

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

Principal Investigators: Nicholas Siefert\*, Rachael Yesenchak, R. Burt Thomas, and Madison Wenzlick

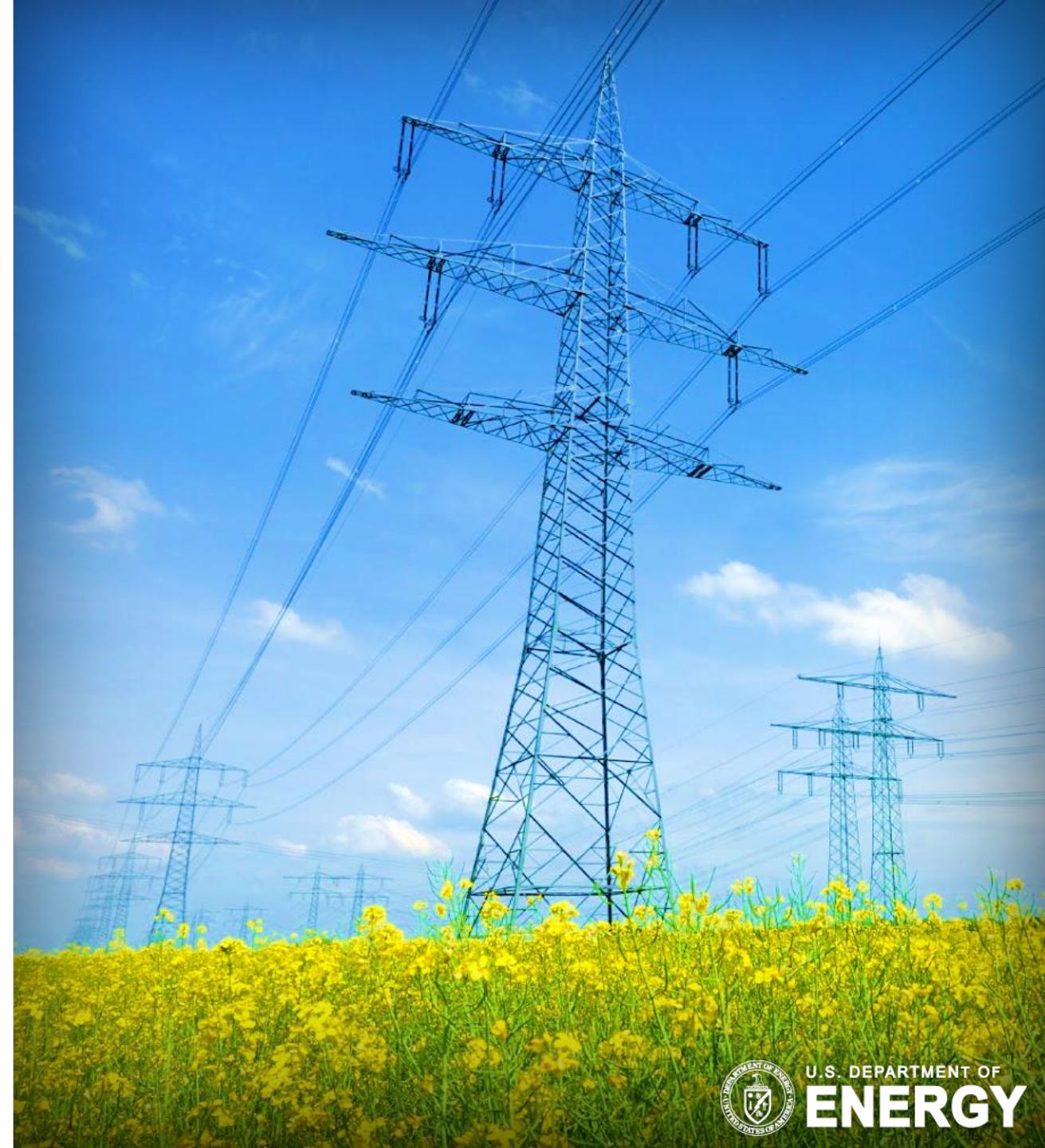
GSA 2023

T88. Urban Geochemistry

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# NEWTS

## DATABASE

NATIONAL ENERGY WATER TREATMENT & SPECIATION

# NEWTS Project Goals



Develop a **national level dataset** of **energy wastewater compositions** that is relevant, useful, and useable

- Help industries and the public understand the value of reuse opportunities, and the benefits of water treatment and management.
- Data must be FAIR (findable, accessible, interoperable, and reusable)
- Seamless integration with widely used modeling software



**What?**



**When & Where?**



**Who?**



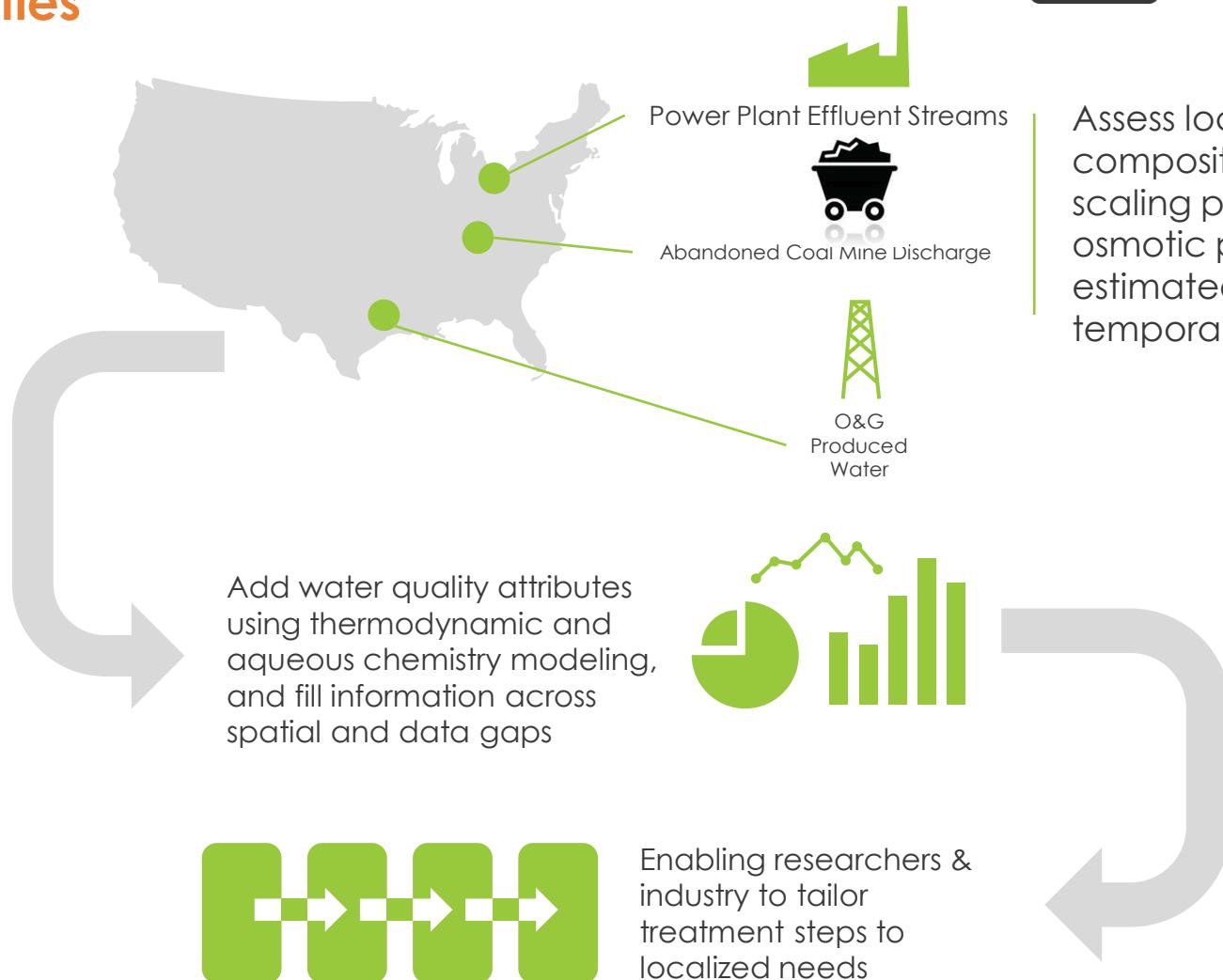
# National Energy Water Treatment & Speciation Database



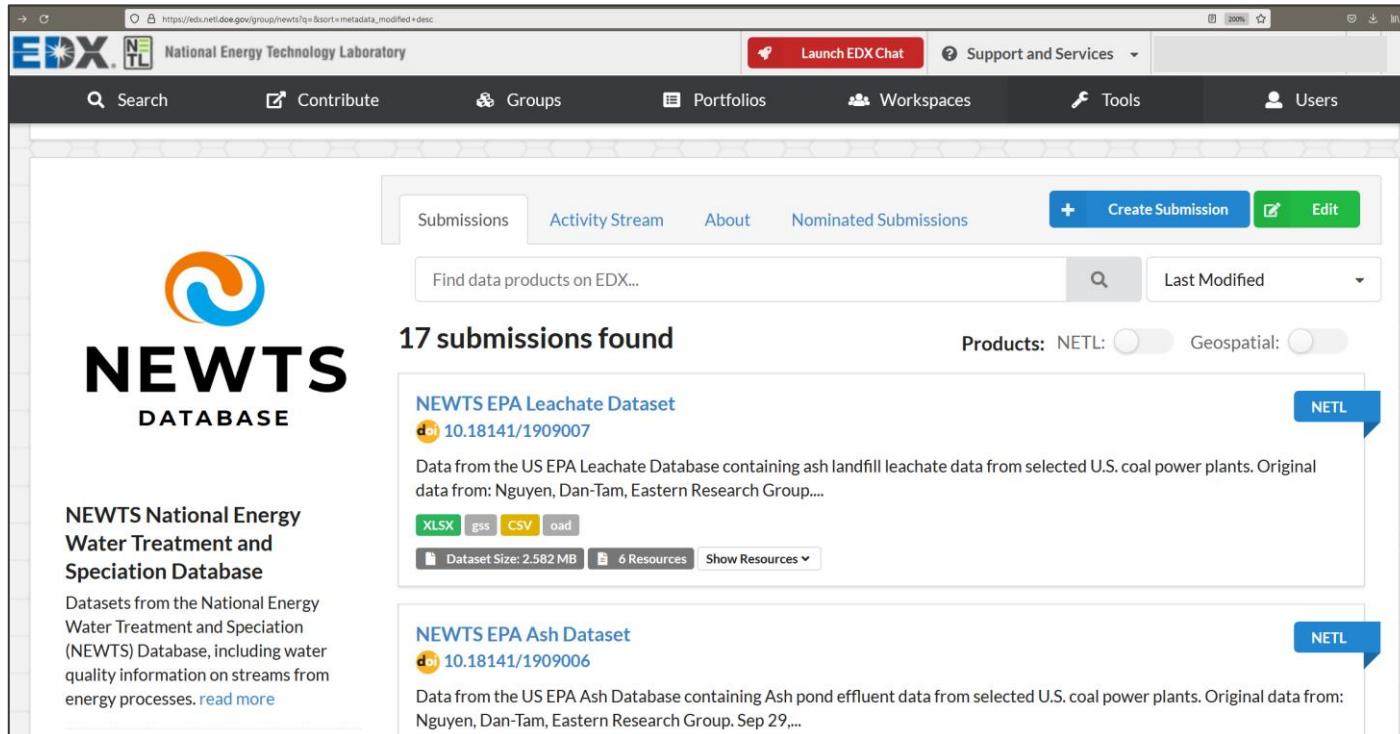
## Leveraging NETL R&D Core Capabilities

### 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 header includes the EDX logo, the NETL logo, and a 'Launch EDX Chat' button. The main content area shows a search bar, navigation links for 'Submissions', 'Activity Stream', 'About', and 'Nominated Submissions', and a 'Create Submission' button. Below this, a search bar with the placeholder 'Find data products on EDX...' and a dropdown menu for 'Last Modified'. A section titled '17 submissions found' lists two datasets: 'NEWTS EPA Leachate Dataset' (version 10.18141/1909007) and 'NEWTS EPA Ash Dataset' (version 10.18141/1909006). Each dataset entry includes a brief description, file formats (XLSX, gss, CSV, oad), dataset size (2.582 MB), and a 'Show Resources' button. A sidebar on the left features the NEWTS Database logo and a brief description of the database.

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

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

The NEWTS Database logo, featuring a stylized orange and blue swirl icon above the text 'NEWTS DATABASE NATIONAL ENERGY WATER TREATMENT & SPECIATION'. The background of the logo is a blurred image of a large industrial facility with many rows of solar panels or similar equipment.

- 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

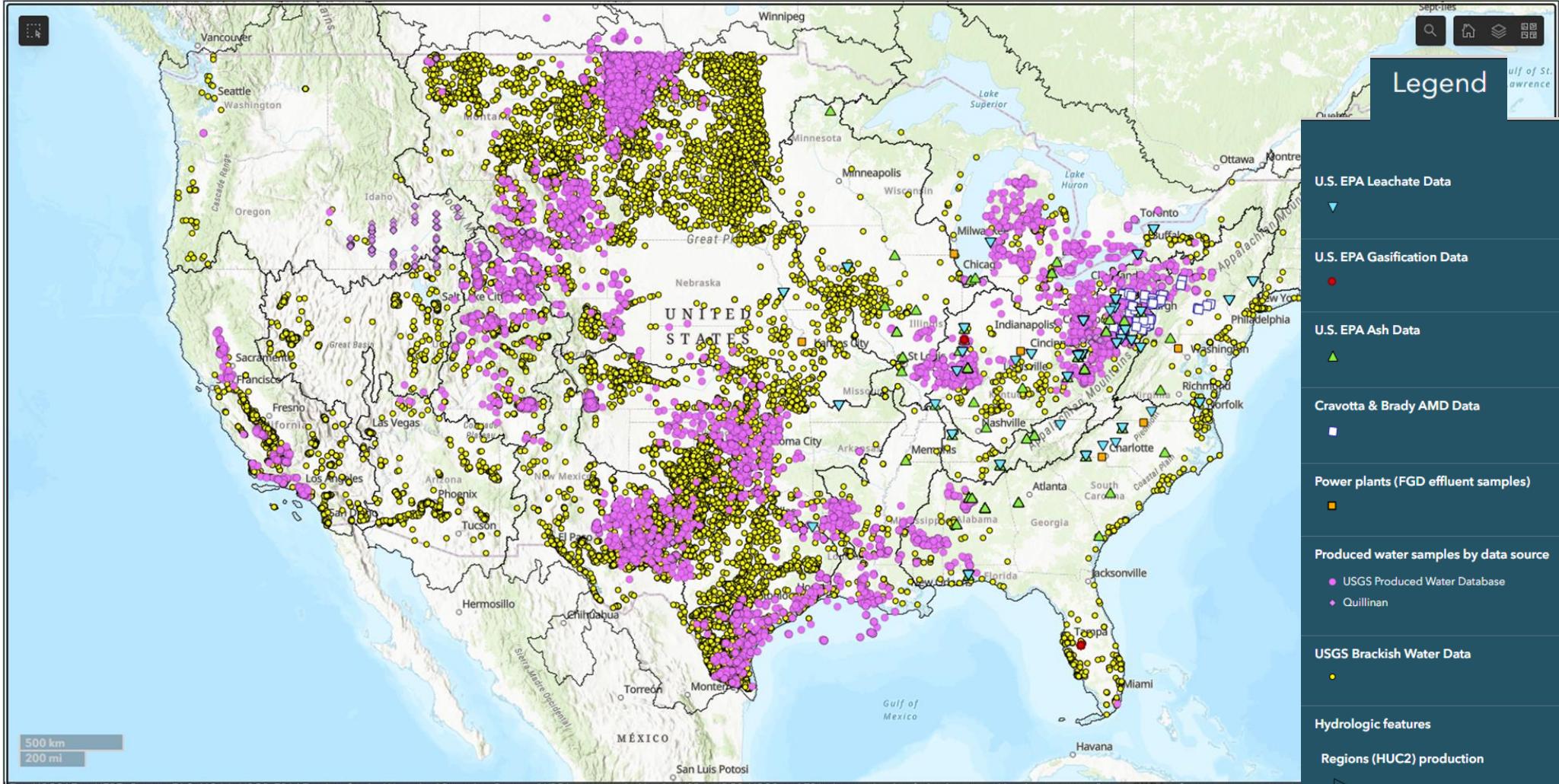
NEWTS Database Dashboard  
National Energy Water Treatment and Speciation



State:  
None

County:  
None

Sedimentary basin:  
None

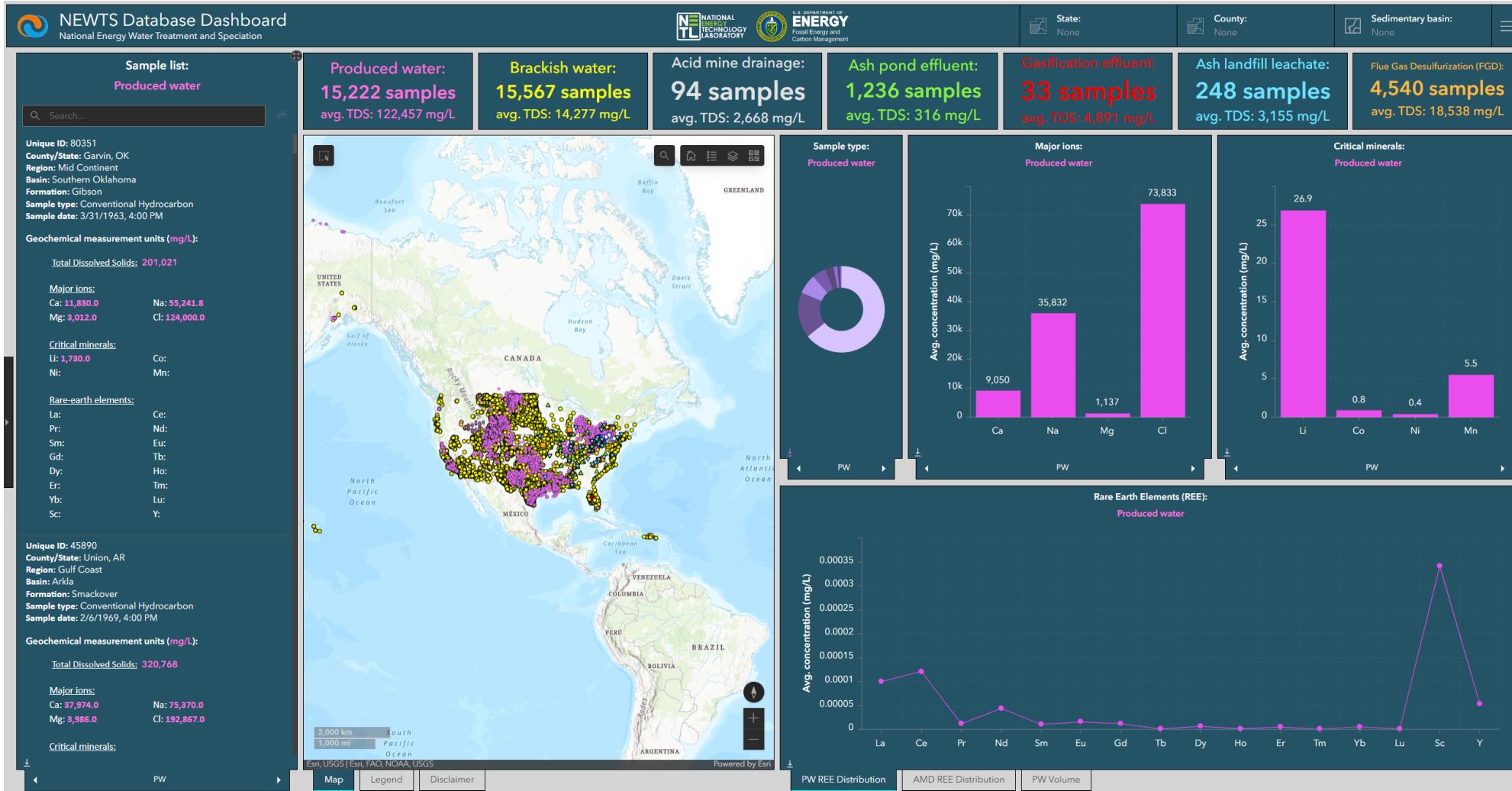


NEWTS Dashboard



Enables data visualization, exploration, and download

# NEWTS Dashboard

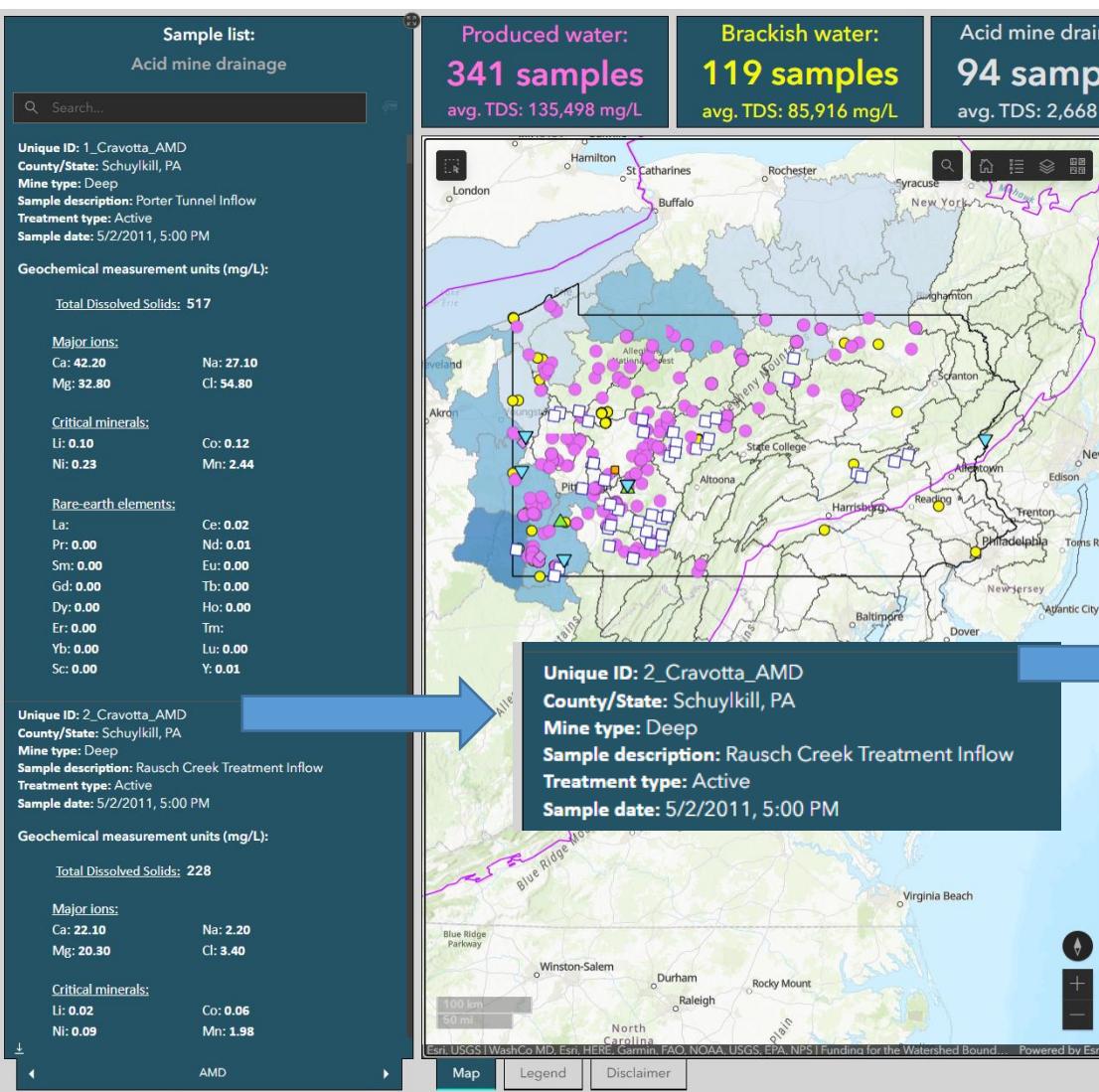


- Filter by spatial location, water type
- View data summaries and time series data
- Get sample list & water quality information

# 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

17 submissions found

**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...



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# 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

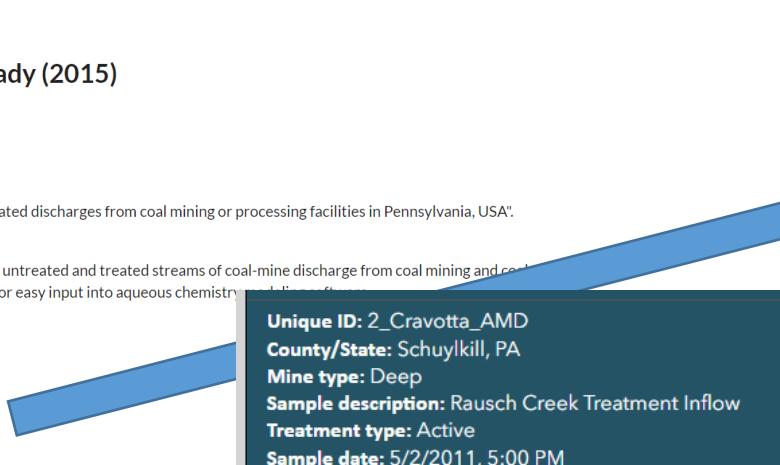
or

or

or

or

or



Unique_ID	ID_Num	1_Cravotta_AMD	2_Cravotta_AMD	3
CSNAME	Descriptio Redox State			
MINE_NUM	<b>Some Mines have multiple Streams</b>			
STAID	Station identifier used by USGS			
Lon_dd				
Lat_dd				
Mine_Type				
Pass				
Minflow_Outflow				
DATE				
TIME				
Alkalinity	Alkalinity	Blank & Total Comb mg/L as CaCO <sub>3</sub>		5.3
TIC	TIC	mol C/L	2.39	1.38
Density		g/mL		
Specific EI COND		µS/cm	802	311
B(OH) <sub>3</sub>	Boron Hydroxide	Not Meas mg/L of B(OH) <sub>3</sub>		
Be(OH) <sub>2</sub>	Beryllium	2 mg/L of Be(OH) <sub>2</sub>	1.86E-02	5.73E-03
Pd(OH) <sub>2</sub>	Palladium	2 mg/L of Pd(OH) <sub>2</sub>		
Al(OH) <sub>3</sub>	Aluminum	3 mg/L of Al(OH) <sub>3</sub>	1.35E+01	2.40E+00
Bi(OH) <sub>3</sub>	Bismuth	Bi_Total 3 mg/L of Bi(OH) <sub>3</sub>		
Cr(OH)(s)	Chromium	Cr_Total (3 mg/L of Cr(OH)	2.62E-03	
Ga(OH)(s)	Gallium	Ga_Total 3 mg/L of Ga(OH)	1.62E-04	5.89E-05
In(OH) <sub>3</sub>	Indium	In_Total 3 mg/L of In(OH) <sub>3</sub>	1.30E-05	1.44E-06
Ru(OH) <sub>4</sub>	Ruthenium	4 mg/L of Ru(OH) <sub>4</sub>		
SiO <sub>2</sub>	Silica	4 mg/L of SiO <sub>2</sub>	2.46E+01	1.81E+01
SnO <sub>2</sub>	Tin	4 mg/L of SnO <sub>2</sub>		
ThO <sub>2</sub>	Thorium	Th_T 4 mg/L of ThO <sub>2</sub>	4.09E-04	4.89E-05
TiO <sub>2</sub>	Titanium	4 mg/L of TiO <sub>2</sub>	3.50E-03	2.00E-03
ZrO <sub>2</sub>	Zirconium	4 mg/L of ZrO <sub>2</sub>	2.70E-05	1.35E-05
Sb(OH) <sub>5</sub>	Antimony hydroxide	5 mg/L of Sb(OH) <sub>5</sub>	1.70E-05	1.70E-05
UO <sub>3</sub>	Uranium	6 mg/L of UO <sub>3</sub>	1.61E-03	3.05E-04
C <sub>6</sub> H <sub>5</sub> OH	Phenol	organic mg/L of C <sub>6</sub> H <sub>5</sub> OH	3.00E-04	
O <sub>2</sub>	Oxygen	0 mg/L of O <sub>2</sub>	10.6	10.7
NH <sub>4</sub> <sup>+</sup>	Ammonium	-3 mg/L of NH <sub>4</sub> <sup>+</sup>	1.54E-01	1.29E-01
Ag <sup>+</sup>	Silver	1 mg/L of Ag <sup>+</sup>		
Cs <sup>+</sup>	Cesium	Cs 1 mg/L of Cs <sup>+</sup>	1.46E-04	8.70E-05
K <sup>+</sup>	Potassium	1 mg/L of K <sup>+</sup>	7.31E+00	1.60E+00
Li <sup>+</sup>	Lithium	1 mg/L of Li <sup>+</sup>	9.85E-02	2.30E-02
Na <sup>+</sup>	Sodium	1 mg/L of Na <sup>+</sup>	2.71E+01	2.20E+00
Rb <sup>+</sup>	Rubidium	1 mg/L of Rb <sup>+</sup>	8.11E-03	3.04E-03
Tl <sup>+</sup>	Thallium	1 mg/L of Tl <sup>+</sup>	7.90E-05	3.40E-05
Ba <sup>2+</sup>	Barium	2 mg/L of Ba <sup>2+</sup>	2.05E-02	2.91E-02
Ca <sup>2+</sup>	Calcium	2 mg/L of Ca <sup>2+</sup>	4.22E+01	2.21E+01
Cd <sup>2+</sup>	Cadmium	2 mg/L of Cd <sup>2+</sup>	8.00E-04	2.10E-04
Original Data_Totals Only	Convert mgperL	mgperL Values	Transpose	<b>Input to OLI</b>
				Charge Balance Redox Species Summary

# 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



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 this 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



# Example Processed Data

## EPA FGD Effluent Dataset

G	H	I	J	K	L	M	N	O	
Date Collected	Lab No	Analyte	CAS_NO	Method	Proced	Units	Non-Det	Amount	J-V
8/24/2010	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	580	
8/25/2010	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	450	
8/26/2010	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	570	
9/29/2010	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	600	
12/8/2010	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	560	
1/12/2011	TA	Nickel	7440-02-0	200.8	Total	ug/L	D	510	
8/23/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	67	
8/24/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	67	
8/25/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	47	
8/26/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	62	
9/29/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	83	
12/8/2010	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	94	
1/12/2011	TA	Nitrate Nitrite as N	STL00217	353.2	Total	mg/L	D	94	
8/23/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	130	
8/24/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	23	
8/25/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	12	
8/26/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	21	
9/29/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	23	
12/8/2010	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	17	
1/12/2011	TA	Nitrogen, Kjeldahl	STL00296	351.2	Total	mg/L	D	15	
8/23/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	3.7	
8/24/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	ND	0	
8/25/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	3.2	
8/26/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	4.3	
9/29/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	1.9	
12/8/2010	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	1.2	
1/12/2011	TA	Phosphorus, Total	7723-14-0	365.1	Total	mg/L	D	2.5	
8/23/2010	TA	Selenite	7723-14-0	360.8	Dissolved	ug/L	D	150	

Raw data: one row per measurement

## EPA FGD Effluent data in NEWTS Template

Unique_ID	Analyte	Procedure Unit	485	486	487	488	489	490
Date Collected	-	-	10/27/2008	10/27/2008	10/27/2008	10/27/2008	10/27/2008	10/27/2008
Sample Point	-	-	Influ after set basin	Influ prior set ba:	Outfall002	Outfall010	Outfall_003	Primary Clarifi Re
Type of Wastewater	-	-	Settling Pond Effluent	Settling Pond Infl	Bio Treatment	Final NPDES	FGD Wastewa FGD	
Sample Description	-	-	Effluent from Settling	Influent to Settlin	Effluent from Final	Internal point	Infl	
Wastewater Classification	-	-	FGD Pond Effluent	FGD Purge	Comingled W	Bio Effluent -	Comingled W	CP Primary Cla FGD
Plant Name	-	-	Roxboro	Roxboro	Roxboro	Roxboro	Roxboro	Pleasant Prairi Ple
Plant ID	-	-	9391	9391	9391	9391	9391	6283
Total Dissolved Solids	Total Diss Total	mg/L						
pH								
Alkalinity mg/L	Alkalinity	Blank & T mg/L as CaCO <sub>3</sub>						
Silica	Silica	mg/L of SiO <sub>2</sub>						
B(OH)3	Boron Hydroxide	mg/L of B(OH) <sub>3</sub>	450.743872	381.5306632	44.15917121	441.019702	4.15279253	
Ag+	Silver	mg/L of Ag <sup>+</sup>	0.0002	0.02	0.0002	0.0002	0.0002	
K+	Potassium	mg/L of K <sup>+</sup>						
Li+	Lithium	mg/L of Li <sup>+</sup>						
Na+	Sodium	mg/L of Na <sup>+</sup>						
NH4+	Ammonium	mg/L of NH <sub>4</sub> <sup>+</sup>						
Ba <sup>2+</sup>	Barium	mg/L of Ba <sup>2+</sup>	0.31	0.579	0.201	0.169	0.045	
Ca <sup>2+</sup>	Calcium	mg/L of Ca <sup>2+</sup>						
Co <sup>2+</sup>	Cobalt	mg/L of Co <sup>2+</sup>	0.011	0.032	0.011	0.011	0.011	
Cu <sup>2+</sup>	Copper	mg/L of Cu <sup>2+</sup>	0.016	0.074	0.016	0.016	0.016	
Hg <sup>2+</sup>	Mercury	mg/L of Hg <sup>2+</sup>	0.00052	0.028	0.00011	0.00012	0.00011	0.0043
Mg <sup>2+</sup>	Magnesium	mg/L of Mg <sup>2+</sup>						
Mn <sup>2+</sup>	Manganese	mg/L of Mn <sup>2+</sup>	0.846	3.5	0.245	0.592	0.154	
Ni <sup>2+</sup>	Nickel	mg/L of Ni <sup>2+</sup>	0.096	0.158	0.018	0.018	0.018	
Pb <sup>2+</sup>	Lead	mg/L of Pb <sup>2+</sup>	0.019	0.032	0.019	0.019	0.019	
Sr <sup>2+</sup>	Strontium	mg/L of Sr <sup>2+</sup>						
Zn <sup>2+</sup>	Zinc	mg/L of Zn <sup>2+</sup>	0.049	0.259	0.038	0.038	0.038	
Al <sup>+++</sup>								
Cr <sup>+++</sup>								
Fe <sup>+3</sup>								
Sn <sup>+4</sup>								
Br-1								
Cl-1								
F-1								
NO3-1								
CrO4-2								
HPO4----								

### Processed data:

- One column per stream
- Easy input into modeling software
- Easy charge balance calculation; data comparison; gap analysis

# 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 CaO03		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)6	Chromium	Cr_Total	3	mg/L of Cr(OH)6	2.62E-03				
24	102.7	69.7	Ga(OH)6	Gallium	Ga_Total	3	mg/L of Ga(OH)6	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

The screenshot shows the Helgeson Direct software interface with the 'Reconcile' module active. The main workspace displays several tables of chemical data:

- Analysis Parameters:**
  - Stream Amount (L): 1.00000
  - Temperature (°C): 28.0000
  - Pressure (atm): 1.0000
- Recorded Properties:**
  - Total Dissolved Solids (mg/L): 12900.0
  - Measured pH: 6.22000
  - Measured Alkalinity (mg HCO<sub>3</sub>/L): 432.000
  - Measured TIC (mol C/L): 118.000
  - Density (g/ml): 0.0
  - Specific Electrical Conductivity (μmho/cm): 13000.0
- Calculation Parameters:**
  - Alkalinity pH Titrant: H<sub>2</sub>SO<sub>4</sub>
  - Alkalinity End Point pH: 4.50000
- Neutrals (mg/L):**
  - H<sub>2</sub>O: 0.0
  - CO<sub>2</sub>: 0.0
  - H<sub>2</sub>S: 0.0
  - B(OH)<sub>3</sub>: 2.39000e-3
  - Be(OH)<sub>2</sub>: 0.0
  - Fe(OH)<sub>2</sub>: 0.0
  - Al(OH)<sub>3</sub>: 0.289000
  - Bi(OH)<sub>3</sub>: 0.0
  - HCO<sub>3</sub>: 6.21000e-5
  - Ga(OH): 1.92000e-4
  - In(OH)<sub>3</sub>: 4.33000e-6
  - Ru(OH)<sub>4</sub>: 8.37000e-5
  - SiO<sub>2</sub>: 19.0000
  - SnO<sub>2</sub>: 0.0
  - ThO<sub>2</sub>: 1.25000e-5
  - TiO<sub>2</sub>: 0.0185000
  - ZrO<sub>2</sub>: 2.81000e-3
  - Sb(OH)<sub>5</sub>: 1.70000e-5
  - UO<sub>3</sub>: 6.42000e-4
  - La(OH)<sub>3</sub>: 0.0
  - O<sub>2</sub>: 7.57000
- Total Ions (mg/L):**
  - Cations (mg/L):**
    - Na<sup>+</sup>: 7.53000
    - Ag<sup>+</sup>: 0.0
    - K<sup>+</sup>: 8.30000e-4

**Measured**

**Actions**

**Reconciliation**

**Specs...**

**Reconcile**

No Reconcile

Reconcile pH

Reconcile pH/Alkalinity

Reconcile pH/Alkalinity/TIC

Calculate Alkalinity

**Calculate**

**Summary**

Unit Set: Metric (mass concentration)

Automatic Chemistry Model

MSE (H<sub>3</sub>O<sup>+</sup> ion) Databanks:

MSE (H<sub>3</sub>O<sup>+</sup> ion)

Using Helgeson Direct

Na/Cl Charge Balance (eq/L):

Cation Charge: 0.187601 eq/L

Anion Charge: -0.189144 eq/L

Imbalance: -1.54318e-3 eq/L

35.478 mg/L of Na<sup>+</sup> is needed to balance.

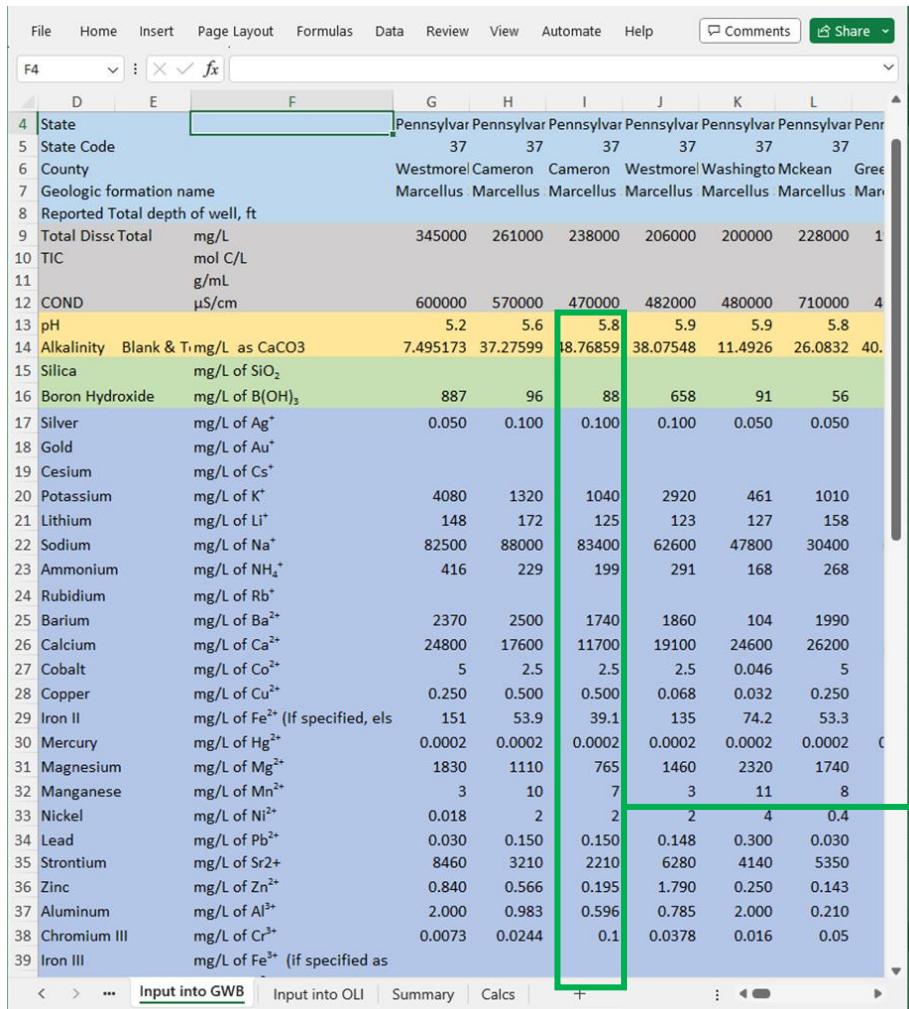
Alkalinity Calculation

25.0000 °C 1.00000 atm

Calculation not done

# Ease of Input into Aqueous Chemistry Software

Geochemist's Workbench example



Sample ID: Pennsylvan  
pH: 5.2  
Carbonate alkalinity: mg/l as CaCO<sub>3</sub>  
SiO<sub>2</sub>(aq): mg/l  
B(OH)<sub>3</sub>: mg/l  
Ag<sup>+</sup>: mg/l  
Au<sup>+</sup>: mg/l  
Cs<sup>+</sup>: mg/l  
K<sup>+</sup>: mg/l  
Li<sup>+</sup>: mg/l  
Na<sup>+</sup>: mg/l  
NH<sub>4</sub><sup>+</sup>: mg/l  
Rb<sup>+</sup>: mg/l  
Ba<sup>++</sup>: mg/l  
Ca<sup>++</sup>: mg/l  
Co<sup>++</sup>: mg/l  
Cu<sup>++</sup>: mg/l  
Fe<sup>++</sup>: mg/l  
Hg<sup>++</sup>: mg/l  
Mg<sup>++</sup>: mg/l  
Mn<sup>++</sup>: mg/l  
Ni<sup>++</sup>: mg/l  
Pb<sup>++</sup>: mg/l  
Sr<sup>++</sup>: mg/l  
Zn<sup>++</sup>: mg/l  
Al<sup>+++</sup>: mg/l  
Cr<sup>+++</sup>: mg/l  
Fe<sup>+++</sup>: mg/l  
V<sup>+++</sup>: mg/l  
Sn<sup>++++</sup>: mg/l  
Br<sup>-</sup>: mg/l  
CH<sub>3</sub>COO<sup>-</sup>: mg/l  
Cl<sup>-</sup>: mg/l  
F<sup>-</sup>: mg/l  
HCO<sub>3</sub><sup>-</sup>: mg/l  
HPO<sub>4</sub><sup>2-</sup>: mg/l  
HS<sup>-</sup>: mg/l

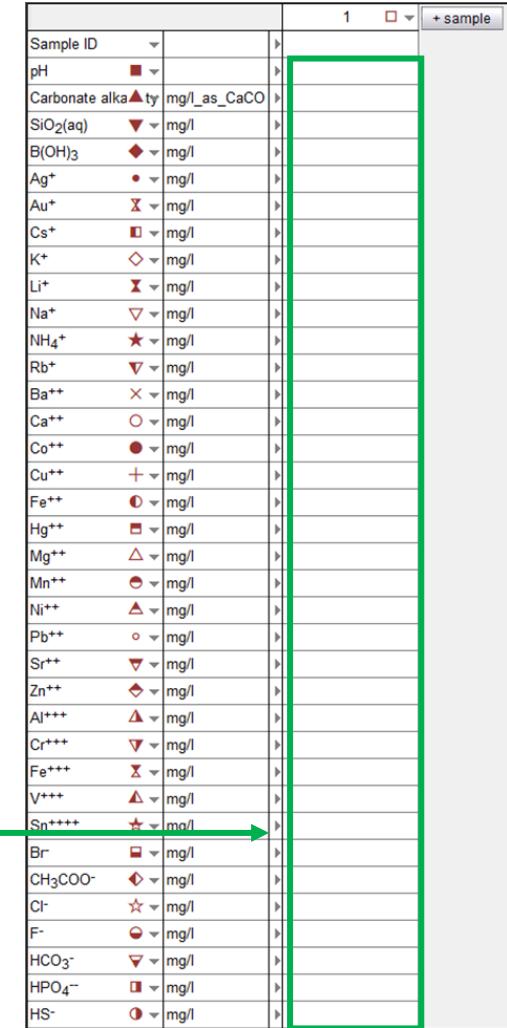
State: Pennsylvan  
State Code: 37  
County: Westmorel  
Geologic formation name: Marcellus  
Reported Total depth of well, ft: 345000  
Total Dissc Total: 345000  
TIC: 261000  
COND: 238000  
pH: 206000  
Alkalinity: 200000  
Silica: 228000  
Boron Hydroxide: 1  
Silver: 37  
Gold: 26  
Cesium: 25  
Potassium: 24  
Lithium: 23  
Sodium: 22  
Ammonium: 21  
Rubidium: 20  
Barium: 20  
Calcium: 19  
Cobalt: 18  
Copper: 17  
Iron II: 16  
Mercury: 15  
Magnesium: 14  
Manganese: 13  
Nickel: 12  
Lead: 11  
Strontium: 10  
Zinc: 9  
Aluminum: 8  
Chromium III: 7  
Iron III: 6

File Home Insert Page Layout Formulas Data Review View Automate Help Comments Share

F4

Input into GWB Input into OLI Summary Calcs

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



Sample ID: Pennsylvan  
pH: 5.2  
Carbonate alkalinity: mg/l as CaCO<sub>3</sub>  
SiO<sub>2</sub>(aq): mg/l  
B(OH)<sub>3</sub>: mg/l  
Ag<sup>+</sup>: mg/l  
Au<sup>+</sup>: mg/l  
Cs<sup>+</sup>: mg/l  
K<sup>+</sup>: mg/l  
Li<sup>+</sup>: mg/l  
Na<sup>+</sup>: mg/l  
NH<sub>4</sub><sup>+</sup>: mg/l  
Rb<sup>+</sup>: mg/l  
Ba<sup>++</sup>: mg/l  
Ca<sup>++</sup>: mg/l  
Co<sup>++</sup>: mg/l  
Cu<sup>++</sup>: mg/l  
Fe<sup>++</sup>: mg/l  
Hg<sup>++</sup>: mg/l  
Mg<sup>++</sup>: mg/l  
Mn<sup>++</sup>: mg/l  
Ni<sup>++</sup>: mg/l  
Pb<sup>++</sup>: mg/l  
Sr<sup>++</sup>: mg/l  
Zn<sup>++</sup>: mg/l  
Al<sup>+++</sup>: mg/l  
Cr<sup>+++</sup>: mg/l  
Fe<sup>+++</sup>: mg/l  
V<sup>+++</sup>: mg/l  
Sn<sup>++++</sup>: mg/l  
Br<sup>-</sup>: mg/l  
CH<sub>3</sub>COO<sup>-</sup>: mg/l  
Cl<sup>-</sup>: mg/l  
F<sup>-</sup>: mg/l  
HCO<sub>3</sub><sup>-</sup>: mg/l  
HPO<sub>4</sub><sup>2-</sup>: mg/l  
HS<sup>-</sup>: 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 <sub>3</sub>	
Silica	Silica	mg/L of SiO <sub>2</sub>	
B(OH) <sub>3</sub>	Boron Hydroxide	mg/L of B(OH) <sub>3</sub>	441.0197022
TiO <sub>2</sub>	Titanium dioxide	mg/L of TiO <sub>2</sub>	
Sb(OH) <sub>5</sub>	Antimony hydroxide	mg/L of Sb(OH) <sub>5</sub>	0.095772536
Al(OH) <sub>3</sub>	Aluminum	mg/L of Al(OH) <sub>3</sub>	1.487777778
Be(OH) <sub>2</sub>	Beryllium	mg/L of Be(OH) <sub>2</sub>	0.003963918
CrO(OH)	Chromium	mg/L of CrO(OH)	0.016346154
Ag <sup>+</sup>	Silver	mg/L of Ag <sup>+</sup>	0.0002
K <sup>+</sup>	Potassium	mg/L of K <sup>+</sup>	
Li <sup>+</sup>	Lithium	mg/L of Li <sup>+</sup>	
Na <sup>+</sup>	Sodium	mg/L of Na <sup>+</sup>	
NH <sub>4</sub> <sup>+</sup>	Ammonium	mg/L of NH <sub>4</sub> <sup>+</sup>	
Tl <sup>+</sup>	Thallium	mg/L of Tl <sup>+</sup>	0.00241
VO <sub>2</sub> <sup>+</sup>	Vanadium	mg/L of VO <sub>2</sub> <sup>+</sup>	0.02279466
Ba <sup>2+</sup>	Barium	mg/L of Ba <sup>2+</sup>	0.408
Ca <sup>2+</sup>	Calcium	mg/L of Ca <sup>2+</sup>	
Cd <sup>2+</sup>	Cadmium	mg/L of Cd <sup>2+</sup>	0.00277
Co <sup>2+</sup>	Cobalt	mg/L of Co <sup>2+</sup>	0.022
Cu <sup>2+</sup>	Copper	mg/L of Cu <sup>2+</sup>	0.016
Hg <sup>2+</sup>	Mercury	mg/L of Hg <sup>2+</sup>	0.00116
Mg <sup>2+</sup>	Magnesium	mg/L of Mg <sup>2+</sup>	
Mn <sup>2+</sup>	Manganese	mg/L of Mn <sup>2+</sup>	1.88
Ni <sup>2+</sup>	Nickel	mg/L of Ni <sup>2+</sup>	0.126
Pb <sup>2+</sup>	Lead	mg/L of Pb <sup>2+</sup>	0.019
Sr <sup>2+</sup>	Strontrium	mg/L of Sr <sup>2+</sup>	
Zn <sup>2+</sup>	Zinc	mg/L of Zn <sup>2+</sup>	0.038
Fe <sup>3+</sup>	Iron	mg/L of Fe <sup>3+</sup>	1.04
Mo <sup>3+</sup>	Molybdenum	mg/L of Mo <sup>3+</sup>	0.0449
Sn <sup>4+</sup>	Tin	mg/L of Sn <sup>4+</sup>	
Br <sup>-1</sup>	Bromide	mg/L of Br <sup>-</sup>	
Cl <sup>-1</sup>	Chloride	mg/L of Cl <sup>-</sup>	4300
F <sup>-1</sup>	Fluoride	mg/L of F <sup>-</sup>	9.4
CN <sup>-1</sup>	Cyanide	mg/L of CN <sup>-</sup>	
NO <sub>3</sub> <sup>-1</sup>	Nitrate	mg/L of NO <sub>3</sub> <sup>-</sup>	
CrO <sub>4</sub> <sup>-2</sup>	Chromate	mg/L of CrO <sub>4</sub> <sup>-2</sup>	
SO <sub>4</sub> <sup>-2</sup>	Sulfate	mg/L of SO <sub>4</sub> <sup>-2</sup>	
SO <sub>3</sub> <sup>-2</sup>	Sulfite	mg/L of SO <sub>3</sub> <sup>-2</sup>	
SeO <sub>4</sub> <sup>-2</sup>	Selenate	mg/L of SeO <sub>4</sub> <sup>-2</sup>	
SeO <sub>3</sub> <sup>-2</sup>	Selenite	mg/L of SeO <sub>3</sub> <sup>-2</sup>	
AsO <sub>4</sub> <sup>-3</sup>	Arsenic(V) Tetraoxid	mg/L of AsO <sub>4</sub> <sup>-3</sup>	
PO <sub>4</sub> <sup>-3</sup>	Phosphate	mg/L of PO <sub>4</sub> <sup>-3</sup>	



## OLI Studio Output Report

### Scaling Tendencies

Row Filter Applied: Values > 1.0e-4

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

Post-Scale Q/K

Pre-Scale Q/K

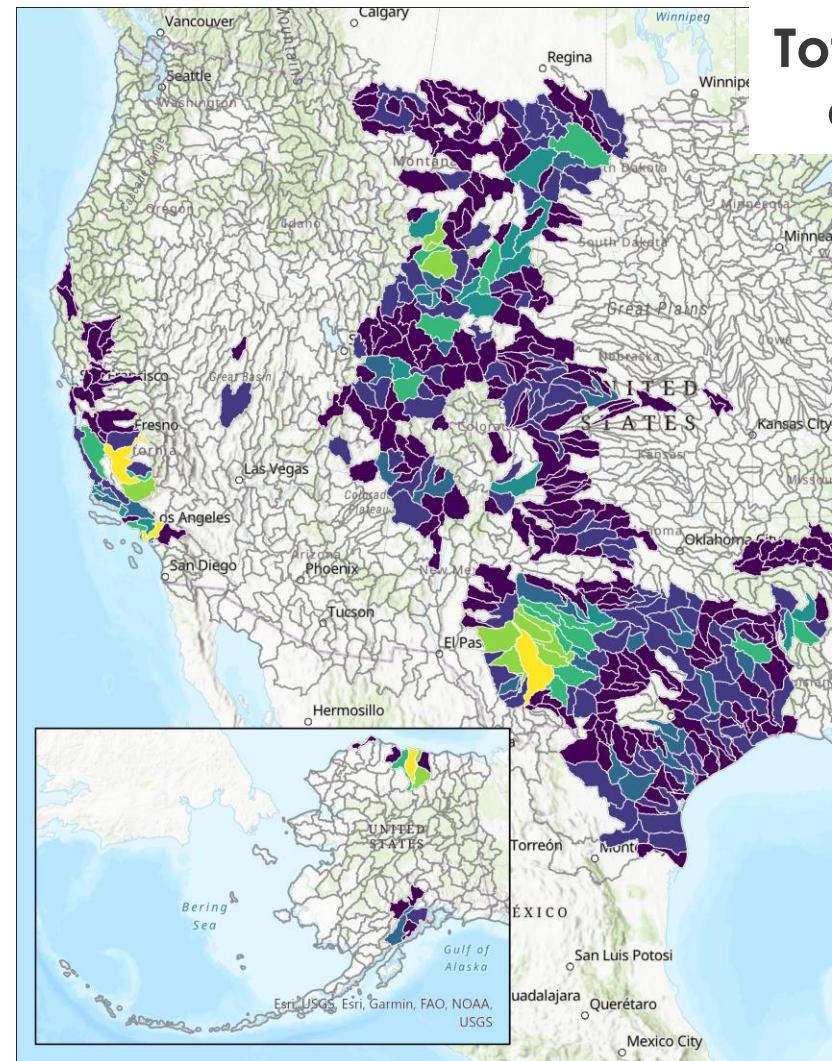
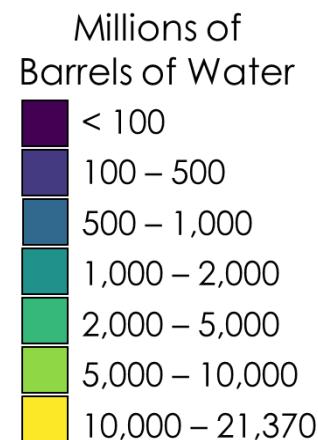
Kinetic induction time for scaling can be estimated for Barite, Gypsum, Calcite, and Celestine) and others (silica) likely in the future



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



**Total Water Production of Producing Wells**

Data Source: Enverus

# Data Catalog and Citing Datasets with DOI#’s



	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, <a href="https://doi.org/10.5066/F72F7KK1">https://doi.org/10.5066/F72F7KK1</a> .	<a href="https://doi.org/10.5066/F72F7KK1">https://doi.org/10.5066/F72F7KK1</a>
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.	<a href="https://www.regulations.gov/c/OW-2009-0819-5640">https://www.regulations.gov/c/OW-2009-0819-5640</a>

## NEWTS EPA Leachate Case Studies

 [10.18141/1909011](https://doi.org/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>

Followers: 0



### Authors

[Nicholas Siefert](#) [Zineb BELARBI](#) [Alison Fritz](#) [Madison Wenzlick](#)

### Citation (Click to Copy)

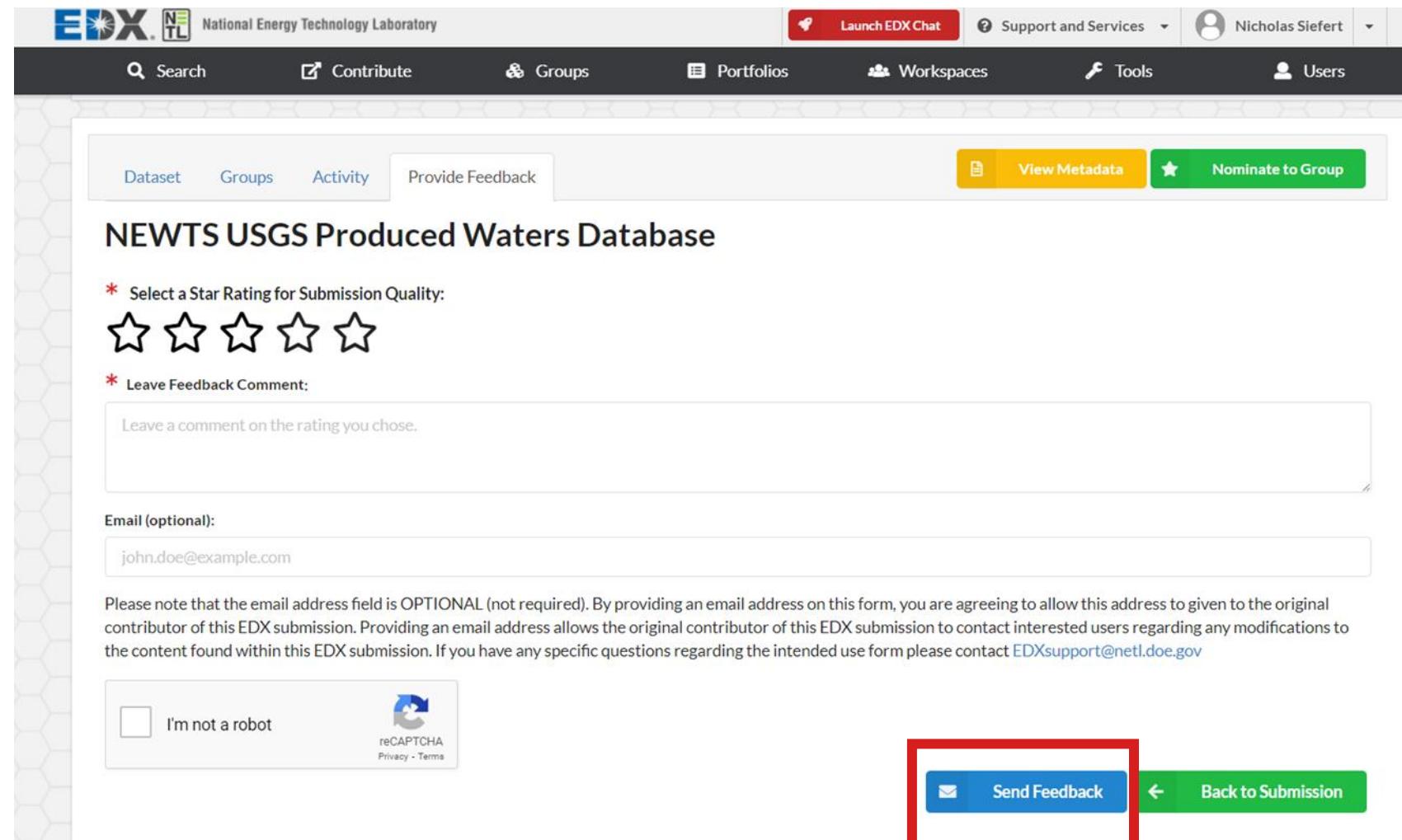
Nicholas Siefert, Zineb Belarbi, Alison Fritz, Madison Wenzlick, NEWTS EPA Leachate Case Studies, 1/13/2023, <https://edx.netl.doe.gov/dataset/newts-epa-leachate-case-studies>, DOI: [10.18141/1909011](https://doi.org/10.18141/1909011)

- Data Catalog summarizes sources for all data sets on EDX

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

# 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, all of which are filled.
- "Leave Feedback Comment": A text input field with the placeholder text "Leave a comment on the rating you chose.".
- "Email (optional)": A text input field containing the email address "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](mailto:EDXsupport@netl.doe.gov)".
- A "reCAPTCHA" verification box with the text "I'm not a robot".
- 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 aqueous chemistry software
3. Submit dataset to EDX using **Create Submission**
4. Nominate to NEWTS Group

The screenshot shows the EDX (NETL's Energy Data eXchange) interface. At the top, there is a navigation bar with the NETL logo, a search bar, and links for 'Launch EDX Chat', 'Support and Services', and 'Nicholas Siebert'. Below the navigation bar, the EDX logo and the text 'NETL's Energy Data eXchange' are displayed. The main content area shows the 'Groups' section, specifically the 'NEWTS National Energy Water...' group. The group page includes a 'Submissions' section with 17 submissions found, a 'Find data products on EDX...' search bar, and a 'Create Submission' button highlighted with a red box. Below the submissions, there are two dataset cards: 'NEWTS USGS Brackish Water Case Studies' and 'NEWTS USGS Brackish Water Database', each with a DOI link, file formats (e.g., CSV, XLSX), dataset size, and resource links.

## Option B

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



# NETL RESOURCES

VISIT US AT: [www.NETL.DOE.gov](http://www.NETL.DOE.gov)



**NEWTS**  
DATABASE

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