunity to learn about a variety of surface water quality modeling tools, and updates on anticipated advances and changes to **models.** Attendees will assist in identifying information technology enhancements for user interfaces, architecture, and maintenance for key models.

See page 2 and visit the workshop webpage for the workshop agenda.

- Coordination of modeling efforts within EPA Office of Research and Development, Office of Water, and Regions
- Hosting modeling training and workshops: <u>https://www.epa.gov/waterdata/surface-</u> <u>water-quality-modeling-training</u>
- Peer reviewing models and data: <u>https://cfpub.epa.gov/si/si_public_record_rep_ort.cfm?Lab=NHEERL&dirEntryId=342391</u>

https://www.epa.gov/waterdata/surface-water-quality-modeling

Guiding Principles for Model and Tool Development

- Customer driven identified as a need through EPA ORD's stakeholder process involving EPA's Office of Water, Regional offices, states, communities, as well as the needs of model/tool users
- Address national priorities
- Solves problems
- Based on the best available science
- Freely available, open, transparent
- Reliable, reproducible, high quality

Looking to the Future: EPA Water Modeling

- Support for Bipartisan Infrastructure Law water system improvements
- Climate change and resilience
- Features to support digital water future
- Integrated water resources modeling
- Stakeholder engagement
- Collaboration with external organizations

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Upcoming EPA positions related to digital water:

- Federal principal investigator to support EPANET
- Federal principal investigator to assess resilience
- ORISE/ORAU research fellows for water infrastructure modeling, tool development, climate change and resilience studies

Diversity, Equity, Inclusion and Accessibility

We all have a role to play in making every member of ORD feel engaged, included, valued, safe and secure. Learn more about Diversity, Equity, Inclusion and Accessibility at ORD.

www.epa.gov/careers/equal-opportunity-employment-epa



Advancing EPA's Storm Water Management Model for the Digital Water Transformation

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US EPA Office of Research and Development Center for Environmental Solutions and Emergency Response

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Legacy of SWMM

- SWMM simulates runoff quantity and quality and routes them through collection system infrastructure
- SWMM has played a pivotal role in flow and pollution control in collection systems since its inception
- SWMM supports studies driven by regulatory imperatives including:
 - Long Term Control Plan development (LTCP)
 - Total Maximum Daily Allocation (TMDL)
 - Municipal Separate Stormwater Systems (MS4)
 - National Pollutant Discharge Elimination System (NPDES)
- Remains the subject of various scientific applications and research efforts



SWMM Core Users



SWMM Traditional Applications

- Traditional application scenarios
 - Design and sizing of drainage systems
 - Control of combined and sanitary sewer overflows
 - Pollutant load estimation and transport as well as BMP and treatment evaluation
 - Estimating inflow and infiltration in sanitary systems
 - Green infrastructure evaluation
- Typically involves calibrating to historical records and evaluating on design/typical year storms for long term engineering design and planning purposes



SWMM's Role in Advancing the Intelligent Collection Systems Paradigm





- Sensing and communication infrastructure deployed at critical locations within collection system
- Controllable assets can be adjusted automatically or with a user-in-the loop in real-time to achieve various near-term and long-term objectives
- Virtual representations digital twins fuse realtime sensor data and models to predict future states under different control scenarios
- SWMM could fill this role, but challenges remain that hamper evaluations (e.g., performance, runtime interactions, real-time data integration, etc.)

SWMM Recent Updates Version 5.1-5.2: Realtime Control Enhancements

- Control rules premise clauses expanded to include:
 - Additional control rule parameters:
 - Current and next rainfall
 - Node attributes including full depth, head, and volume
 - Conduit attributes including length, slope, full depth, full flow and velocity
 - Named variable as aliases and math expressions for more sophisticated real time control implementations
 - Variable D1 = Node Node1 Depth
 - Variable D2 = Node Node2 Depth
 - Expression $HGL = \frac{D1+D2}{2.0} + 23.7$
 - If Expression HGL <> 24 THEN ORIFICE OR1 SETTING = PID 0.10.010.0



SWMM Recent Updates Version 5.1-5.2: Dual Drainage System Modeling



- Flow from runoff component is applied as oneway inflow into downstream nodes
- Flooding is accumulated over a user prescribed area on nodes.
- This is a poor approximation of what happens in reality, where dynamic floods flow on streets and over the landscape



- As a step towards coupling of the under drainage and streets, a new streets cross-section for links and inlet types are available in SWMM
- FHWA "Urban Drainage Design Manual" (HEC-22), the de facto standard for inlet analysis has been implemented
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Future SWMM Advancements to Support Developing Intelligent Collection Systems



Advancing SWMM's Geospatial and Runtime Interaction Capabilities

Goal

- A transparent and flexible GIS-based data model for SWMM inputs and outputs. Advance SWMM's API and runtime scripting interaction capabilities to support:
 - Multi-scenario, what-if evaluations
 - Realtime sensor data assimilation
 - Resilience evaluations
- Data-driven or AI/ML based model and controls integration **Approach**
- A GIS-based data model that represents the natural and built infrastructure as well as their topological relationships.
- A transparent and flexible output and model state persistence
- Python bindings for an expanded SWMM API



Improving the Computational Performance of SWMM

Goal

 Improve SWMM's computational performance for large systems and high-resolution modeling, and multiscenario and stochastic evaluations

Approach

- Modern approaches to writing efficient and highperformance computational code emphasize spatial and temporal locality of data in memory for fast access and transformation (i.e., "cache friendly") using dataoriented design
 - Vectorizing data and using Single Instruction, Multiple Data (SIMD)
 - Using struct of arrays (SOA) instead of arrays of structs (AOS)
 - Use of data managed contiguous arrays instead of linked lists for data that are frequently accessed or modified
- A preliminary testing of these approaches has shown a lot of promise with reductions of 20-30% in computational time

Frequent Cache Misses



Cache Friendly Data Layout



Improving the Fidelity of SWMM's Hydraulic Routing and Water Quality Formulations

Goal

Advance SWMM's formulation to improve the degree of fidelity paid to underlying routing and water quality processes in an efficient manner **Approach**

- Efficient and accurate numerical methods for hydraulics that resolve sub-pipe dynamics, handle transitions from open-channel to pressurized flows, and promote mass conservation and convergence
- Implementing full advection-reaction-dispersion formulation that can handle the different flow regimes in collection systems
- Advancing a heat transport and multi-species reaction capability for SWMM



Improving the Fidelity of SWMM's Overland Processes

Goal

- A spatially explicit multi-process and multi-scale overland flow quantity and quality model to facilitate:
 - Coupled 1D/2D inundation studies
 - Integration of the vast databases of publicly available remotely sensed and derived products e.g., radar-based rainfall, land use, soil moisture, etc.
 - Spatially explicit evaluation of GI and other sustainable urban development approaches

Approach

- Implement coupling infrastructure to allow coupling arbitrary 2D models to SWMM
- Implement a spatially explicit multi-scale and multi-process overland flow-infiltration 2D model
 - The Penn State Integrated Hydrologic Model (PIHM) is being evaluated for adaptation and adoption
 - It solves for flow over triangular irregular network (TIN) mesh
 - Benefit of the TIN mesh is that we are add more resolution where needed (e.g., spatially explicit implementation of GI) and coarsen the mesh in areas where not needed



Conclusions

- EPA ORD will continue to maintain and advance SWMM for the digital water transformation
- Advancements will go through EPA's rigorous internal review process to ensure continued confidence in the use of SWMM
- We plan to continue conversations with our stakeholders throughout the development process to make sure their views are considered in this process
- We are excited about the future of SWMM and invite practitioners, researchers, to provide feedback and suggestions on future directions



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Advancing EPA's Drinking Water Modeling Tools for the Digital Water Transformation

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Drinking Water Distribution System Modeling

- Simulates hydraulics within water distribution network
- Models decay/growth of single substance
- More than 50,000 downloads per year
- Components utilized for multiple commercial software packages
- Latest official release: version 2.2 in July 2020

https://www.epa.gov/waterresearch/epanet

EPANET

Application for Modeling Drinking Water Distribution Systems

EPANET is a software application used throughout the world to model water distribution systems. It was developed as a tool for understanding the movement and fate of drinking water constituents within distribution systems, and can be used for many different types of applications in distribution systems analysis. Today, engineers and consultants use EPANET to design and size new water infrastructure, retrofit existing aging infrastructure, optimize operations of tanks and pumps, reduce energy usage, investigate water quality problems, and prepare for emergencies. It can also be used to model contamination threats and evaluate resilience to security threats or natural disasters.

- On this Page
- Software, Compatibility, and Manuals
- <u>Capabilities</u>
- <u>Applications</u>
- Related Resources
- <u>Technical Support</u>



EPANET Typical Uses and Applications

Solving Regulatory Problems



Optimizing Operations to Improve Water Quality





Preparing for Emergencies



Real-time Operations and Decision Making



EPANET Version 2.2 Recent Updates

- Improved solution performance and accuracy
 - Pressure dependent demand analysis
 - Water quality mass balance
 - Handling of low flows
 - Convergence criteria
- External contributors
- Testing and quality assurance
- Updated user interface



EPANET Extensions: EPANET-MSX

- Used to model
 - Adsorption/desorption on pipe walls
 - Attachment to biofilms
 - Chemical reactions
 - Biological growth and decay
- EPANET-MSX 2.0 updates
 - Compatible with EPANET 2.2
 - Added dispersion
 - Added parallelization
 - Added mass balance reporting
 - Added sub-second timesteps

https://github.com/USEPA/EPANETMSX



EPANET Extensions: Real-time Tools

- EPANET-RTX is suite of software libraries to integrate EPANET with SCADA operational data
- RTX enables real-time analytics for automated:
 - Forward and hind casting
 - Model calibration
 - Simulation & comparison of operational decisions
 - Continuous comparison between model and sensor/data outputs, and analysis, allows for more accurate predictions



EPANET Extensions: Resilience Analysis

- Water Network Tool for Resilience (WNTR): simulates disaster scenarios such as earthquakes, power outages, floods, and contamination incidents
- Predicts damage to infrastructure
- Calculates resilience metrics
- Evaluates response and mitigation strategies to improve resilience





WNTR Version 1.0 Recent Updates

WNTR Pipe Break Der	no
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Capability	Description	This demonstration covers how to run simple pipe break analysis using WNTR. 1 Simulation set up 1a Import packages		
Model I/O	 Read/write water network models to/from standard formats Dictionary, NetworkX Graph, GeoPandas GeoDataFrame EPANET INP file, JSON file, GeoJSON and Shapefile files 	<pre>Numpy and Matplotlib are required to support data handling and graphics/plotting. In []: import matplotlib import matplotlib.opDot as plt import matplotlib.colormaps['viridis'] bCreate a water network model If adapting code for a different INP file, code for 1b and 1c need to be changed to reflect the correct file path and desired simulation parameters.</pre>		
Geospatial analysis	Integrate GIS data into resilience analysis to build water network models, and define scenarios and metrics	<pre>In []: # Identify file path to inp file inp_file * 'fretworks/Net3.inp' # Create water network model un = wnfr.network.WaterNetworkModel(inp_file) # Calculate population per junction population = wnfr.metrics.population(wn) 1c Define pipe break parameters</pre>		
Simulation	Run EPANET simulations in interactive mode to integrate WNTR with third-party simulators that customize controls	The parameters minimum_pressure and required_pressure are used for PDD simulations. Nodes with pressures below minimum pressure will not receive any water, and node pressures need to be at least the required pressure to receive all of the requested demand.		
Resilience metrics	Compute additional metrics (modified resilience index, tank capacity, pump energy) and improve computation efficiency	Analy the D Wate Edited by June		
Demos	Added Jupyter notebook demo, available in software repository and published in <i>Embracing Analytics in the Drinking Water Industry</i>	Covers a broad spectrum analytics topics in an eas		

Embracing Analytics in the Drinking Water Industry

Covers a broad spectrum of water industry analytics topics in an easy-to-follow manne

WNTR Geospatial Analysis Capabilities

- **Goal**: Integrate geospatial data into WNTR for model development, scenario generation, and community-centric resilience metrics
- Read/write
 - Read GIS files into WNTR to define water network model
 - Write water network model to GIS files
- Coordinate projections
 - Convert coordinate reference system (CRS)
- Spatial joins
 - Associate GIS data with node and edges of water network model
- Visualization
 - Append simulation results to GIS files
 - Load GIS files into GIS platforms for visualization



dependency on GeoPandas

WNTR Interactive Simulation Capabilities

- Interactive Mode uses EPANET toolkit and Controller to interact with simulation
 - Example controllers include SCADA, cyberphysical simulator, power flow model, or user
 - Some or all of EPANET Rules/Controls can be relinquished to Controller
 - Controls modified using EPANET toolkit or though direct modification of model
 - Intermediate simulation results can include sensor readings or resilience metrics
 - Stop criteria can include conditions like pump status, tank level, and water service availability



WNTR Simulation Capabilities

- **Goal:** Efficient simulation capabilities that can pass simulation results and custom controls between WNTR and external tools
 - Power-flow models
 - Cyber-physical models
 - Table top exercises
- Interactive simulation capabilities
 - Advance to next timestep and check conditions
 - Pause simulation using flexible criteria
 - Change model operations and solver options (including timestep and changes not supported by traditional Rules/Controls)

Power distribution model



Sensor readings are used to record system status and pause the model



Water distribution model

Future Enhancements for Drinking Water Model Tools

- Integrate EPANET-MSX into WNTR
- Enhancement capabilities to pull in other data sources
- Expand capabilities to simulate additional disaster and response scenarios
- Add economic data metrics to evaluate repair and mitigation actions
- Incorporate optimization algorithms to help prioritize response and mitigation actions

Conclusions

- Maintain and advance EPANET for digital water transformation
- Review advancements to ensure continued confidence in EPANET
- Continue conversations with our partners throughout development process to make sure their views are considered
- Invite EPANET practitioners, researchers, and others to provide feedback and suggestions on future directions



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Integrated Modeling and Adaptive Planning of Water Infrastructure for Sustainability and Resilience in a Digital Water Age

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Models and Tools for Water Systems



Systems Sustainability in Multiple Objectives



- Sustainability in three pillars: System resilience, environmental effects, and socioeconomics
- Climate change and environmental justice are prominent factors, but not yet fully considered in water systems planning and design
- How to adapt the water and other urban infrastructure of large physical footprints is a daunting challenge
- ORD/WID researchers are working from both urban-scale planning and system-specific engineering methods and techniques

Quantify through Systems Modeling at Three Scales



Physical models and physics-informed AI modeling for multi-scaled water infrastructure to improve resilience and sustainability

- Watershed scale models IWM. *Variables* in climate, LULC, stream flow and surface water quality
- Urban scale model SUD. *Variables* in urban climate, green house gas (GHG) emissions, population, services, and land use policies
- Drinking water models EPANET/WNTR, WTP-cam. Variables in water demand, water quality, operation resilience, and environmental justice (EJ)
- Stormwater / collection system models SWMM, SWC. Variables in urban hydrology/climate, LULC, green and gray infrastructure, EJ
- Waster Reuse model NEWR. Variables in economic activities, waste stream, treatment process, compliance criteria, reuse and water availability

Effects of Climate and Urban Changes on Water Systems

Climate Change

- Complex climate impacts, often location specific, mostly occur in hydrology (water quantity and quality) and hydraulics.
- Water quality, availability, and hydraulics all affect water systems both in planning and operation phases
- Climate impacts can be shortterm disruptive and longterm impactive on water sustainability

Urban Growth/LCLU Changes

- Exacerbate climate impacts, such as urban head island effects, GHG emission, etc.
- Urban systems and population are also vulnerable to climate impacts making effective and practical adaptation necessary
- Climate justice and EJ are social dimensions to consider
- Three water systems and transportation often define urban forms of structure difficult to change and adapt once built

Impact Analysis



Systems Modeling for Urban Infrastructure Impacts



SUD helps water planning

- The models simulate LULC, transportation and population distribution under future climate and urban development scenarios
- Outputs define water demand, wastewater and stormwater generation, and help in infrastructure siting and layout
- Optimizing water infrastructure master planning in the adaptive process

SUD helps water operations

- Enable EJ and GHG emission analysis
- Assist in system adaptation and water quality monitoring for resilience against changes in economics, population and climate-induced source water changes

SUD Development for Operation Adaptation: Water Quality, Demand and Supplies



- SUD modules integrate remote sensing, sensor-based water quality monitoring and system engineering for better operations
- Large data processing and data fusion of satellite sensing, water sensors, operational data
- The use of process-informed AI (ML, ANN, etc.) techniques
- How to best use AI in process parameterization, solution space identification, process optimization, etc.?

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SUD Development for Planning Adaptation: GHG, EJ and Infrastructure Sustainability



Optimal urban adaptation changes population distribution, reduce GHG emissions, and differently affects communities. Case study in Cincinnati, Ohio



Multi-dimensional adaptation for water system and community resilience against SLR and storm surge. Case studies in Chesapeake Bay & Mattapoisett



- Growth policy, socioeconomic, and LULC define water and other urban infrastructures, their configuration, layout and sustainability.
- Adaptive planning achieves optimal GHG emission reduction, water infrastructure services, and climate justice – the EJ factor
- Adaption scenarios are computersimulated and analyzed due to large physical and financial footprints of urban infrastructure
- SUD modeling based on physical processes. Can AI and ML techniques be applied for better modeling?

Digital Water & Infrastructure Adaptation

- Help systems modeling in model integration
- Reduce output uncertainty by better parameterization, especially on climate and socioeconomic changes
- Better configuration and result visualization in scenario analysis
- Integration of data acquisition, data fusion, and computation for timely decision making
- Support for infrastructure improvements in planning, operations and compliances



Advancing EPA Modeling for Drinking Water, Stormwater, and Infrastructure Improvements

- Continued support for SWMM, EPANET, WNTR and other models under EPA's Safe and Sustainable Water Resources (SSWR) research program
- Efforts driven by EPA program office, regional, and state needs, as well as by users and other stakeholders
- Enhancements underway to further support next generation digital water applications
- Building and preparing our future workforce