



National Energy Water Treatment & Speciation (NEWTS): A Water & Critical Mineral Database and Dashboard

Nicholas Siefert and NEWTS Team

PWS 2024 Session#6: Produced Water Quality & Analysis

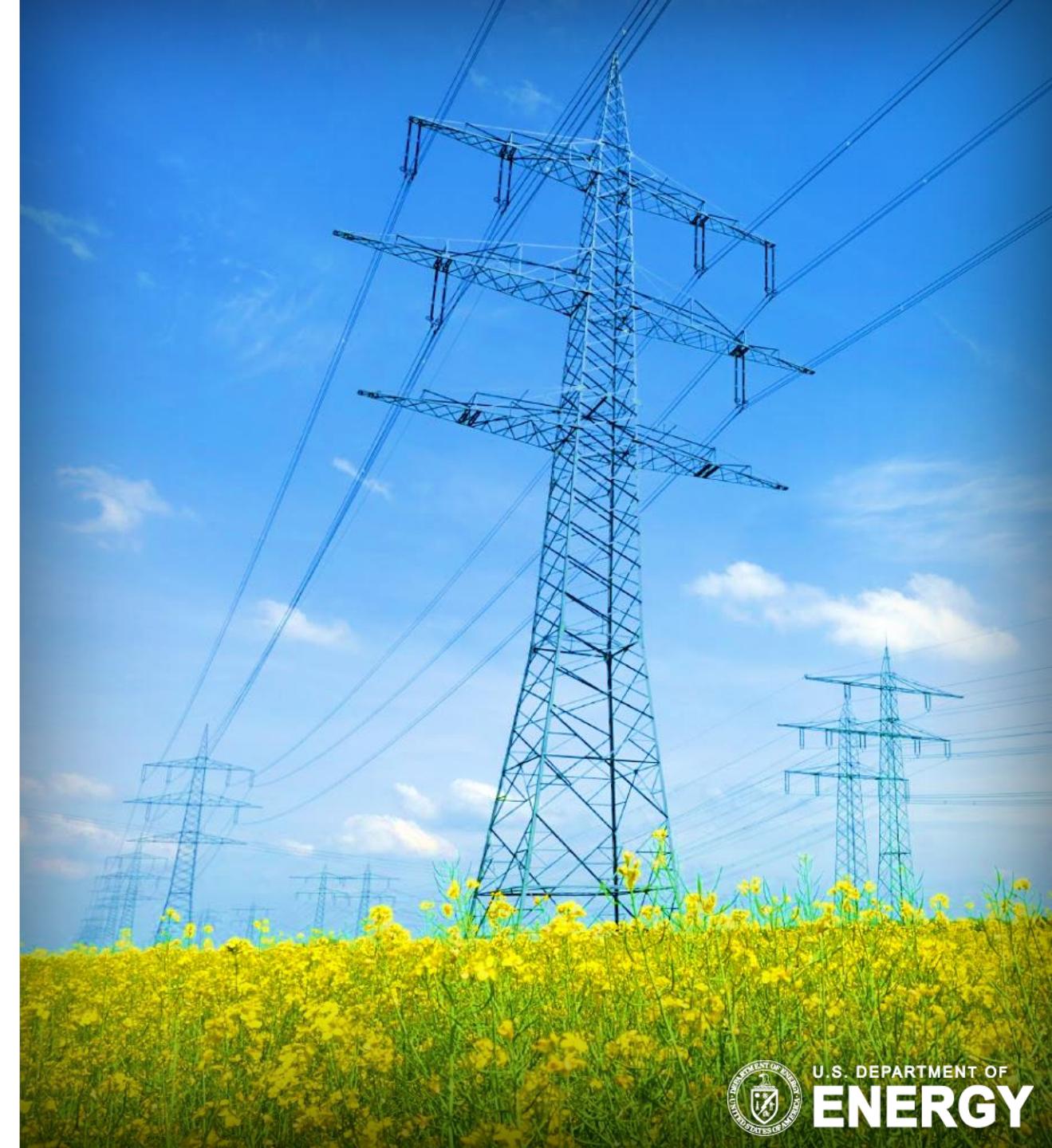
Thursday February 8, 2024



Fossil Energy and
Carbon Management



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NEWTS

DATABASE

NATIONAL ENERGY WATER TREATMENT & SPECIATION (NEWTS)

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Motivation for NEWTS Database

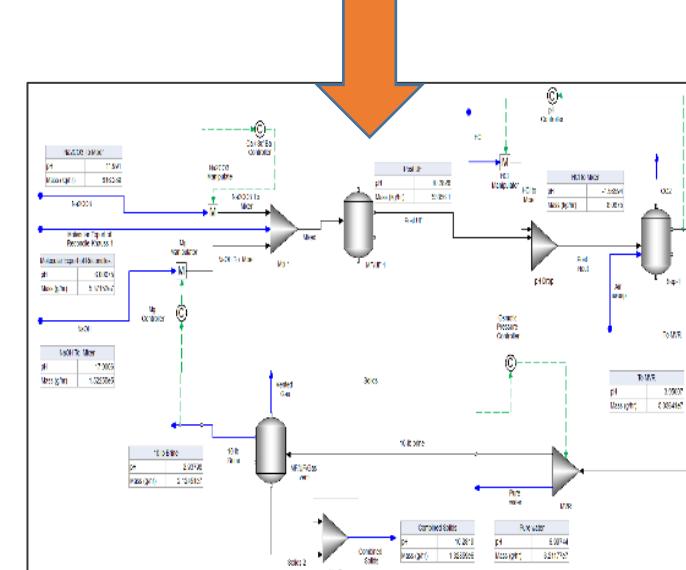
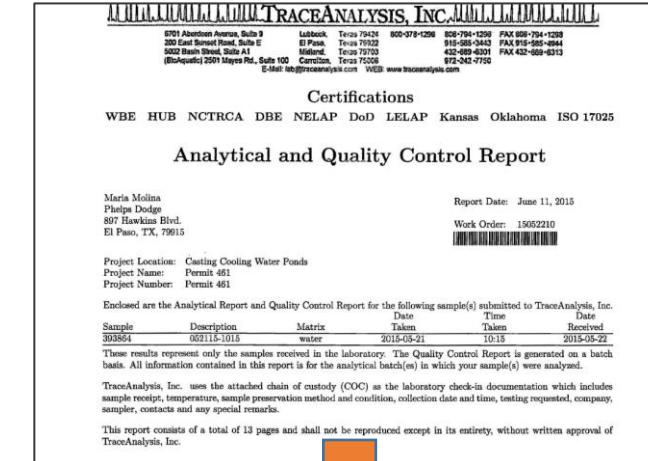


Prior state of energy-water data

- Energy process wastewater data were **disparate, incomplete, and difficult to access and to use**
- Regulated by different **federal and state agencies**
 - Many datasets were not easily downloadable
- Many datasets listed elements, not the species (B vs. B(OH)₃) or redox state (Fe(II) vs. Fe(III))
- Existing datasets were **not formatted** for input into modeling and water treatment software



- High-quality, detailed datasets are necessary to design **treatment technologies** and to understand cross-industry wastewater **re-use opportunities**



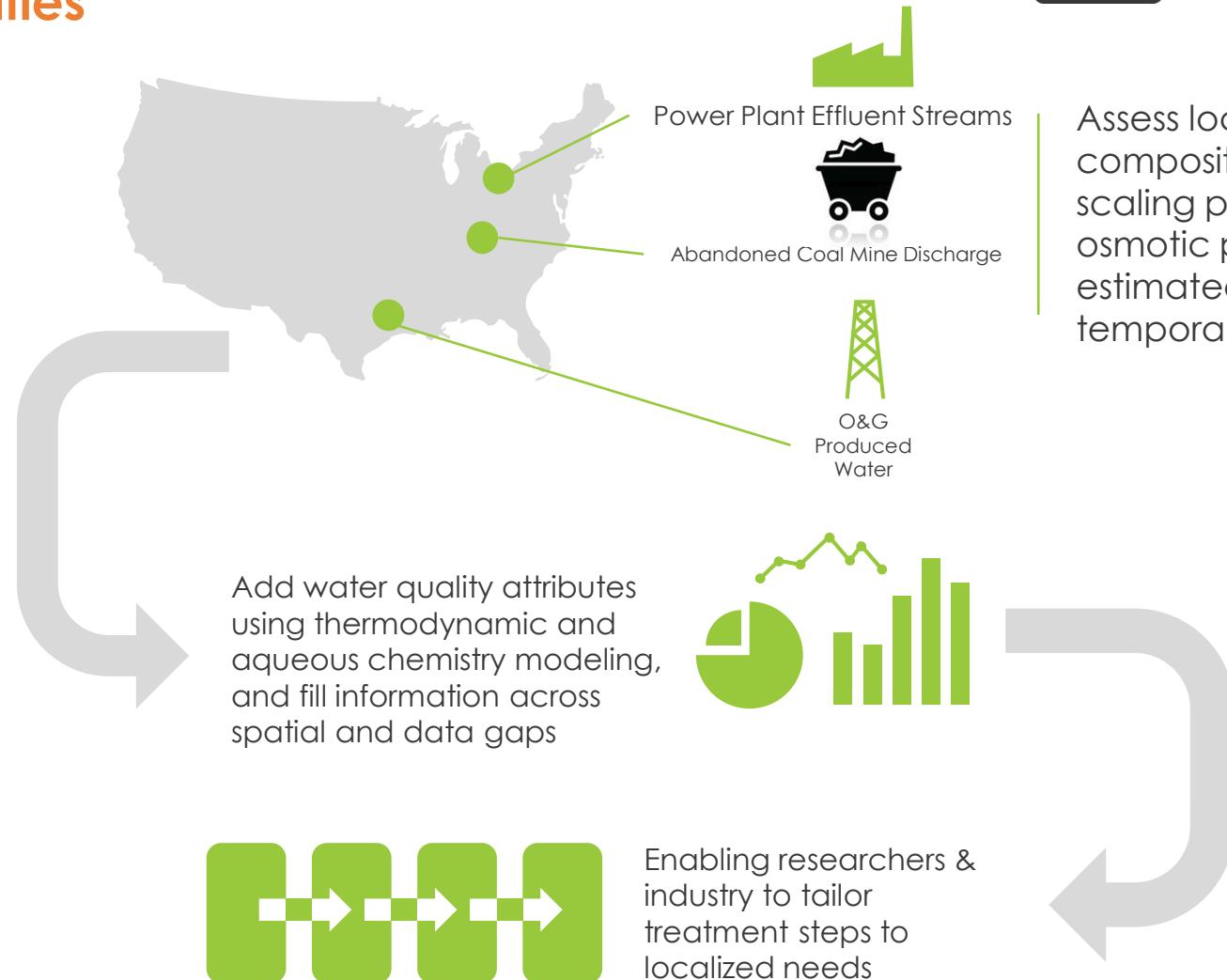
National Energy Water Treatment & Speciation Database



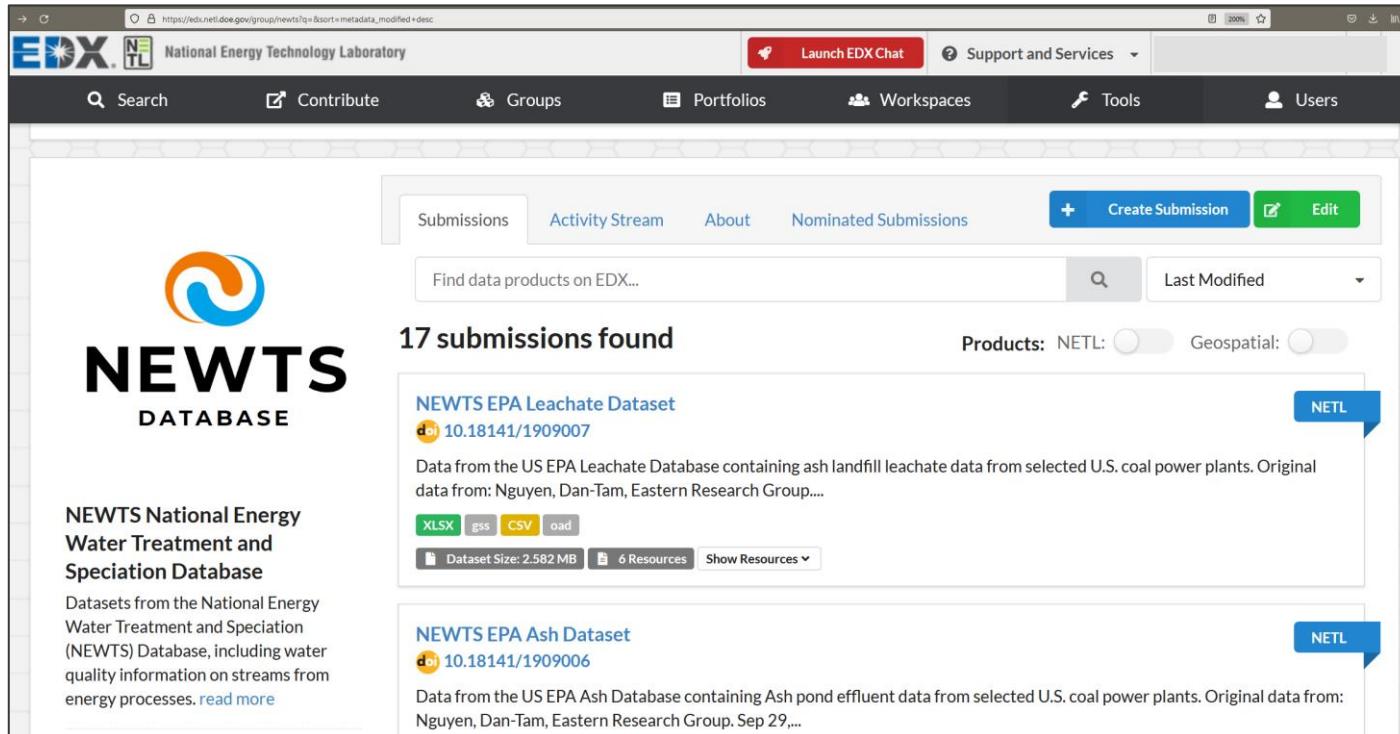
Leveraging NETL R&D Core Capabilities

Solution: Develop a Nationwide Energy Wastewater Data System

- Supplemented with thermodynamic & chemical modeling
- Includes **waste streams** such as:
 - USGS oil & gas produced water
 - Energy sector effluent (FGD, etc.)
 - Acid mine drainage (OSMRE)
 - Landfill leachate
 - And more
- Enables design of localized treatment
- **Publicly Available Data** hosted & displayed through **NETL's EDX**, and a custom visualization dashboard



NEWTS Public Group on EDX

A screenshot of the NEWTS Public Group on EDX website. The page shows a search interface with a 'Create Submission' button and a 'Last Modified' dropdown. Below this, a search bar and a 'Find data products on EDX...' button are visible. A message '17 submissions found' is displayed. Two datasets are listed: 'NEWTS EPA Leachate Dataset' (version 10.18141/1909007) and 'NEWTS EPA Ash Dataset' (version 10.18141/1909006). Each dataset entry includes a small thumbnail, a download link (XLSX, gss, CSV, oad), a dataset size (2.582 MB), and a '6 Resources' link. A 'Show Resources' dropdown is also present. The left sidebar features the NEWTS Database logo and a brief description of the database, along with a 'read more' link. A QR code is located at the bottom left of the page.The NEWTS Database logo is displayed, featuring a stylized orange and blue swirl icon above the text 'NEWTS DATABASE NATIONAL ENERGY WATER TREATMENT & SPECIATION'. The background of the logo shows a blurred image of a large industrial facility with many rows of solar panels or similar equipment under a cloudy sky.

- NEWTS Data Catalog
- [Overview Video](#)
- Training Videos

<https://edx.netl.doe.gov/group/newts>

- EPA FGD, Ash, Leachate, Gasification datasets + case studies
- USGS Brackish Waters & Produced Waters databases + case studies
- Acid mine drainage data
- Assessment of REEs in geothermal and oil & gas produced brines
- Templates for each dataset for input into OLI Studio & Geochemist's WorkBench

NEWTS Dashboard

NEWTS Database Dashboard
National Energy Water Treatment and Speciation



State:
None



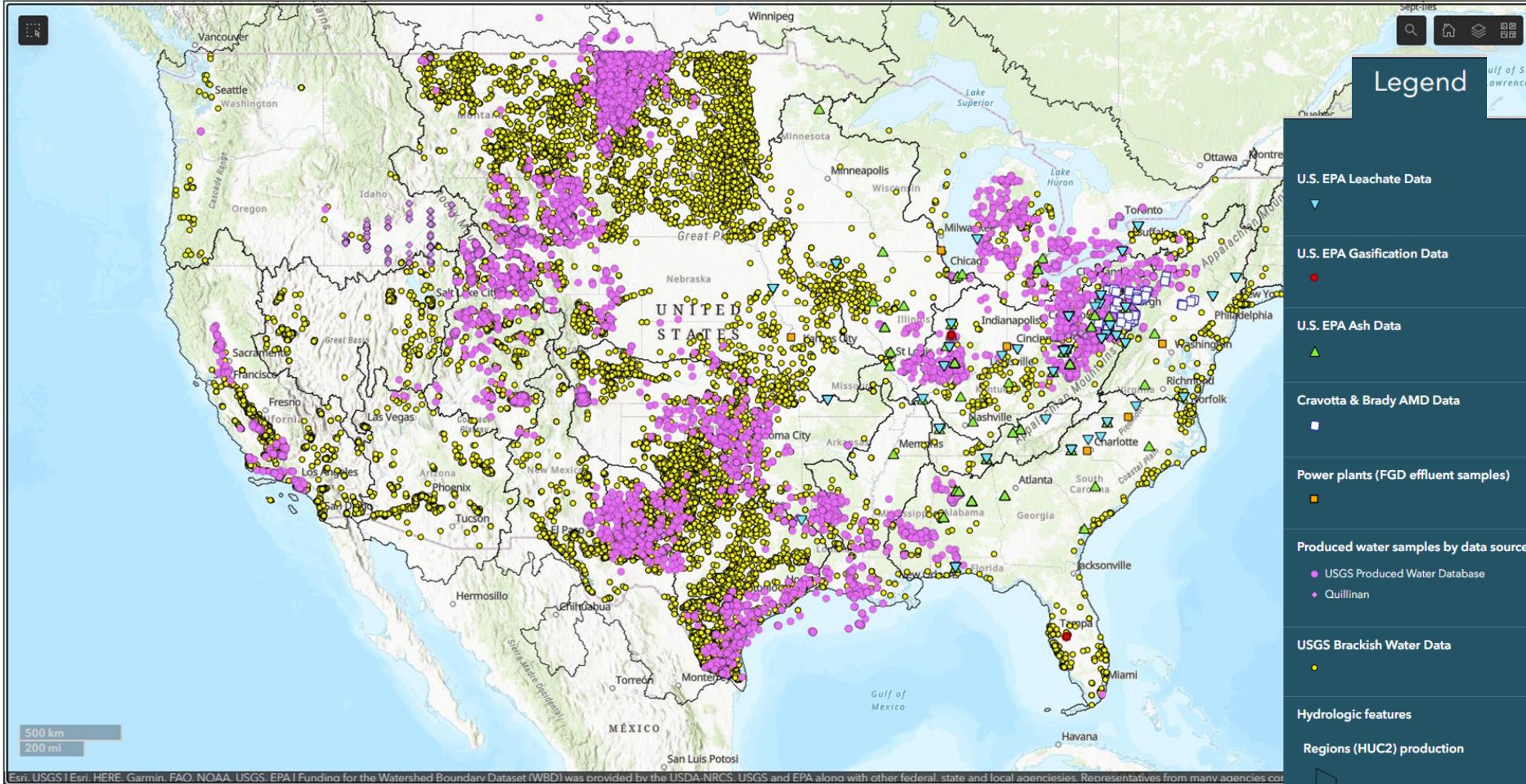
County:
None



Sedimentary basin:
None



NEWTS Dashboard

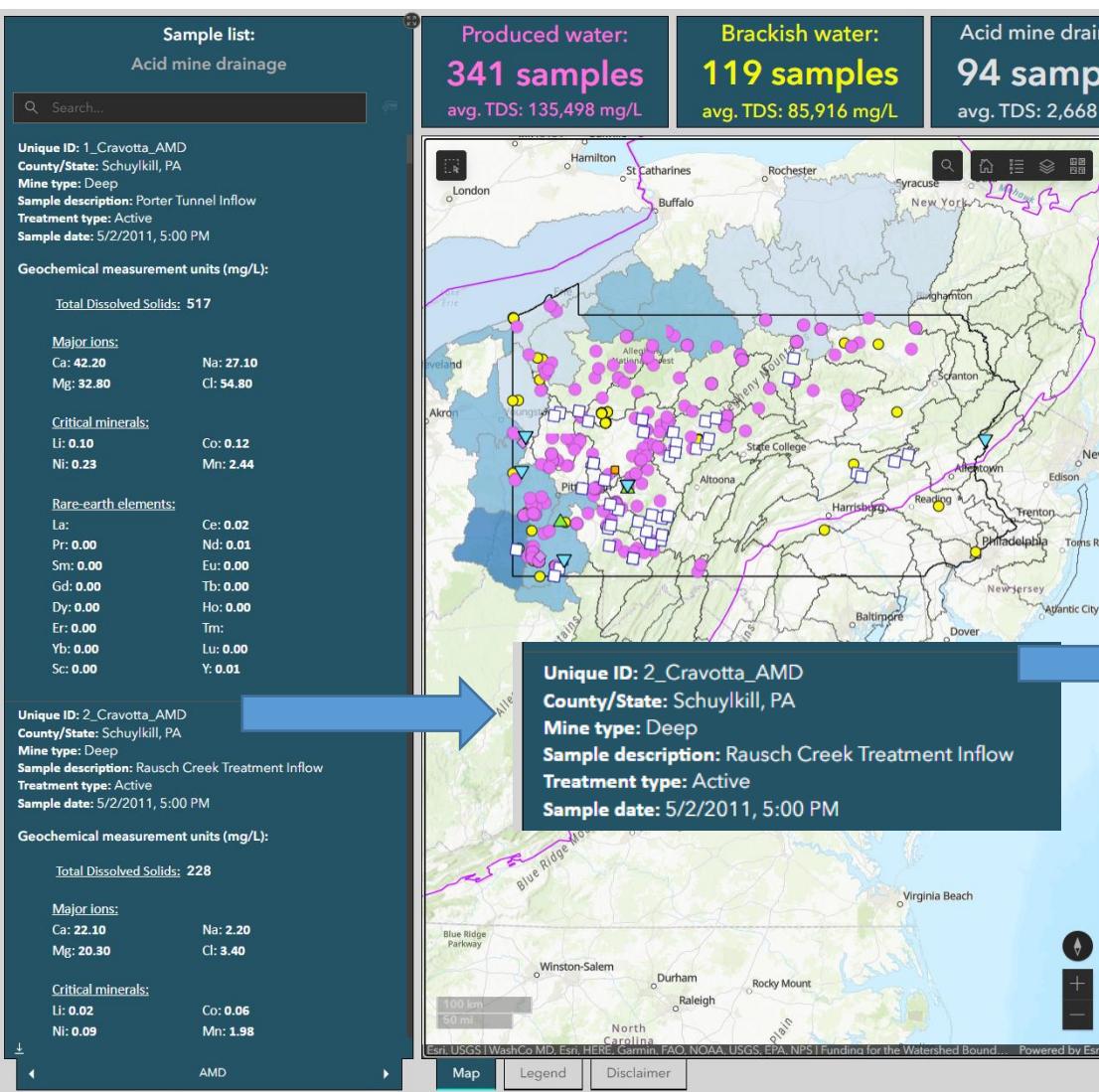


Enables data visualization, exploration, and download

Connecting NEWTS Dashboard to the Database



<https://edx.netl.doe.gov/group/newts>



Submissions Activity Stream About Nominated Submissions + Create Submission Edit

Find data products on EDX... Relevance

17 submissions found

Products: NETL: Geospatial:

NEWTS DATABASE

NEWTS National Energy Water Treatment and Speciation Database
Datasets from the National Energy Water Treatment and Speciation

Case studies from the USGS Brackish Water Database. Includes OLI Studio and Geochemist's Workbench files. Original data from: Qi, S.L., and Harris, A.C., 2017, Geochemical...

NEWTS USGS Brackish Water Case Studies
DOI: 10.18141/1890176

Case studies from the USGS Brackish Water Database. Includes OLI Studio and Geochemist's Workbench files. Original data from: Qi, S.L., and Harris, A.C., 2017, Geochemical...

NEWTS Coal Mine Drainage Dataset from Cravotta Brady (2015)
DOI: 10.18141/1964003

Data from Cravotta, Brady, "Priority pollutants and associated constituents in untreated and treated discharges from coal mining or processing facilities in Pennsylvania, USA"....

NEWTS Database Dashboard
DOI: 10.18141/1963919

The NEWTS (National Energy Water Treatment and Speciation) database dashboard displays sites across the nation where energy-related wastewater stream samples and composition...

Connecting NEWTS Dashboard to the Database

<https://edx.netl.doe.gov/group/newts>



NEWTS Coal Mine Drainage Dataset from Cravotta Brady (2015)

doi 10.18141/1964003

License(s):

License Not Specified

Data from Cravotta, Brady, "Priority pollutants and associated constituents in untreated and treated discharges from coal mining or processing facilities in Pennsylvania, USA". Applied Geochemistry, 2015. <https://doi.org/10.1016/j.apgeochem.2015.03.001>

Dataset includes information on water quality composition including inorganic compounds from untreated and treated streams of coal-mine discharge from coal mining and coal processing locations. Data is provided in the original version as well as in a summarized version for easy input into aqueous chemistry modeling software.

Followers: 0

Follow

cravottabradypa-amd_data_all-tabs.xlsx
 License Not Specified

cb-pa-amd_lion-minning-grove-inflow_id_num-18.oad
 License Not Specified

cb-pa-amd_pbs-job-8-inflow_id-num-25.oad
 License Not Specified

cravotta_oli_input_data_only.csv
 License Not Specified

cb-pa-amd_consol-renton-mine-inflow_id_num-39.oad
 License Not Specified

oli-template-for-cravotta-brady-2015.oad
 License Not Specified

Unique ID: 2_Cravotta_AMD
County/State: Schuylkill, PA
Mine type: Deep
Sample description: Rausch Creek Treatment Inflow
Treatment type: Active
Sample date: 5/2/2011, 5:00 PM

or

or

or

or

or



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CRV002	237			

Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment



Integrating data streams with open source & commercial aqueous chemistry modeling software to:

- Provide high quality case studies for modeling
- Information on precipitates and speciation
- Provide thermodynamic context including pH, osmotic pressure, and activity coefficients, etc.
- Enable direct integration with treatment modeling software for ease of use

Software include:

- OLI Studio
- Geochemist's Workbench
- DuPont Wave
- NAWI Water-Tap3



U.S. DEPARTMENT OF
ENERGY

Case Studies publicly available on

[EDX NEWTS Group](#)

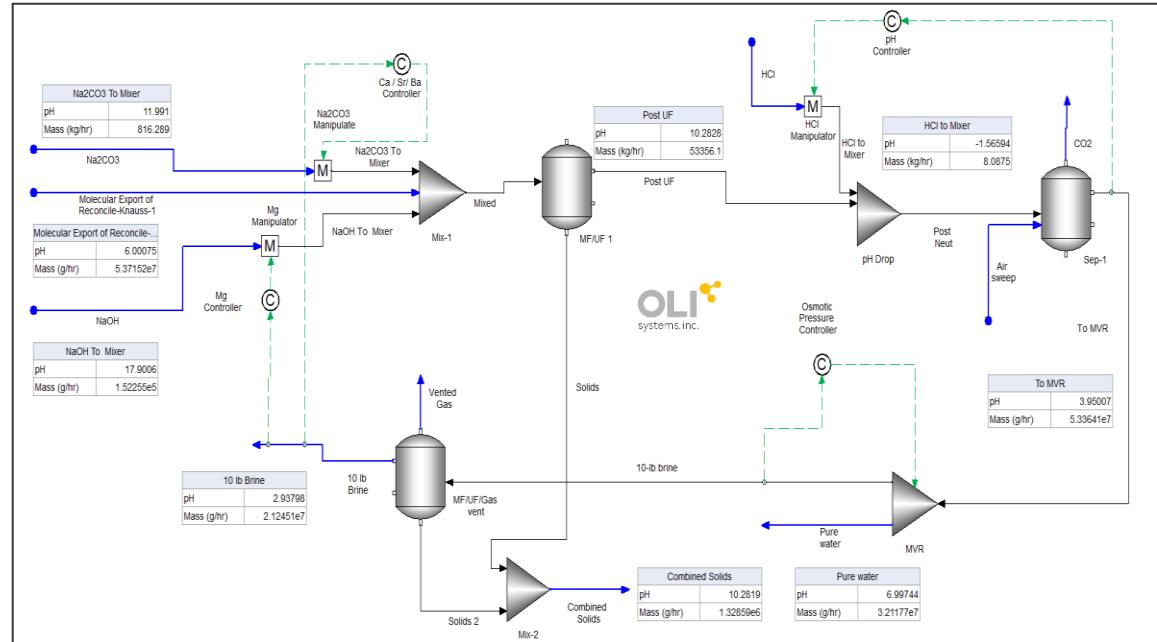
The screenshot shows the NEWTS Database interface. At the top, there is a navigation bar with 'Data and Resources' and buttons for 'Download Checked' and 'Check All'. Below this is a search bar labeled 'Filter resources by name...'. A dropdown menu shows 'Date: Newest → Oldest'. The main content area displays a list of datasets with columns for 'File Type', 'Name', and 'License'. Below the list is a table titled 'Datasets from the National Energy Water Treatment and Speciation Database' with columns for 'Analyte', 'Procedure', 'Units', 'Wght. Avg.', 'Input', 'Converted Units', and 'Converted Avg.'. The table lists various chemical elements and their properties.

Analyte	Procedure	Units	Wght. Avg.	Input	Converted Units	Converted Avg.
Alkalinity, HCO3		mg/L	48.03	HCO3-	mg/L	48.03
Aluminum	Total	ug/L			mg/L	
Ammonia as N	Total	mg/L			mg/L	
Antimony	Total	ug/L			mg/L	
Arsenic	Total	ug/L	190.00	AsO4-3	mg/L	0.35
Beryllium	Total	ug/L			mg/L	
Boron	Total	ug/L	167,106.67	B as B(OH)3	mg/L	167.11
Bromide	Total	mg/L	27.35	Br-	mg/L	0.03
Cadmium	Total	ug/L	0.00	Cd+2	mg/L	0.00
Calcium	Total	ug/L	2,079,500.00	Ca+2	mg/L	2,079.50
Chemical Oxygen Demand	Total	mg/L			mg/L	
Chloride	Total	mg/L	2,389.67	Cl-	mg/L	2,389.67
Chromium	Total	ug/L	200.07	Cr(OH)3	mg/L	0.40
Cobalt	Total	ug/L		Co+2	mg/L	
Copper	Total	ug/L	158.62	Cu+2	mg/L	0.16
Lithium	Total	mg/L	290.25	Li+	mg/L	0.29
Magnesium	Total	ug/L	1,014,700.00	Mg+2	mg/L	1,014.70
Manganese	Total	ug/L			mg/L	
Mercury	Total	ng/L	89,133.33	Hg+2	mg/L	0.09

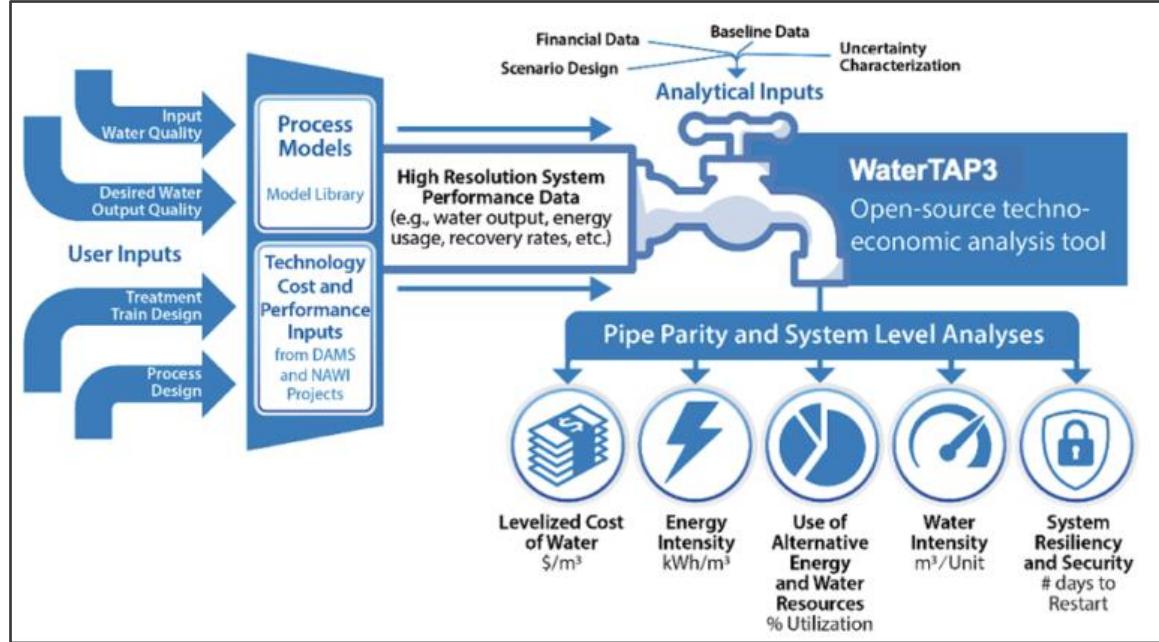


Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment



Input Water Stream



Input Water Quality



National Alliance
for Water Innovation

Ease of Input into Aqueous Chemistry Software

OLI Studio example



- Templates have been created so that water stream compositions can be easily input into OLI Studio and GWB Geochemist's Spreadsheet (GSS)

F9	File	Home	Insert	Page Layout	Formulas	Data	Review	View	Automate	Help	Comments	Share
	A	B	C	D	E	F	G	H	I	J	AF	AG
1	MW of mo	MW of el	SNAME	Descripti	Redox State		Porter	Tur	Rausch	Cr Silver	PBS Job 8	PBS Trent
2			MINE_NUM				1	2	3	22	23	
3			STAID				4.04E+14	4.04E+14	4.04E+14	4E+14	4E+14	
4			Lon_dd				40.60056	40.62994	40.73417	40.40333	40.01122	4
5			Lat_dd				-76.5058	-76.554	-76.1233	-78.8122	-78.9285	-7
6			Mine_Type				Deep	Deep	Deep	Surface	Surface	
7			Passive_Active				Active	Active	Passive	Active	Active	Act
8			Chemical_trt				CaO	CaO	Wetlands	NaOH	NaOH	Na
9			Inflow_Outflow				I	I	I	I	I	I
10			DATE				110503	110503	110503	110525	110525	
11			TIME				1000	1230	1430	1215	1345	
12	TDS	Total Dissolu	Total	mg/L			517.25	228	389.5	1952.5	1305	
13	PH	pH					3.51	6.26	5.99	6.38	5.76	
14	Alkalinity	Alkalinity	Blank & Total	Comt	mg/L as CaCO3		5.3	36	122	31.3		
15	TIC	TIC		mol	C/L		2.39	1.38	18.9	40.4	20.3	
16	Density			g/mL								
17	Specific E	COND		µS/cm			802	311	504	2150	1490	
18	61.84	10.811	B(OH)3	Boron	Hydroxide	Not Meas	mg/L of B(OH)3					
19	43.03	9.01	Be(OH)2	Beryllium		2	mg/L of Be(OH)2	1.86E-02	5.73E-03	1.15E-02	8.60E-03	
20	140.436	106.42	Pd(OH)2	Palladium		2	mg/L of Pd(OH)2					
21	78	27	Al(OH)3	Aluminum		3	mg/L of Al(OH)3	1.35E+01	2.40E+00	5.66E+00	4.28E+00	
22	260.004	208.98	Bi(OH)3	Bismuth	Bi_Total	3	mg/L of Bi(OH)3					
23	85	52	Cr(OH)2	Chromium	Cr_Total	3	mg/L of Cr(OH)2	2.62E-03				
24	102.7	69.7	Ga(OH)2	Gallium	Ga_Total	3	mg/L of Ga(OH)2	1.62E-04	5.89E-05	8.84E-05	3.24E-04	1.52E-03
25	165.8	114.8	In(OH)3	Indium	In_Total	3	mg/L of In(OH)3	1.30E-05	1.44E-06		2.89E-06	
26	169.102	101.07	Ru(OH)4	Ruthenium		4	mg/L of Ru(OH)4					
27	60	60	SiO2	Silica		4	mg/L of SiO2	2.46E+01	1.81E+01	2.81E+01	1.60E+01	2.61E+01
28	150.71	118.71	TiO2	Tin		4	mg/L of SnO2					
29	264.04	232.04	ThO2	Thorium	Th_T	4	mg/L of ThO2	4.09E-04	4.89E-05	7.97E-06	1.12E-04	3.
30	79.9	47.9	TiO2	Titanium		4	mg/L of TiO2	3.50E-03	2.00E-03	2.50E-03	2.50E-03	5.67E-03
31	123.2	91.2	ZrO2	Zirconium		4	mg/L of ZrO2	2.70E-05	1.35E-05	2.70E-05	6.75E-05	1.
32	206.76	121.76	Sb(OH)5	Antimony	hydroxide	5	mg/L of Sb(OH)5	1.70E-05	1.70E-05	3.40E-05	8.49E-05	
33	286.03	238.03	UO3	Uranium		6	mg/L of UO3	1.61E-03	3.05E-04	2.64E-04	2.16E-05	9.96E-04
34	94.11	94.11	C6H5OH	Phenol		organic	mg/L of C6H5OH	3.00E-04				
35	16	16	O2	Oxygen		0	mg/L of O2	10.6	10.7	1.68	1.5	5.79
36	18	14	NH4+	Ammonium		-3	mg/L of NH4+	1.54E-01	1.29E-01	2.83E-01	2.31E-01	1.17E-00
37	107.9	107.9	Ag+	Silver		1	mg/L of Ag+					
38	132.9	132.9	Cs+	Cesium	Cs	1	mg/L of Cs+	1.46E-04	8.70E-05	1.94E-04	1.50E-05	1.79E-04
39	39.1	39.1	K+	Potassium		1	mg/L of K+	7.31E+00	1.60E+00	1.30E+00	3.14E+00	5.75E+00
40	6.941	6.941	Li+	Lithium		1	mg/L of Li+	9.85E-02	2.30E-02	4.50E-02	2.40E-02	3.10E-02
41	22.9897	22.9897	Na+	Sodium		1	mg/L of Na+	2.71E+01	2.20E+01	2.40E+00	3.95E+00	9.85E+00
42	85.468	85.468	Rb+	Rubidium		1	mg/L of Rb+	8.11E-03	3.04E-03	2.51E-03	2.99E-03	1.39E-02
43	204.38	204.38	Tl+	Thallium		1	mg/L of Tl+	7.90E-05	3.40E-05	2.30E-05	1.44E-04	3.
44	137.3	137.3	Ra2+	Barium		2	mg/L of Ra2+	2.05E-02	2.91E-02	2.02E-02	1.11E-02	2.89E-02

Reconcile

Description **Reconciliation** **Molecular Basis** **Report**

Variable	Value
Analysis Parameters	
Stream Amount (L)	1.00000
Temperature (°C)	25.0000
Pressure (atm)	1.0000
Recorded Properties	
Total Dissolved Solids (mg/L)	12900.0
Measured pH	6.22000
Measured Alkalinity (mg HCO_3/L)	432.000
Measured TIC (mol C/L)	118.000
Density (g/mL)	0.0
Specific Electrical Conductivity ($\mu\text{mho}/\text{cm}$)	13000.0
Calculation Parameters	
Alkalinity pH Titrant	H_2SO_4
Alkalinity End Point pH	4.50000
Neutrals (mg/L)	
H_2O	0.0
CO_2	0.0
H_2S	0.0
$\text{B}(\text{OH})_3$	2.39000e-3
$\text{Be}(\text{OH})_2$	0.0
$\text{P}(\text{OH})_2$	0.0
$\text{Al}(\text{OH})_3$	0.289000
$\text{B}(\text{OH})_3$	0.0
HClO_2	6.21000e-5
GaOOH	1.92000e-4
$\text{In}(\text{OH})_3$	4.33000e-5
$\text{Ru}(\text{OH})_4$	8.37000e-5
SiO_2	19.0000
SnO_2	0.0
ThO_2	1.25000e-5
TiO_2	0.0185000
ZrO_2	2.61000e-5
$\text{Sb}(\text{OH})_5$	1.70000e-5
UO_3	6.42000e-4
V_2O_5	0.0
O_2	7.57000
Total Ions (mg/L)	
Cations (mg/L)	
NH_4^+	7.53000
Ag^+	0.0
K^+	8.30000e-4
Measured	11.8000

Advanced Search Add as Stream Export

Reconciliation

Specs...

Reconcile

Reconcile pH

Reconcile pH/Alkalinity

Reconcile pH/Alkalinity/TIC

Calculate Alkalinity

Calculate

Summary

Unit Set: Metric (mass concentration)

Automatic Chemistry Model

MSE (H3O+ ion) Databanks:

MSE (H_3O^+ ion)

Using Helgeson Direct

Na/Cl Charge Balance (eq/L):

Cation Charge: 0.187601 eq/L

Anion Charge: -0.189144 eq/L

Imbalance: -1.543186e-3 eq/L

35.478 mg/L of Na^+ is needed to balance.

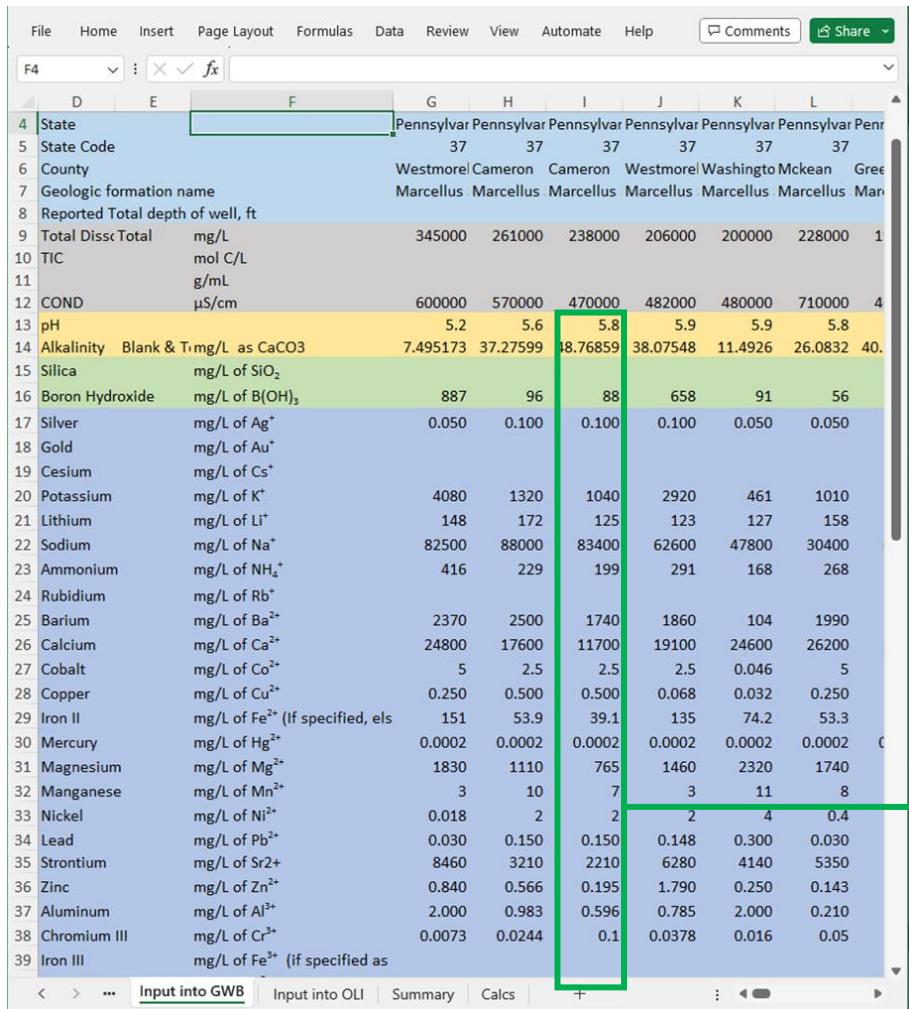
Alkalinity Calculation

25.0000 °C 1.00000 atm

Calculation not done

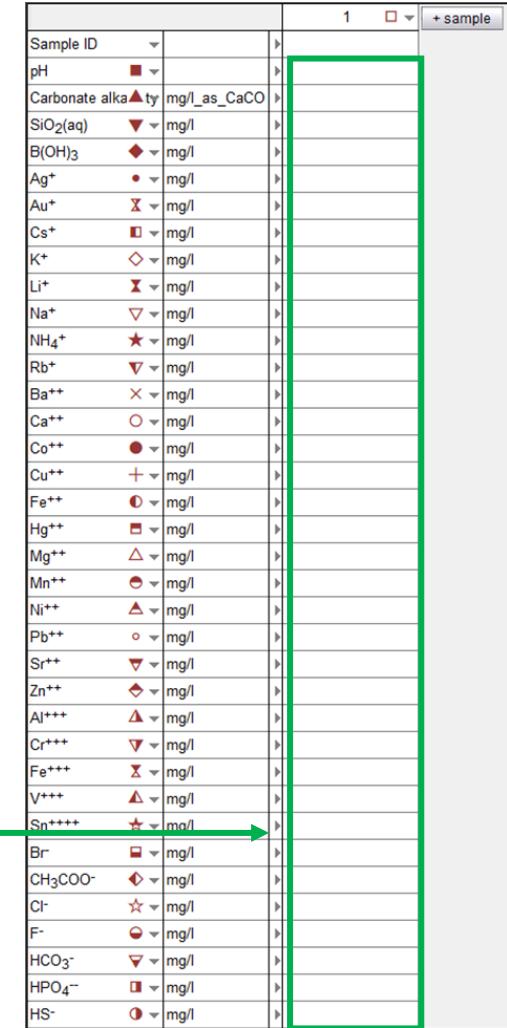
Ease of Input into Aqueous Chemistry Software

Geochemist's Workbench example



State	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan
5 State Code	37	37	37	37	37	37
6 County	Westmorel	Camer	Camer	Westmorel	Washingto	McKean
7 Geologic formation name	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus
8 Reported Total depth of well, ft						
9 Total Dissc Total	mg/L	345000	261000	238000	206000	200000
10 TIC	mol C/L					
11	g/mL					
12 COND	µS/cm	600000	570000	470000	482000	480000
13 pH		5.2	5.6	5.8	5.9	5.9
14 Alkalinity	Blank & T ₁ mg/L as CaCO ₃	7.495173	37.27599	48.76859	38.07548	11.4926
15 Silica	mg/L of SiO ₂					
16 Boron Hydroxide	mg/L of B(OH) ₃	887	96	88	658	91
17 Silver	mg/L of Ag ⁺	0.050	0.100	0.100	0.100	0.050
18 Gold	mg/L of Au ⁺					
19 Cesium	mg/L of Cs ⁺					
20 Potassium	mg/L of K ⁺	4080	1320	1040	2920	461
21 Lithium	mg/L of Li ⁺	148	172	125	123	127
22 Sodium	mg/L of Na ⁺	82500	88000	83400	62600	47800
23 Ammonium	mg/L of NH ₄ ⁺	416	229	199	291	168
24 Rubidium	mg/L of Rb ⁺					
25 Barium	mg/L of Ba ²⁺	2370	2500	1740	1860	104
26 Calcium	mg/L of Ca ²⁺	24800	17600	11700	19100	24600
27 Cobalt	mg/L of Co ²⁺	5	2.5	2.5	2.5	0.046
28 Copper	mg/L of Cu ²⁺	0.250	0.500	0.500	0.068	0.032
29 Iron II	mg/L of Fe ²⁺ (If specified, els	151	53.9	39.1	135	74.2
30 Mercury	mg/L of Hg ²⁺	0.0002	0.0002	0.0002	0.0002	0.0002
31 Magnesium	mg/L of Mg ²⁺	1830	1110	765	1460	2320
32 Manganese	mg/L of Mn ²⁺	3	10	7	3	11
33 Nickel	mg/L of Ni ²⁺	0.018	2	2	4	0.4
34 Lead	mg/L of Pb ²⁺	0.030	0.150	0.150	0.148	0.300
35 Strontium	mg/L of Sr ²⁺	8460	3210	2210	6280	4140
36 Zinc	mg/L of Zn ²⁺	0.840	0.566	0.195	1.790	0.250
37 Aluminum	mg/L of Al ³⁺	2.000	0.983	0.596	0.785	2.000
38 Chromium III	mg/L of Cr ³⁺	0.0073	0.0244	0.1	0.0378	0.016
39 Iron III	mg/L of Fe ³⁺ (if specified as					

- Templates have been created so that water stream compositions can be easily input into OLI Studio and GWB Geochemist's Spreadsheet (GSS)



Sample ID		
pH	■	
Carbonate alkalinity	▲ mg/l as CaCO ₃	
SiO ₂ (aq)	▼ mg/l	
B(OH) ₃	◆ mg/l	
Ag ⁺	● mg/l	
Au ⁺	✗ mg/l	
Cs ⁺	■ mg/l	
K ⁺	◇ mg/l	
Li ⁺	✗ mg/l	
Na ⁺	▼ mg/l	
NH ₄ ⁺	★ mg/l	
Rb ⁺	▼ mg/l	
Ba ⁺⁺	✗ mg/l	
Ca ⁺⁺	○ mg/l	
Co ⁺⁺	● mg/l	
Cu ⁺⁺	✚ mg/l	
Fe ⁺⁺	● mg/l	
Hg ⁺⁺	■ mg/l	
Mg ⁺⁺	△ mg/l	
Mn ⁺⁺	● mg/l	
Ni ⁺⁺	▲ mg/l	
Pb ⁺⁺	○ mg/l	
Sr ⁺⁺	▼ mg/l	
Zn ⁺⁺	◆ mg/l	
Al ⁺⁺⁺	▲ mg/l	
Cr ⁺⁺⁺	▼ mg/l	
Fe ⁺⁺⁺	✗ mg/l	
V ⁺⁺⁺	▲ mg/l	
Sn ⁺⁺⁺⁺	★ mg/l	
Br ⁻	■ mg/l	
CH ₃ COO ⁻	◆ mg/l	
Cl ⁻	★ mg/l	
F ⁻	● mg/l	
HCO ₃ ⁻	▼ mg/l	
HPO ₄ ²⁻	■ mg/l	
HS ⁻	● mg/l	

Aqueous Chemistry Modeling: Case Studies



Using OLI Studio to evaluate scale tendency of FGD effluent from Roxboro plant

Input into OLI Studio

Unique_ID	Analyte	Procedure Unit	270
Date Collected	-	-	7/28/2008
Sample Point	-	-	Influent after set basin
Type of Wastewater	-	-	Settling Pond Effluent
Sample Description	-	-	Effluent from Settling Pond
Wastewater Classification	-	-	FGD Pond Effluent
Plant Name	-	-	Roxboro
Plant ID	-	-	9391
Total Dissolved Solids Total	Total Diss. Total	mg/L	
pH			
#REF!	#REF!	Blank & T mg/L as CaCO ₃	
Silica	Silica	mg/L of SiO ₂	
B(OH) ₃	Boron Hydroxide	mg/L of B(OH) ₃	441.0197022
TiO ₂	Titanium dioxide	mg/L of TiO ₂	
Sb(OH) ₅	Antimony hydroxide	mg/L of Sb(OH) ₅	0.095772536
Al(OH) ₃	Aluminum	mg/L of Al(OH) ₃	1.487777778
Be(OH) ₂	Beryllium	mg/L of Be(OH) ₂	0.003963918
CrO(OH)	Chromium	mg/L of CrO(OH)	0.016346154
Ag ⁺	Silver	mg/L of Ag ⁺	0.0002
K ⁺	Potassium	mg/L of K ⁺	
Li ⁺	Lithium	mg/L of Li ⁺	
Na ⁺	Sodium	mg/L of Na ⁺	
NH ₄ ⁺	Ammonium	mg/L of NH ₄ ⁺	
Tl ⁺	Thallium	mg/L of Tl ⁺	0.00241
VO ₂ ⁺	Vanadium	mg/L of VO ₂ ⁺	0.02279466
Ba ²⁺	Barium	mg/L of Ba ²⁺	0.408
Ca ²⁺	Calcium	mg/L of Ca ²⁺	
Cd ²⁺	Cadmium	mg/L of Cd ²⁺	0.00277
Co ²⁺	Cobalt	mg/L of Co ²⁺	0.022
Cu ²⁺	Copper	mg/L of Cu ²⁺	0.016
Hg ²⁺	Mercury	mg/L of Hg ²⁺	0.00116
Mg ²⁺	Magnesium	mg/L of Mg ²⁺	
Mn ²⁺	Manganese	mg/L of Mn ²⁺	1.88
Ni ²⁺	Nickel	mg/L of Ni ²⁺	0.126
Pb ²⁺	Lead	mg/L of Pb ²⁺	0.019
Sr ²⁺	Strontrium	mg/L of Sr ²⁺	
Zn ²⁺	Zinc	mg/L of Zn ²⁺	0.038
Fe ³⁺	Iron	mg/L of Fe ³⁺	1.04
Mo ³⁺	Molybdenum	mg/L of Mo ³⁺	0.0449
Sn ⁴⁺	Tin	mg/L of Sn ⁴⁺	
Br ⁻¹	Bromide	mg/L of Br ⁻	
Cl ⁻¹	Chloride	mg/L of Cl ⁻	4300
F ⁻¹	Fluoride	mg/L of F ⁻	9.4
CN ⁻¹	Cyanide	mg/L of CN ⁻	
NO ₃ ⁻¹	Nitrate	mg/L of NO ₃ ⁻	
CrO ₄ ⁻²	Chromate	mg/L of CrO ₄ ⁻²	
SO ₄ ⁻²	Sulfate	mg/L of SO ₄ ⁻²	
SO ₃ ⁻²	Sulfite	mg/L of SO ₃ ⁻²	
SeO ₄ ⁻²	Selenate	mg/L of SeO ₄ ⁻²	
SeO ₃ ⁻²	Selenite	mg/L of SeO ₃ ⁻²	
AsO ₄ ⁻³	Arsenic(V) Tetraoxid	mg/L of AsO ₄ ⁻³	
PO ₄ ⁻³	Phosphate	mg/L of PO ₄ ⁻³	



OLI Studio Output Report

Scaling Tendencies

Row Filter Applied: Values > 1.0e-4

Solids	Post-Scale
Fe(OH) ₃ (Bernalite)	1.00000
Ba SO ₄ (Barite)	1.00000
Pb SO ₄ (Anglesite)	0.0195029
B(OH) ₃	0.0101386
AgCl	1.96141e-3
Al(OH) ₃ (Gibbsite)	1.47368e-4

Post-Scale Q/K

Pre-Scale Q/K

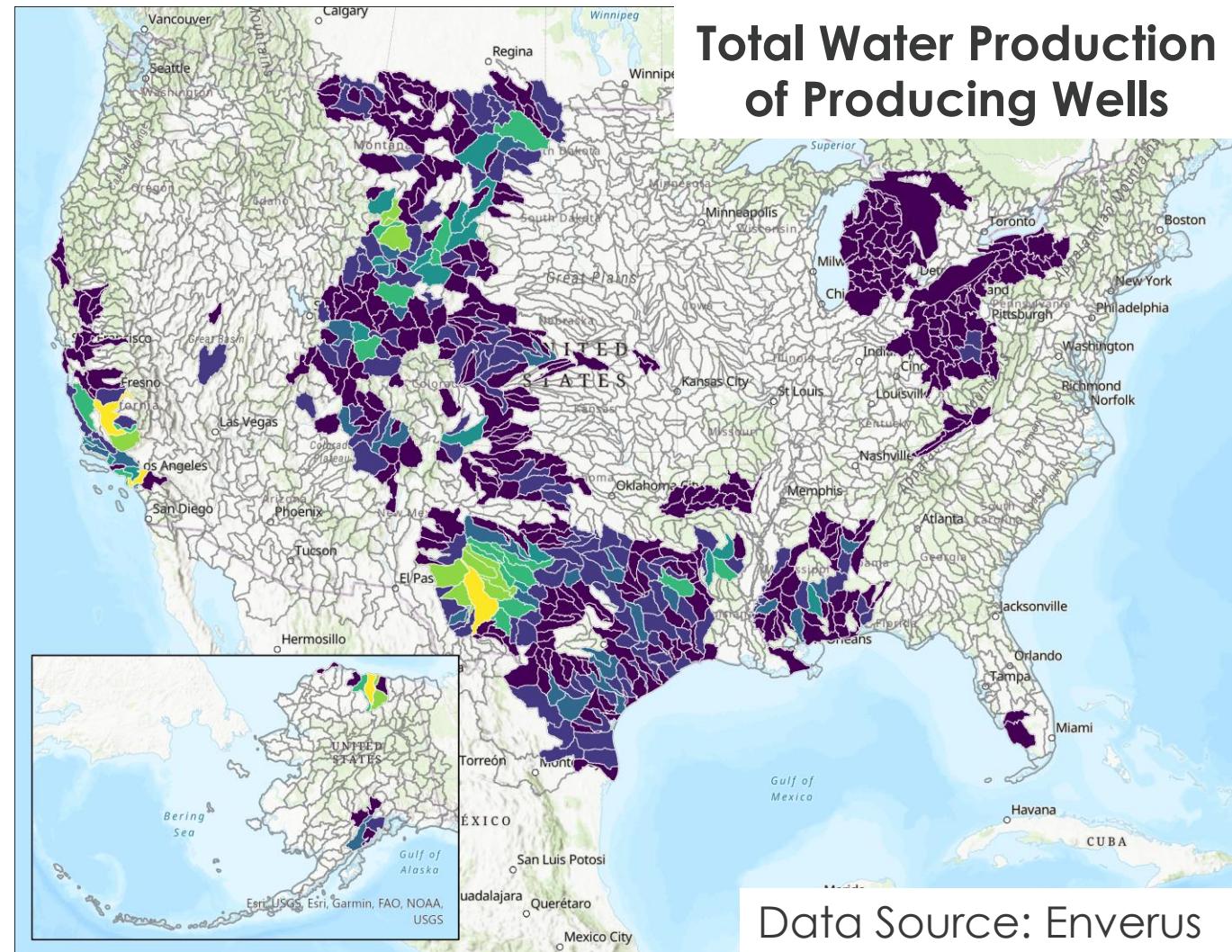
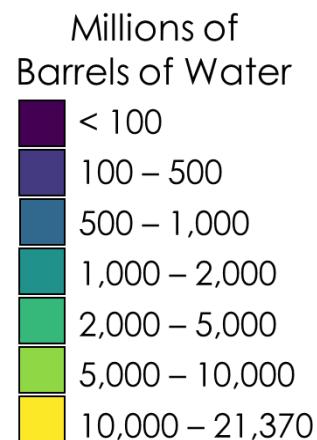
Kinetic induction time for scaling can be estimated for Barite, Gypsum, Calcite, and Celestine with others (silica) likely in the future



U.S. DEPARTMENT OF
ENERGY

Integrating water volume data

- Acquired **5,096,329 well records** (Enverus)
- Spatially aggregated **5,044,327 records** to **Hydrologic Unit Code 8 (HUC 8) subbasins** (grey outlines on map)
- Reducing to **HUC 2** values for CM level estimates
- Production data spatially compiled by **well status** (i.e., active, injecting, abandoned)
 - Well count
 - **Cumulative production**
 - Water, Oil, Gas
 - **Vertical depth statistics**
 - Supports at-depth composition
 - **Temporal trends**
 - Producing months statistics

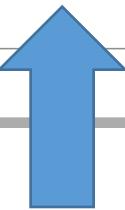


Data Catalog and Citing Datasets with DOI#’s

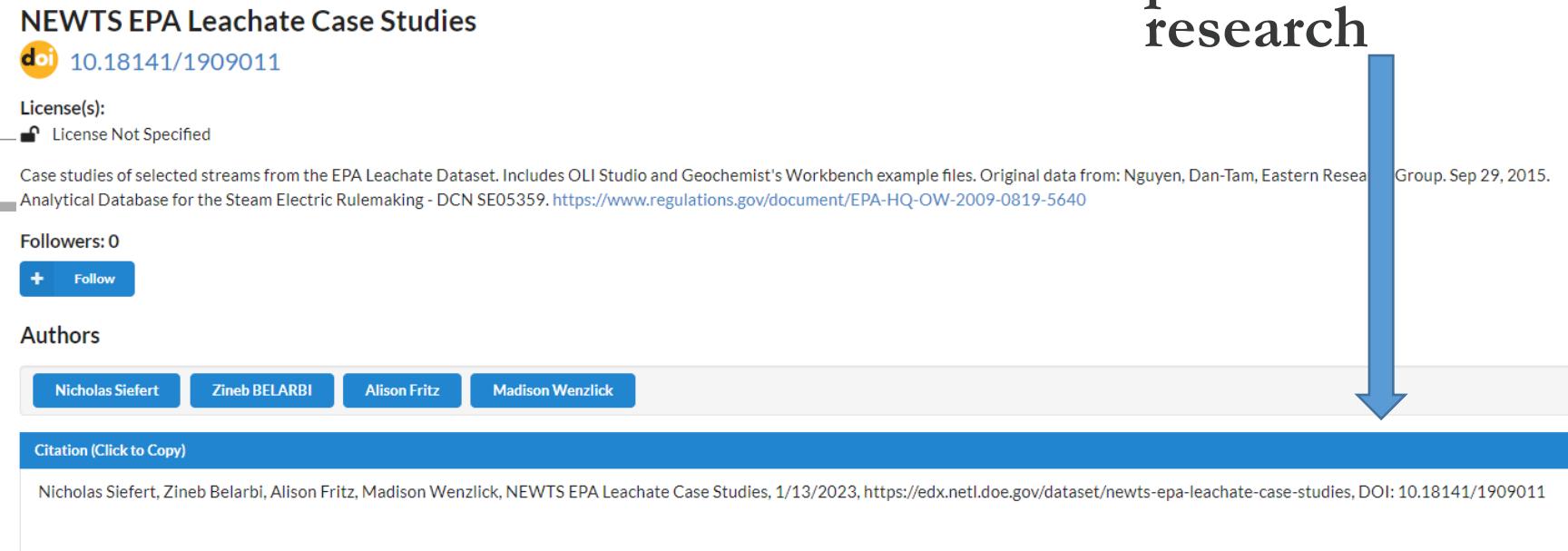


- Most NEWTS datasets have unique DOI#’s with citations
- Please cite if using data in publishable research

	Data	NEWTS Dataset File Name	Original Data Citation	URL
0	USGS Brackish Water Database	usgs-brackish-water_all-tabs.xlsx	Qi, S.L., and Harris, A.C., 2017, Geochemical Database for the Brackish Groundwater Assessment of the United States: U.S. Geological Survey data release, https://doi.org/10.5066/F72F7KK1 .	https://doi.org/10.5066/F72F7KK1
1	EPA FGD Effluent Database	epa-fgd-effluent_all-tabs.xlsx	Nguyen, Dan-Tam, Eastern Research Group. Sep 29, 2015. Analytical Database for the Steam Electric Rulemaking - DCN SE05359.	https://www.regulations.gov/document/EPA-HQ-OW-2009-0819-5640



- Data Catalog summarizes sources for all data sets on EDX



NEWTS EPA Leachate Case Studies

doi 10.18141/1909011

License(s):

License Not Specified

Case studies of selected streams from the EPA Leachate Dataset. Includes OLI Studio and Geochemist's Workbench example files. Original data from: Nguyen, Dan-Tam, Eastern Research Group. Sep 29, 2015. Analytical Database for the Steam Electric Rulemaking - DCN SE05359. <https://www.regulations.gov/document/EPA-HQ-OW-2009-0819-5640>

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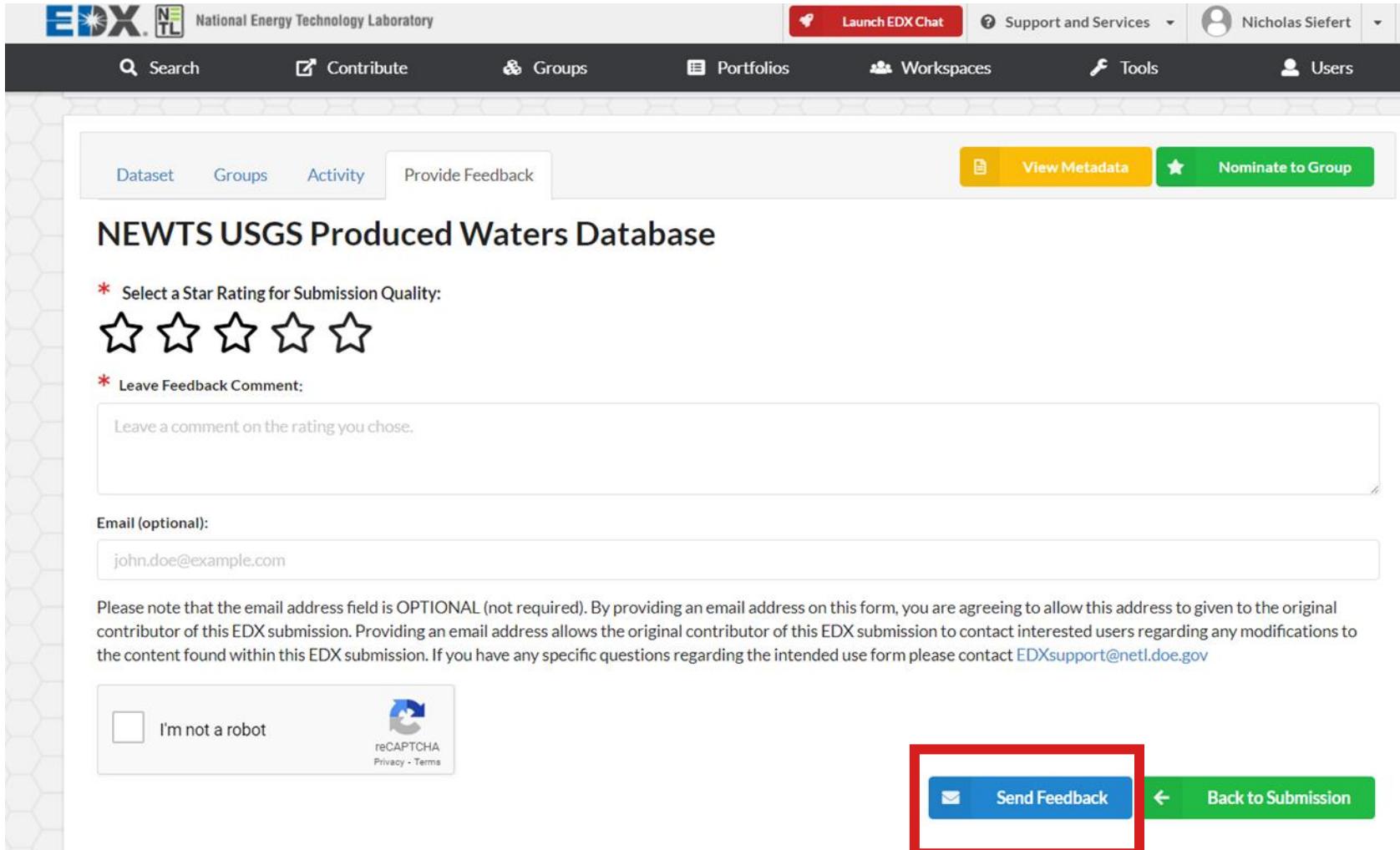
Citation (Click to Copy)

Nicholas Siefert, Zineb Belarbi, Alison Fritz, Madison Wenzlick, NEWTS EPA Leachate Case Studies, 1/13/2023, <https://edx.netl.doe.gov/dataset/newts-epa-leachate-case-studies>, DOI: 10.18141/1909011



Providing Feedback

- Preferred option: Comments on submissions can be sent through the EDX site
- Or reach out to dataset authors listed for each resource



The screenshot shows the EDX platform interface. At the top, there is a navigation bar with the EDX logo, the text "National Energy Technology Laboratory", and links for "Launch EDX Chat", "Support and Services", and a user profile for "Nicholas Siefert". Below the navigation bar, there is a secondary navigation bar with links for "Search", "Contribute", "Groups", "Portfolios", "Workspaces", "Tools", and "Users".

The main content area displays a dataset titled "NEWTS USGS Produced Waters Database". It includes a section for "Provide Feedback" with the following fields:

- "Select a Star Rating for Submission Quality": A row of five stars, with the first four filled and the last one outlined.
- "Leave Feedback Comment": A text input field with the placeholder "Leave a comment on the rating you chose." and a scrollable area below it.
- "Email (optional)": A text input field containing "john.doe@example.com".
- A note below the email field: "Please note that the email address field is OPTIONAL (not required). By providing an email address on this form, you are agreeing to allow this address to be given to the original contributor of this EDX submission. Providing an email address allows the original contributor of this EDX submission to contact interested users regarding any modifications to the content found within this EDX submission. If you have any specific questions regarding the intended use of this form, please contact EDXsupport@netl.doe.gov".
- A "reCAPTCHA" verification box with the text "I'm not a robot" and a checkbox.
- A "Send Feedback" button, which is highlighted with a red box.
- A "Back to Submission" button.

Creating your own data submission



Option A

1. Create an EDX account
2. Format dataset for easy input into aqueous chemistry software
3. Submit dataset to EDX using **Create Submission**
4. Nominate to NEWTS Group

The screenshot shows the EDX platform interface. At the top, the NETL logo and the text "NETL's Energy Data eXchange" are visible. Below the header, there is a navigation bar with links for "Search", "Contribute", "Groups", "Portfolios", "Workspaces", "Tools", and "Users". The main content area shows the "Groups" section for "NEWTS National Energy Water Treatment and Speciation Database". A red box highlights the "Create Submission" button in the top right corner of the group's submission list. The submission list displays 17 submissions, with two specific entries shown in detail: "NEWTS USGS Brackish Water Case Studies" and "NEWTS USGS Brackish Water Database". Both entries include a DOI link, file formats (e.g., CSV, XLSX), dataset size, and resource counts.

Option B

1. Contact NEWTS team to assist in data formatting and submission to EDX and NEWTS group



Acknowledgment:

We thank the organizers of the 2024 Produced Water Society.

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NETL RESOURCES

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