

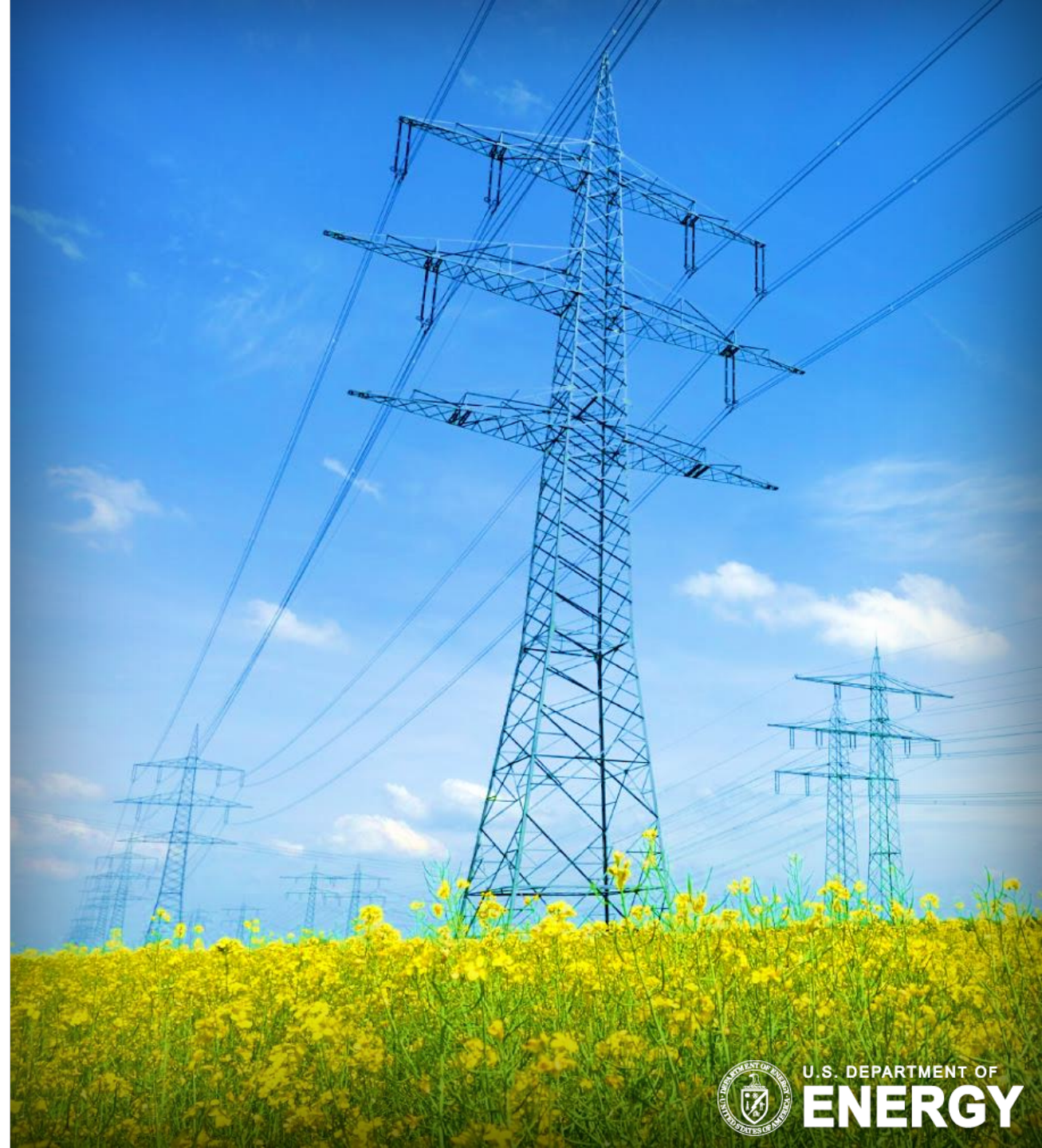
# National Energy Water Treatment & Speciation (NEWTS) : A Water & Critical Mineral Database and Dashboard

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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?**

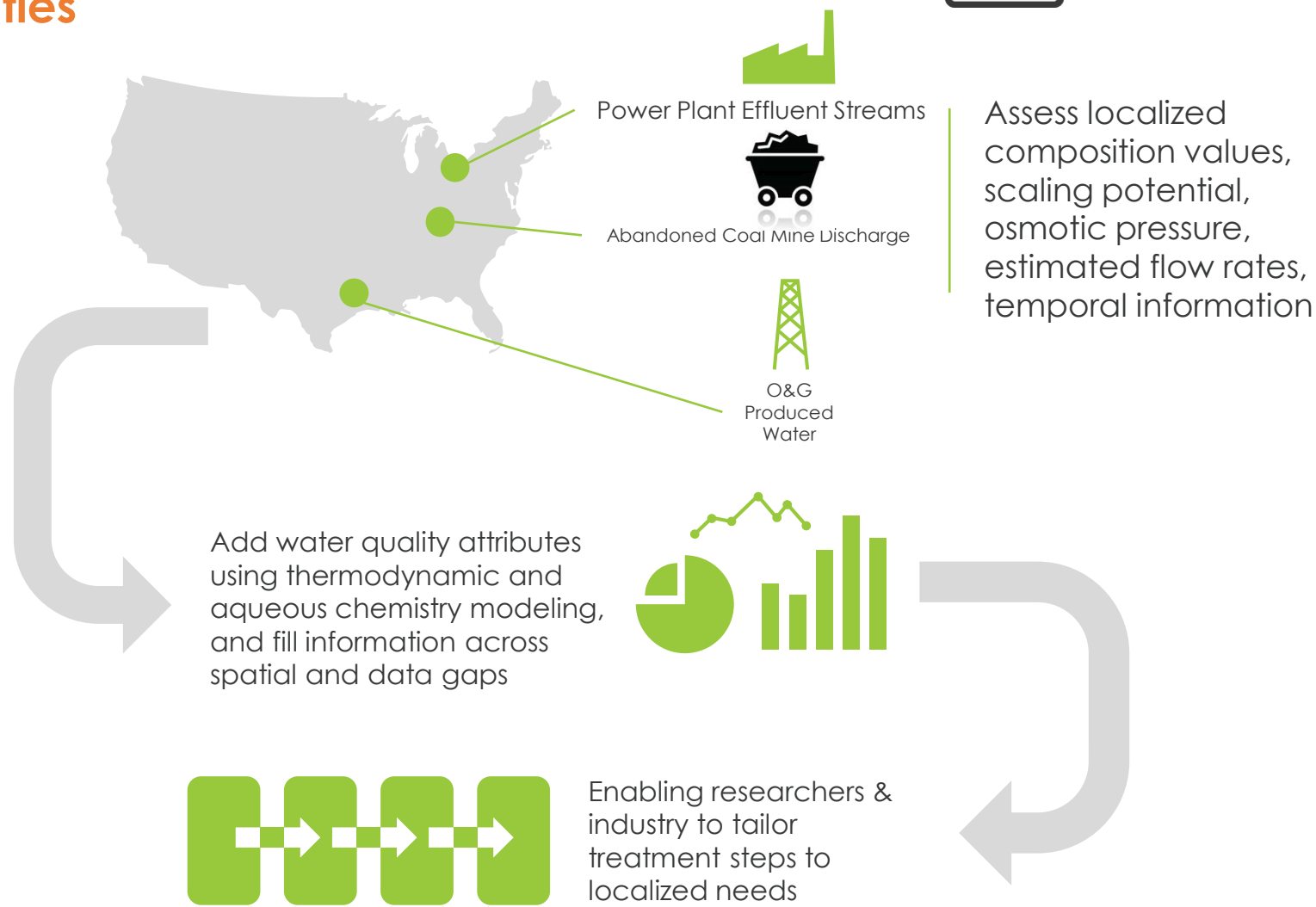


# National Energy Water Treatment & Speciation Database

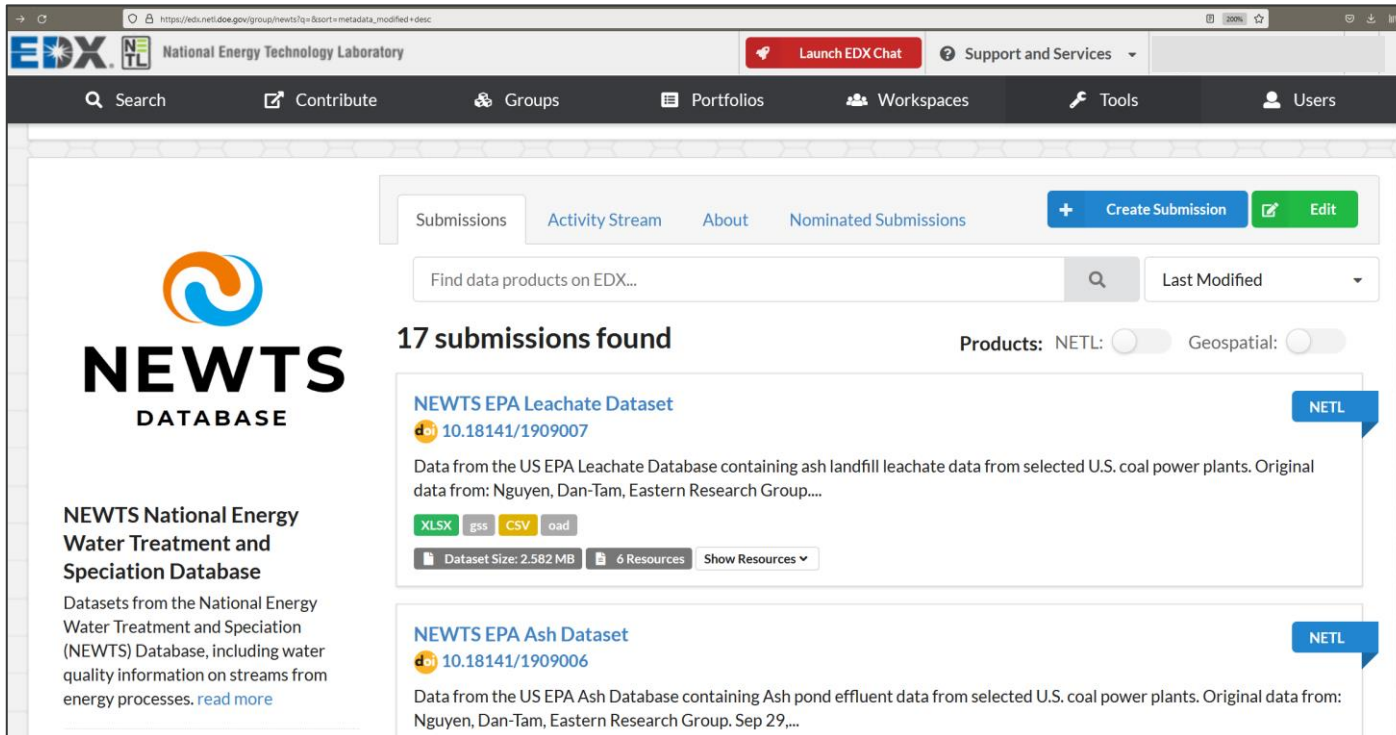
## Leveraging NETL R&D Core Capabilities

### 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



NEWTS  
DATABASE

NEWTS National Energy Water Treatment and Speciation Database

Datasets from the National Energy Water Treatment and Speciation (NEWTS) Database, including water quality information on streams from energy processes. [read more](#)

17 submissions found

Products: NETL: ☐ Geospatial: ☐

**NEWTS EPA Leachate Dataset**  
DOI: 10.18141/1909007

Data from the US EPA Leachate Database containing ash landfill leachate data from selected U.S. coal power plants. Original data from: Nguyen, Dan-Tam, Eastern Research Group...

[XLSX](#) [gss](#) [CSV](#) [oad](#)

Dataset Size: 2.582 MB 6 Resources [Show Resources](#)

**NEWTS EPA Ash Dataset**  
DOI: 10.18141/1909006

Data from the US EPA Ash Database containing Ash pond effluent data from selected U.S. coal power plants. Original data from: Nguyen, Dan-Tam, Eastern Research Group. Sep 29,...



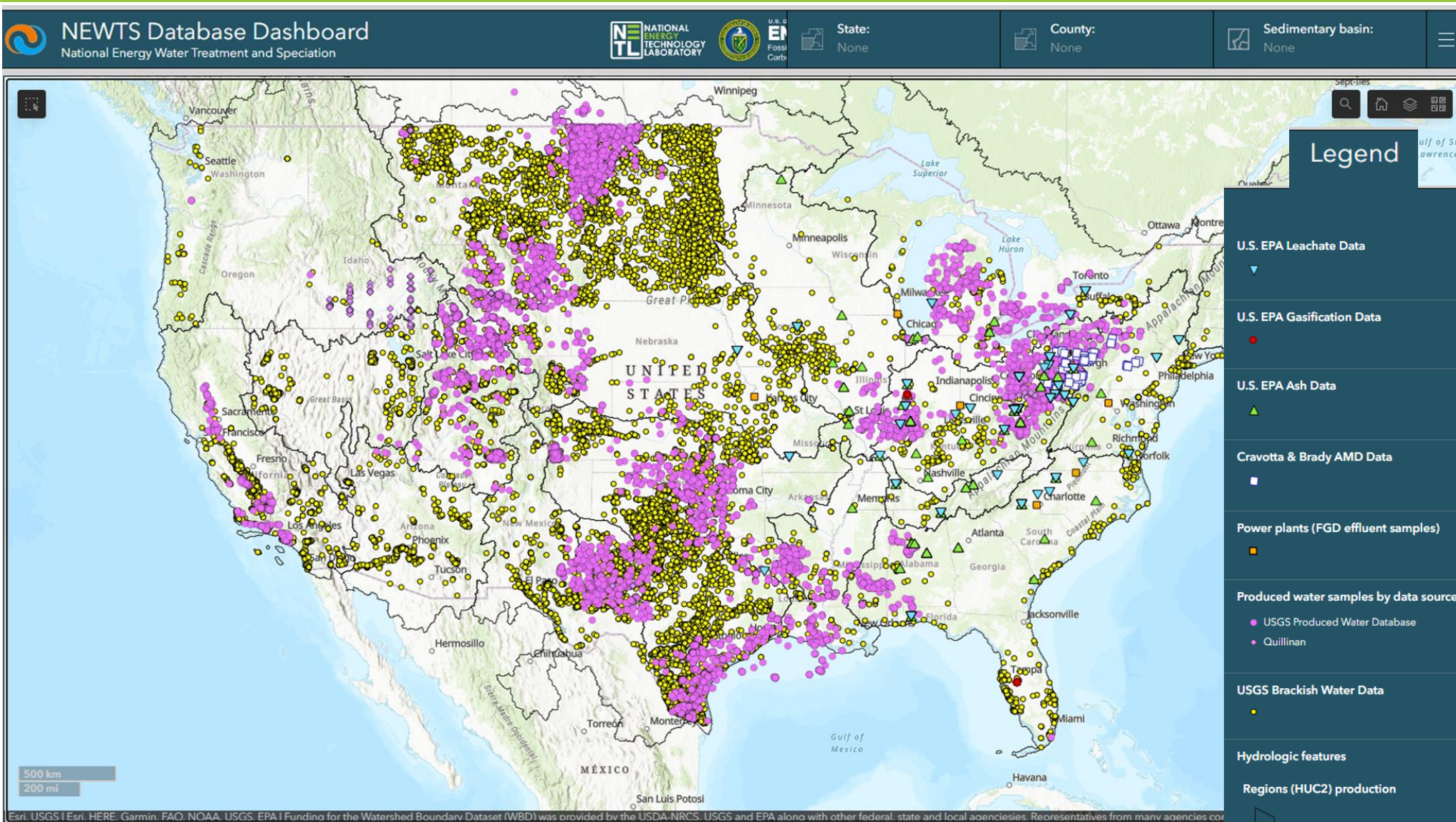
- NEWTS Data Catalog
- [Overview Video](#)
- Training Videos

<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

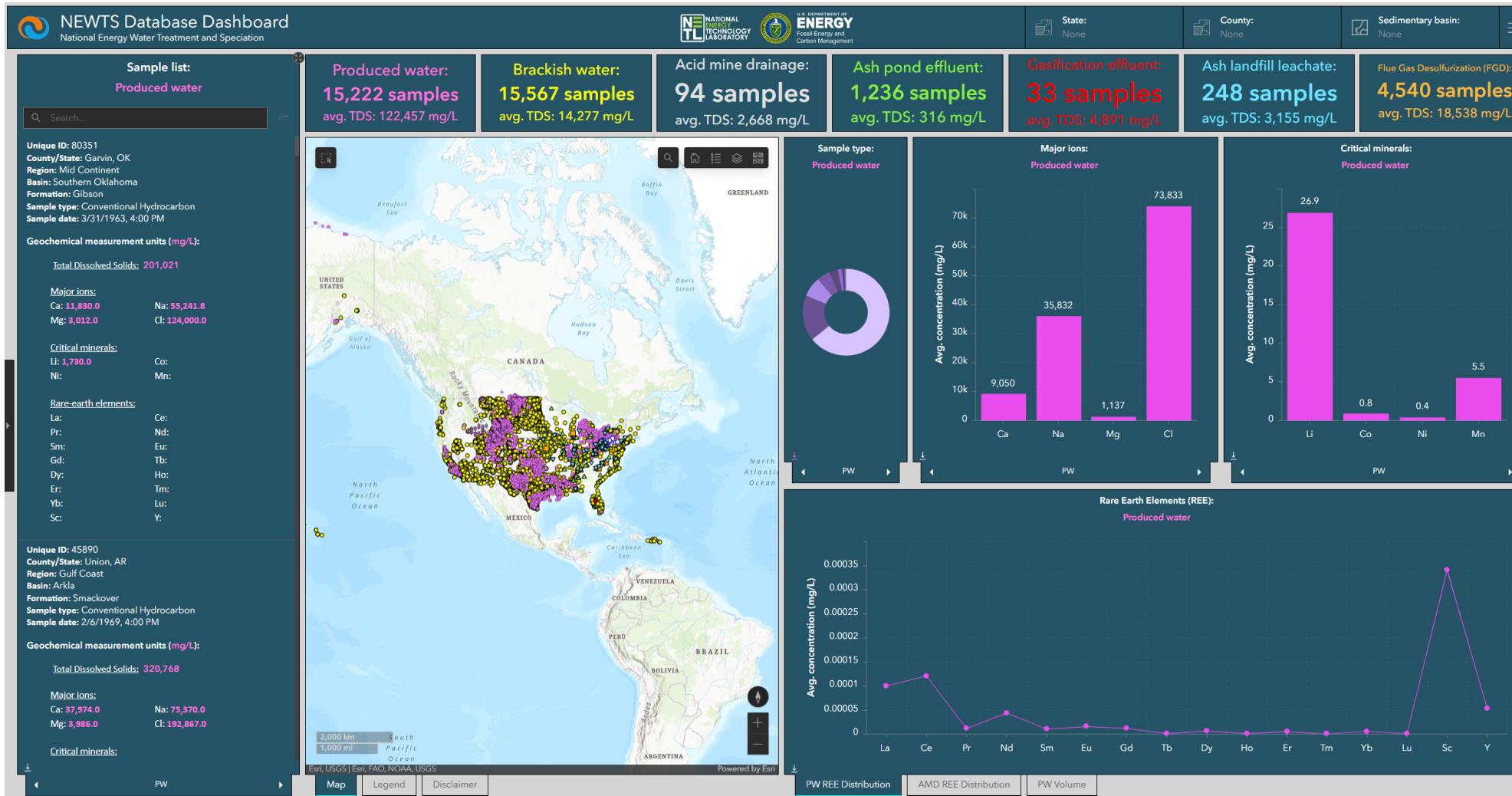


## NEWTS Dashboard



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>

**Sample list:**  
Acid mine drainage

Search...

Unique ID: 1\_Cravotta\_AMD  
County/State: Schuylkill, PA  
Mine type: Deep  
Sample description: Porter Tunnel Inflow  
Treatment type: Active  
Sample date: 5/2/2011, 5:00 PM

**Geochemical measurement units (mg/L):**

Total Dissolved Solids: 517

**Major ions:**  
Ca: 42.20 Na: 27.10  
Mg: 32.80 Cl: 54.80

**Critical minerals:**  
Li: 0.10 Co: 0.12  
Ni: 0.23 Mn: 2.44

**Rare-earth elements:**  
La: Ce: 0.02  
Pr: 0.00 Nd: 0.01  
Sm: 0.00 Eu: 0.00  
Gd: 0.00 Tb: 0.00  
Dy: 0.00 Ho: 0.00  
Er: 0.00 Tm: 0.00  
Yb: 0.00 Lu: 0.00  
Sc: 0.00 Y: 0.01

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

**Geochemical measurement units (mg/L):**

Total Dissolved Solids: 228

**Major ions:**  
Ca: 22.10 Na: 2.20  
Mg: 20.30 Cl: 3.40

**Critical minerals:**  
Li: 0.02 Co: 0.06  
Ni: 0.09 Mn: 1.98

**Produced water:**  
**341 samples**  
avg. TDS: 135,498 mg/L

**Brackish water:**  
**119 samples**  
avg. TDS: 85,916 mg/L

**Acid mine drainage:**  
**94 samples**  
avg. TDS: 2,668 mg/L

Groups / NEWTS National Energy Water...

**NEWTS DATABASE**

NEWTS National Energy Water Treatment and Speciation Database

Datasets from the National Energy Water Treatment and Speciation

quality information on streams from energy processes. [read more](#)

Followers: 8 Submissions: 17

Submissions Activity Stream About Nominated Submissions [+ Create Submission](#) [Edit](#)

Find data products on EDX...  Relevance

Products: NETL: ☒ Geospatial: ☐

17 submissions found

**NEWTS USGS Brackish Water Case Studies**  
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...  
gss oad TXT XLSX  
Dataset Size: 1.179 MB 6 Resources Show Resources

**NEWTS Coal Mine Drainage Dataset from Cravotta Brady (2015)**  
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"...  
XLSX oad CSV  
Dataset Size: 2.269 MB 6 Resources Show Resources

**NEWTS Database Dashboard**  
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...  
HTML  
Dataset Size: 0 bytes 1 Resource Show Resources

# 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.

Followers: 0

+ Follow

☐  **cravottabrady2015\_pa-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

Unique_ID	ID_Num	1_Cravotta_AMD	2_Cravotta_AMD	3
SNAME	Descriptio Redox State	1	2	
MINE_NUM	Some Mines have multiple Streams	1	2	
STAD	Station identifier used by USGS	4.03619E+14	4.03748E+14	
Lon_dd		40.60056	40.62994	
Lat_dd		-76.50583	-76.55399	
Mine_Type		Deep	Deep	
Passive		Active	Active	
CaO		CaO	CaO	
Inflow_Outflow		I	I	
DATE		110503	110503	
TIME		1000	1230	
Alkalinity	Alkalinity	Blank & Total Comb	mg/L as CaCO3	5.3
TIC	TIC		mol C/L	2.39
Density			g/mL	1.38
Specific El COND			μS/cm	802
B(OH)3	Boron Hydroxide	Not Meas	mg/L of B(OH)3	311
Be(OH)2	Beryllium	2	mg/L of Be(OH)2	1.86E-02
Pd(OH)2	Palladium	2	mg/L of Pd(OH)2	5.73E-03
Al(OH)3	Aluminum	3	mg/L of Al(OH)3	1.35E+01
Bi(OH)3	Bismuth	Bi_Total	3	2.40E+00
CrO(OH)3	Chromium	Cr_Total	3	2.62E-03
GaO(OH)3	Gallium	Ga_Total	3	1.62E-04
In(OH)3	Indium	In_Total	3	5.89E-05
Ru(OH)4	Ruthenium		4	1.30E-05
SiO2	Silica		4	1.44E-06
SnO2	Tin		4	2.46E+01
ThO2	Thorium	Th_T	4	1.81E+01
TiO2	Titanium		4	4.09E-04
ZrO2	Zirconium		4	4.89E-05
Sb(OH)5	Antimony hydroxide		5	3.50E-03
UO3	Uranium		6	2.70E-05
C6H5OH	Phenol	organic	mg/L of C6H5OH	1.35E-05
O2	Oxygen		0	1.70E-05
NH4+1	Ammonium	-3	mg/L of NH4+	1.70E-05
Ag+1	Silver	1	mg/L of Ag+	3.05E-04
Cs+1	Cesium	Cs	1	1.61E-03
K+1	Potassium		1	3.00E-04
Li+1	Lithium		1	10.6
Na+1	Sodium		1	1.54E-01
Rb+1	Rubidium		1	1.29E-01
Tl+1	Thallium		1	1.46E-04
Ba+2	Barium		2	8.70E-05
Ca+2	Calcium		2	7.31E+00
Co+2	Cobalt		2	1.60E+00
Cr+3	Chromium		3	9.85E-02
Fe+2	Iron		2	2.30E-02
Mn+2	Manganese		2	2.71E+01
Ni+2	Nickel		2	2.20E+00
Pb+2	Lead		2	8.11E-03
Se+4	Selenium		4	3.04E-03
Si+4	Silicon		4	7.90E-05
Sr+2	Strontium		2	3.40E-05
Te+4	Tellurium		4	2.05E-02
Ti+4	Titanium		4	2.91E-02
V+5	Vanadium		5	4.22E+01
Zn+2	Zinc		2	2.21E+01

# 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



## NEWTS DATABASE

NEWTS National Energy Water  
Treatment and Speciation  
Database











Datasets from the National Energy Water

Data and Resources

[Download Checked](#) [Check All](#)

Filter resources by name...

Date: Newest → Oldest

<input type="checkbox"/>		spece8_output_gss_fgd-case-study_miami-fort-july-12-2010.txt	 License Not Specified	<a href="#">Preview</a> or <a href="#">Download</a>
<input type="checkbox"/>		fgd-case-study-9391.oad	 License Not Specified	<a href="#">Preview</a> or <a href="#">Download</a>
<input type="checkbox"/>		fgd-case-study-1952.oad	 License Not Specified	<a href="#">Preview</a> or <a href="#">Download</a>
<input type="checkbox"/>		fgd-case-study_1956.oad	 License Not Specified	<a href="#">Preview</a> or <a href="#">Download</a>
<input type="checkbox"/>		fgd-case-study-621.oad	 License Not Specified	<a href="#">Preview</a> or <a href="#">Download</a>

Analyte	Procedure	Units	Wght. Avg	Input	Converted Units	Converted Avg.
Alkalinity, HCO <sub>3</sub>		mg/L	48.03	HCO <sub>3</sub> -	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	AsO <sub>4</sub> -3	mg/L	0.35
Beryllium	Total	ug/L			mg/L	
Boron	Total	ug/L	167,106.67	B as B(OH) <sub>3</sub>	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 Dem	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) <sub>3</sub>	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 Collecte	Lab Na	Analyte	CAS_NO	Method	Proced	Units	Non-De	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	Selenium	7782-49-2	200.8	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 Rea	
Type of Wastewater	-	-	Settling Pond Effluent	Settling Pond Infl Bio Treatment Bio	Treatment Final NPDES	FGD Wastewa FGD		
Sample Description	-	-	Effluent from Settling Poi	Influent to Settlin Effluent from	Effluent from Final NPDES	Internal point Infl		
Wastewater Classification	-	-	FGD Pond Effluent	FGD Purge	Comingled We Bio Effluent -	Comingled V CP Primary Cla FGD		
Plant Name	-	-	Roxboro	Roxboro	Roxboro	Roxboro	Roxboro	Pleasant Prairi Plea
Plant ID	-	-	9391	9391	9391	9391	9391	6283
Total Dissolved Solids Total	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+2	Barium	mg/L of Ba <sup>2+</sup>	0.31	0.579	0.201	0.169	0.045	
Ca+2	Calcium	mg/L of Ca <sup>2+</sup>						
Co+2	Cobalt	mg/L of Co <sup>2+</sup>	0.011	0.032	0.011	0.011	0.011	
Cu+2	Copper	mg/L of Cu <sup>2+</sup>	0.016	0.074	0.016	0.016	0.016	
Hg+2	Mercury	mg/L of Hg <sup>2+</sup>	0.00052	0.028	0.00011	0.00012	0.00011	0.0043
Mg+2	Magnesium	mg/L of Mg <sup>2+</sup>						
Mn+2	Manganese	mg/L of Mn <sup>2+</sup>	0.846	3.5	0.245	0.592	0.154	
Ni+2	Nickel	mg/L of Ni <sup>2+</sup>	0.096	0.158	0.018	0.018	0.018	
Pb+2	Lead	mg/L of Pb <sup>2+</sup>	0.019	0.032	0.019	0.019	0.019	
Sr+2	Strontium	mg/L of Sr <sup>2+</sup>						
Zn+2	Zinc	mg/L of Zn <sup>2+</sup>	0.049	0.259	0.038	0.038	0.038	
Al+++								
Cr+++								
Fe+3								
Sn+4								
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)

File	Home	Insert	Page Layout	Formulas	Data	Review	View	Automate	Help	Comments	Share
F9											
A	B	C	D	E	F	G	H	I	J	AF	AG
1	MW of mo	MW of el	SNAME	Descriptor	Redox State		Porter Tur	Rausch Cr	Silver Cre	PBS Job 8	PBS Trent
2			MINE_NUM				1	2	3	22	23
3			STAD				4.04E+14	4.04E+14	4.04E+14	4E+14	4E+14
4			Lon_dd				40.60056	40.62994	40.73417	40.04333	40.0112
5			Lat_dd				-76.5058	-76.554	-76.1233	-78.8122	-78.9285
6			Mine_Type				Deep	Deep	Deep	Surface	Surface
7			Passive_Active				Active	Active	Passive	Active	Active
8			Chemical_trt				CaO	CaO	Wetlands	NaOH	NaOH
9			Inflow_Outflow								
10			DATE				110503	110503	110503	110525	110525
11			TIME				1000	1230	1430	1215	1345
12			TDS	Total Dissolv	Total	mg/L	517.25	228	389.5	1952.5	1305
13			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			uS/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	3	mg/L of Bi(OH)3					
23	85	52	Cr(OH)3	Chromium	3	mg/L of Cr(OH)3	2.62E-03				
24	102.7	69.7	Ga(OH)3	Gallium	3	mg/L of Ga(OH)3	1.62E-04	5.89E-05	8.84E-05	3.24E-04	1.52E-03
25	165.8	114.8	In(OH)3	Indium	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			1.67E-05		
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	SnO2	Tin	4	mg/L of SnO2					
29	264.04	232.04	ThO2	Thorium	4	mg/L of ThO2	4.09E-04	4.89E-05	7.97E-06		1.12E-04
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
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				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	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	5.76E+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+00	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
44	137.3	137.3	Ba+	Barium	2	mg/L of Ba+	2.05E-02	2.91E-02	2.07E-02	1.11E-02	2.89E-02

Navigator  
Document1\*  
cravotta & Brady 2015.

Streams  
WaterAnalysis  
Reconcile

Reconcile

Description Reconciliation Molecular Basis Report

Variable Analysis Parameters Value

Stream Amount (L) 1.00000

Temperature (°C) 25.0000

Pressure (atm) 1.00000

Recorded Properties

Total Dissolved Solids (mg/L) 12900.0

Measured pH 8.22000

Measured Alkalinity (mg HCO3/L) 432.000

Measured TIC (mol C/L) 118.000

Density (g/ml) 0.0

Specific Electrical Conductivity (umho/cm) 13000.0

Calculation Parameters

Alkalinity pH Titrant H2SO4

Alkalinity End Point pH 4.50000

Neutrals (mg/L)

H2O 0.0

CO2 0.0

H2S 0.0

Bi(OH)3 2.39000E-3

Be(OH)2 0.0

Al(OH)3 0.289000

Bi(OH)3 0.0

HCO2 8.21000E-3

Ga(OH)3 1.82000E-4

In(OH)3 4.33000E-6

Ru(OH)4 8.37000E-6

SiO2 19.0000

SnO2 0.0

ThO2 1.25000E-6

TiO2 0.0165000

ZrO2 2.81000E-5

Sb(OH)5 1.70000E-5

UO3 6.42000E-4

O2 7.57000

Total Ions (mg/L)

Cations (mg/L)

NH4+ 7.53000

Ag+ 0.0

K+ 8.30000E-4

11.8000

Measured

Advanced Search Add as Stream Export

Reconciliation

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 (H3O+ ion) Databanks:

MSE (H3O+ 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+ 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

File	Home	Insert	Page Layout	Formulas	Data	Review	View	Automate	Help	Comments	Share
F4											
4	State		Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan
5	State Code		37	37	37	37	37	37	37	37	37
6	County		Westmorel	Cameron	Cameron	Westmorel	Washingto	McKean	Gree		
7	Geologic formation name		Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus
8	Reported Total depth of well, ft										
9	Total Dissc Total	mg/L	345000	261000	238000	206000	200000	228000	1		
10	TIC	mol C/L									
11		g/mL									
12	COND	μS/cm	600000	570000	470000	482000	480000	710000	4		
13	pH		5.2	5.6	5.8	5.9	5.9	5.8			
14	Alkalinity	Blank & T, mg/L as CaCO3	7.495173	37.27599	18.76859	38.07548	11.4926	26.0832	40.		
15	Silica	mg/L of SiO <sub>2</sub>									
16	Boron Hydroxide	mg/L of B(OH) <sub>3</sub>	887	96	88	658	91	56			
17	Silver	mg/L of Ag <sup>+</sup>	0.050	0.100	0.100	0.100	0.050	0.050			
18	Gold	mg/L of Au <sup>+</sup>									
19	Cesium	mg/L of Cs <sup>+</sup>									
20	Potassium	mg/L of K <sup>+</sup>	4080	1320	1040	2920	461	1010			
21	Lithium	mg/L of Li <sup>+</sup>	148	172	125	123	127	158			
22	Sodium	mg/L of Na <sup>+</sup>	82500	88000	83400	62600	47800	30400			
23	Ammonium	mg/L of NH <sub>4</sub> <sup>+</sup>	416	229	199	291	168	268			
24	Rubidium	mg/L of Rb <sup>+</sup>									
25	Barium	mg/L of Ba <sup>2+</sup>	2370	2500	1740	1860	104	1990			
26	Calcium	mg/L of Ca <sup>2+</sup>	24800	17600	11700	19100	24600	26200			
27	Cobalt	mg/L of Co <sup>2+</sup>	5	2.5	2.5	2.5	0.046	5			
28	Copper	mg/L of Cu <sup>2+</sup>	0.250	0.500	0.500	0.068	0.032	0.250			
29	Iron II	mg/L of Fe <sup>2+</sup> (If specified, els	151	53.9	39.1	135	74.2	53.3			
30	Mercury	mg/L of Hg <sup>2+</sup>	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002			
31	Magnesium	mg/L of Mg <sup>2+</sup>	1830	1110	765	1460	2320	1740			
32	Manganese	mg/L of Mn <sup>2+</sup>	3	10	7	3	11	8			
33	Nickel	mg/L of Ni <sup>2+</sup>	0.018	2	2	2	4	0.4			
34	Lead	mg/L of Pb <sup>2+</sup>	0.030	0.150	0.150	0.148	0.300	0.030			
35	Strontium	mg/L of Sr <sup>2+</sup>	8460	3210	2210	6280	4140	5350			
36	Zinc	mg/L of Zn <sup>2+</sup>	0.840	0.566	0.195	1.790	0.250	0.143			
37	Aluminum	mg/L of Al <sup>3+</sup>	2.000	0.983	0.596	0.785	2.000	0.210			
38	Chromium III	mg/L of Cr <sup>3+</sup>	0.0073	0.0244	0.1	0.0378	0.016	0.05			
39	Iron III	mg/L of Fe <sup>3+</sup> (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		1	+ sample
pH			
Carbonate alka	mg/l as CaCO		
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>-</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	-	-	-	Influ 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 n Total Dissi 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)3	Boron Hydroxide	mg/L of B(OH) <sub>3</sub>	441.0197022	
TiO2	Titanium dioxide	mg/L of TiO <sub>2</sub>		
Sb(OH)5	Antimony hydroxide	mg/L of Sb(OH) <sub>5</sub>	0.095772536	
Al(OH)3	Aluminum	mg/L of Al(OH) <sub>3</sub>	1.487777778	
Be(OH)2	Beryllium	mg/L of Be(OH) <sub>2</sub>	0.003963918	
CrO(OH)	Chromium	mg/L of CrO(OH)	0.016346154	
Ag+1	Silver	mg/L of Ag <sup>+</sup>	0.0002	
K+1	Potassium	mg/L of K <sup>+</sup>		
Li+1	Lithium	mg/L of Li <sup>+</sup>		
Na+1	Sodium	mg/L of Na <sup>+</sup>		
NH4+1	Ammonium	mg/L of NH <sub>4</sub> <sup>+</sup>		
Tl+1	Thallium	mg/L of Tl <sup>+</sup>	0.00241	
VO2+1	Vanadium	mg/L of VO <sub>2</sub> <sup>+</sup>	0.02279466	
Ba+2	Barium	mg/L of Ba <sup>2+</sup>	0.408	
Ca+2	Calcium	mg/L of Ca <sup>2+</sup>		
Cd+2	Cadmium	mg/L of Cd <sup>2+</sup>	0.00277	
Co+2	Cobalt	mg/L of Co <sup>2+</sup>	0.022	
Cu+2	Copper	mg/L of Cu <sup>2+</sup>	0.016	
Hg+2	Mercury	mg/L of Hg <sup>2+</sup>	0.00116	
Mg+2	Magnesium	mg/L of Mg <sup>2+</sup>		
Mn+2	Manganese	mg/L of Mn <sup>2+</sup>	1.88	
Ni+2	Nickel	mg/L of Ni <sup>2+</sup>	0.126	
Pb+2	Lead	mg/L of Pb <sup>2+</sup>	0.019	
Sr+2	Strontium	mg/L of Sr <sup>2+</sup>		
Zn+2	Zinc	mg/L of Zn <sup>2+</sup>	0.038	
Fe+3	Iron	mg/L of Fe <sup>3+</sup>	1.04	
Mo+3	Molybdenum	mg/L of Mo <sup>3+</sup>	0.0449	
Sn+4	Tin	mg/L of Sn <sup>4+</sup>		
Br-1	Bromide	mg/L of Br <sup>-</sup>		
Cl-1	Chloride	mg/L of Cl <sup>-</sup>	4300	
F-1	Fluoride	mg/L of F <sup>-</sup>	9.4	
CN-1	Cyanide	mg/L of CN <sup>-</sup>		
NO3-1	Nitrate	mg/L of NO <sub>3</sub> <sup>-</sup>		
CrO4-2	Chromate	mg/L of CrO <sub>4</sub> <sup>2-</sup>		
SO4-2	Sulfate	mg/L of SO <sub>4</sub> <sup>2-</sup>	1200	
SO3-2	Sulfite	mg/L of SO <sub>3</sub> <sup>2-</sup>		
SeO4-2	Selenate	mg/L of SeO <sub>4</sub> <sup>2-</sup>		
SeO3-2	Selenite	mg/L of SeO <sub>3</sub> <sup>2-</sup>		
AsO4-3	Arsenic(V) Tetraoxid	mg/L of AsO <sub>4</sub> <sup>3-</sup>		
PO4-3	Phosphate	mg/L of PO <sub>4</sub> <sup>3-</sup>		



## OLI Studio Output Report

### Scaling Tendencies

Row Filter Applied: Values > 1.0e-4

Post-Scale Q/K

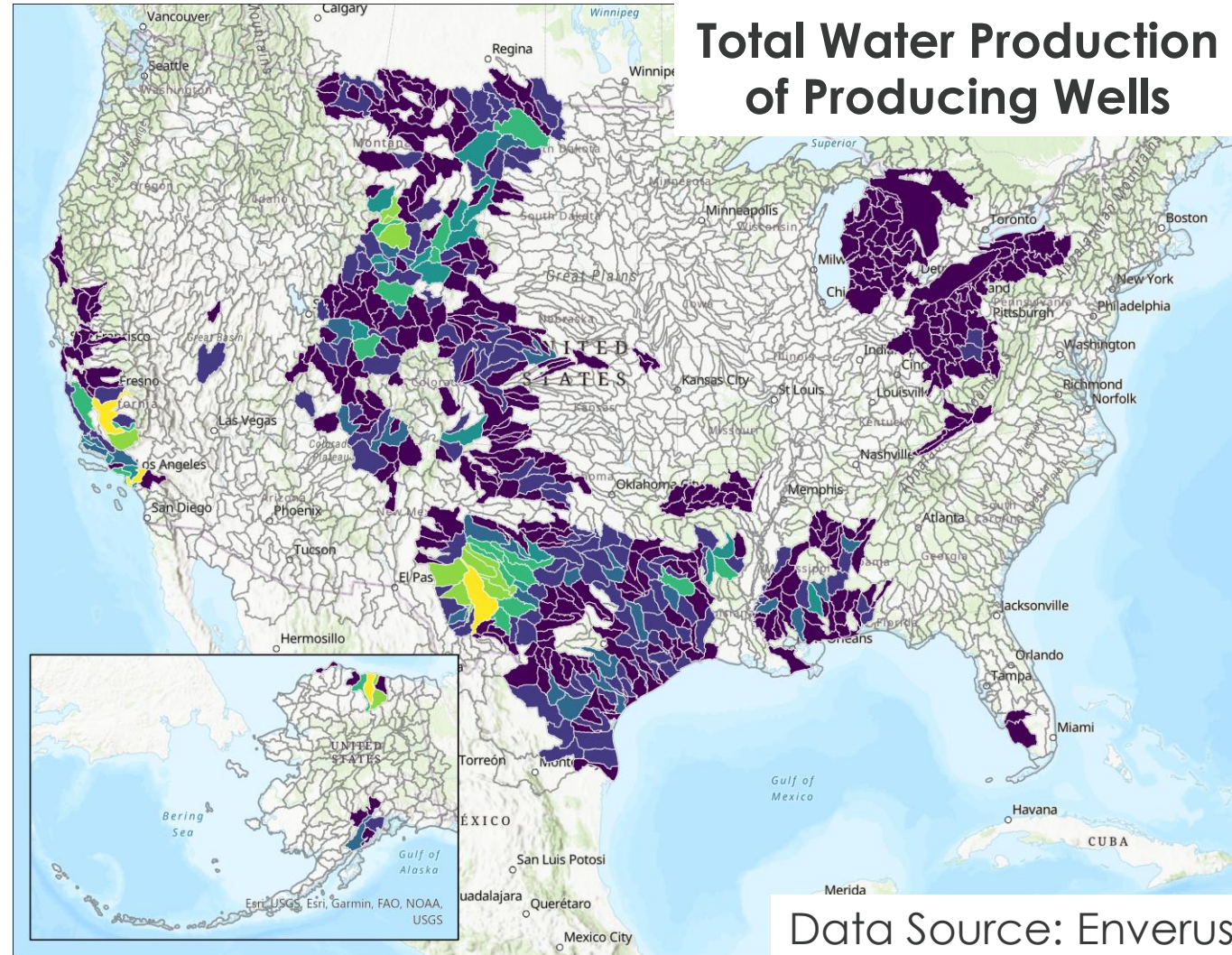
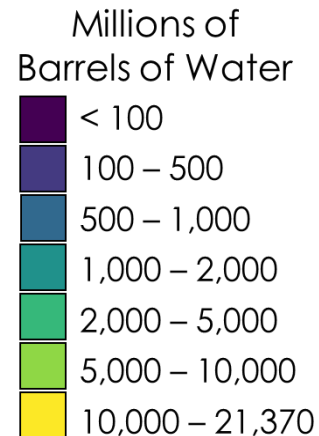
Pre-Scale Q/K

Solids	Post-Scale
Fe(OH)3 (Bernalite)	1.00000
BaSO4 (Barite)	1.00000
PbSO4 (Anglesite)	0.0195029
B(OH)3	0.0101386
AgCl	1.96141e-3
Al(OH)3 (Gibbsite)	1.47368e-4

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

# 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, <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/collection/OW-2009-0819-5640">https://www.regulations.gov/collection/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

 Follow

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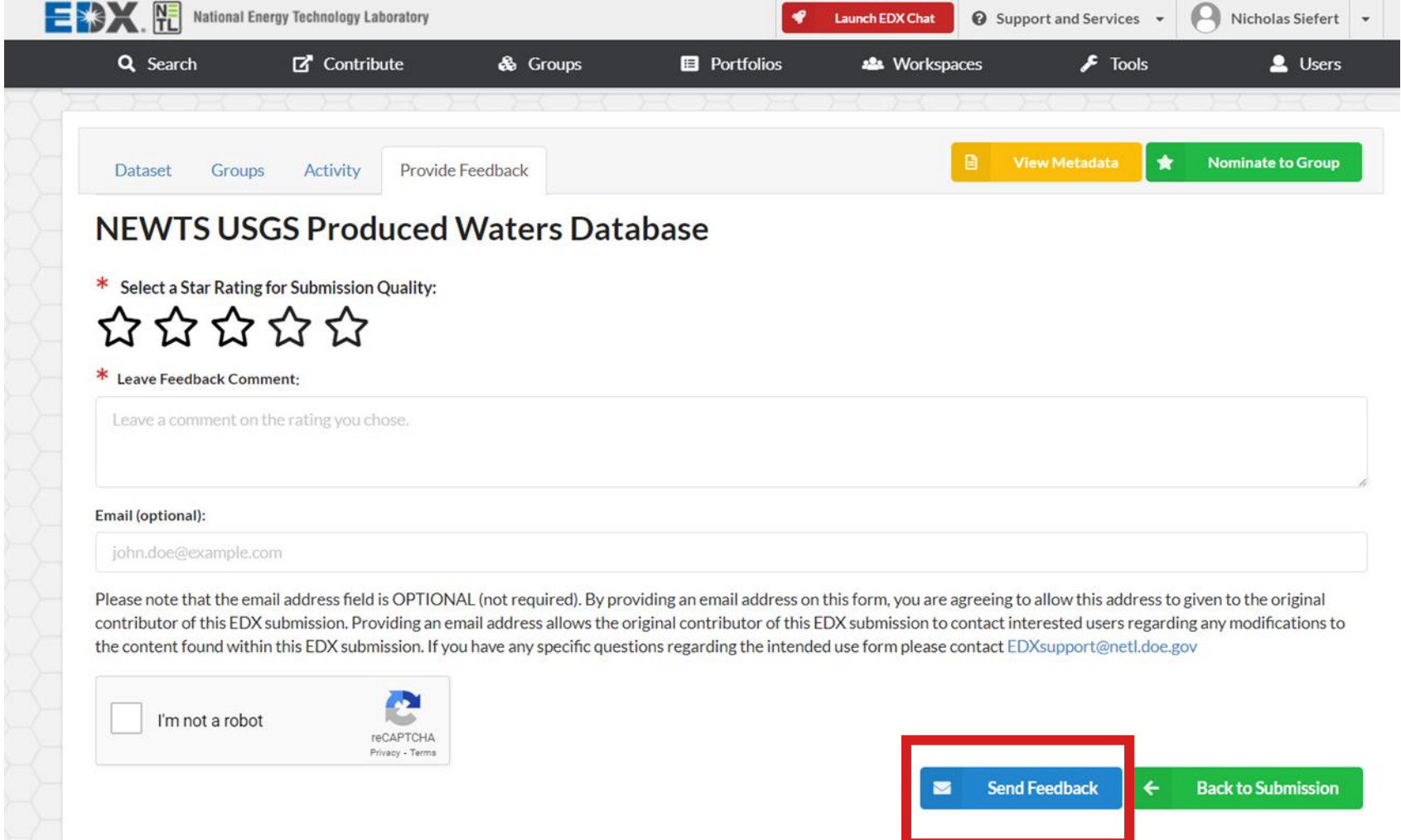
### Citation (Click to Copy)

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

- Data Catalog summarizes sources for all data sets on EDX

# 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 'Provide Feedback' form on the EDX website. The form is titled 'NEWTS USGS Produced Waters Database'. It includes a star rating section with five stars, a text area for a feedback comment, and an optional email field. The 'Send Feedback' button is highlighted with a red box. The 'Back to Submission' button is also visible.

EDX National Energy Technology Laboratory

Launch EDX Chat Support and Services Nicholas Siefert

Search Contribute Groups Portfolios Workspaces Tools Users

Dataset Groups Activity Provide Feedback View Metadata Nominate to Group

### NEWTS USGS Produced Waters Database

\* Select a Star Rating for Submission Quality:

☆ ☆ ☆ ☆ ☆

\* Leave Feedback Comment:

Leave a comment on the rating you chose.

Email (optional):

john.doe@example.com

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 form please contact [EDXsupport@netl.doe.gov](mailto:EDXsupport@netl.doe.gov)

☐ I'm not a robot reCAPTCHA Privacy - Terms

Send Feedback Back to Submission

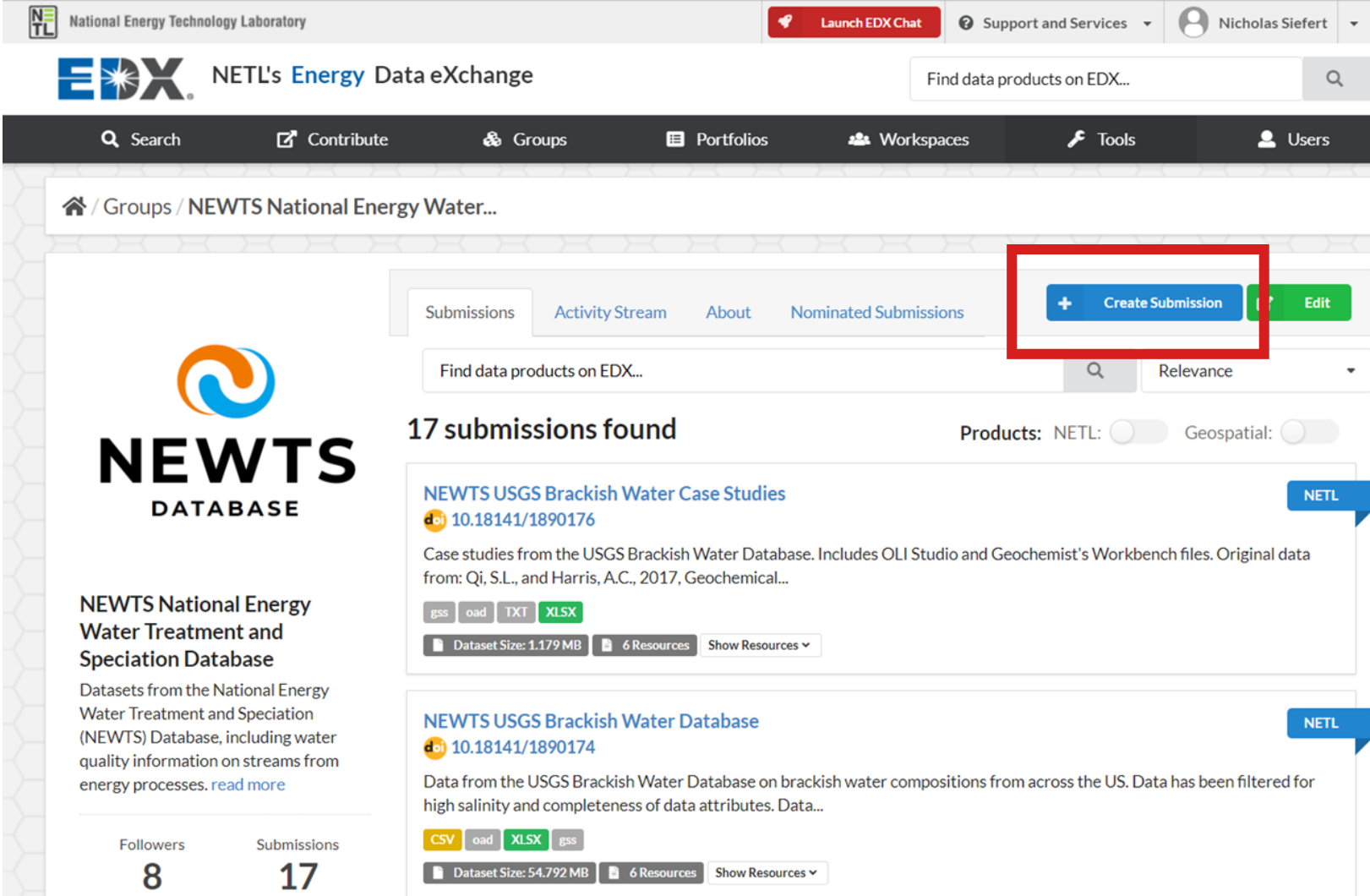
# Creating your own data submission

## 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

## Option B

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



The screenshot shows the EDX (Energy Data eXchange) interface. At the top, there's a header with the NETL logo, "National Energy Technology Laboratory", and a "Launch EDX Chat" button. Below this is the "EDX" logo and "NETL's Energy Data eXchange". A search bar is present with the text "Find data products on EDX...". The main navigation bar includes "Search", "Contribute", "Groups", "Portfolios", "Workspaces", "Tools", and "Users". The current page is for the "NEWTS National Energy Water Treatment and Speciation Database" group. The group page shows the group logo, name, and a description: "NEWTS National Energy Water Treatment and Speciation Database. Datasets from the National Energy Water Treatment and Speciation (NEWTS) Database, including water quality information on streams from energy processes. [read more](#)". It also shows "Followers: 8" and "Submissions: 17". On the right side, there's a "Submissions" tab with a "Create Submission" button highlighted by a red box. Below the tab, there's a search bar and a "Relevance" dropdown. The results show "17 submissions found". Two submissions are listed: "NEWTS USGS Brackish Water Case Studies" and "NEWTS USGS Brackish Water Database". Each submission entry includes a dataset size, number of resources, and a "Show Resources" button.

# NETL RESOURCES

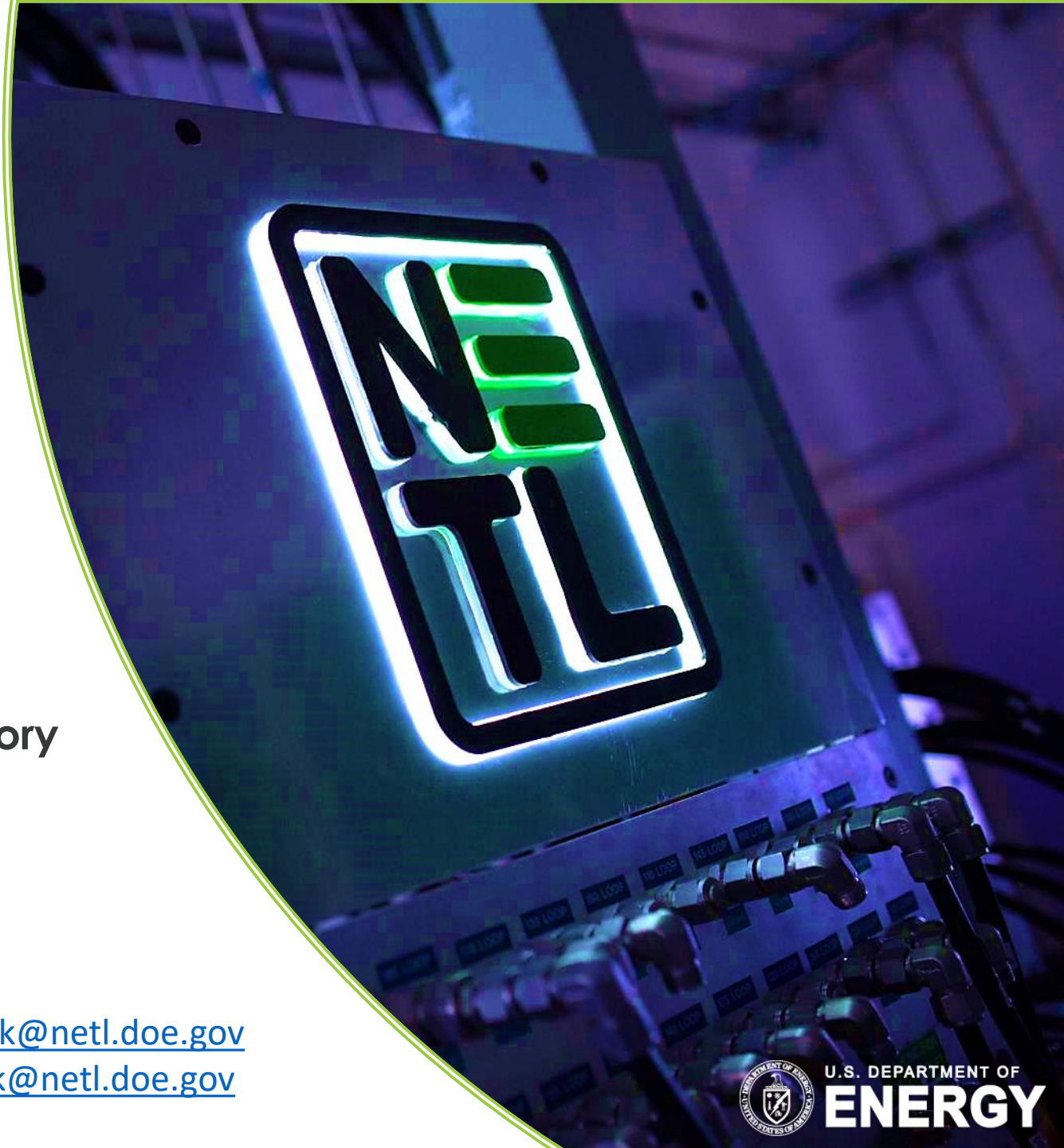
VISIT US AT: [www.NETL.DOE.gov](http://www.NETL.DOE.gov)



**NEWTS**  
DATABASE

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