



# 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



U.S. DEPARTMENT OF  
**ENERGY**

Fossil Energy and  
Carbon Management



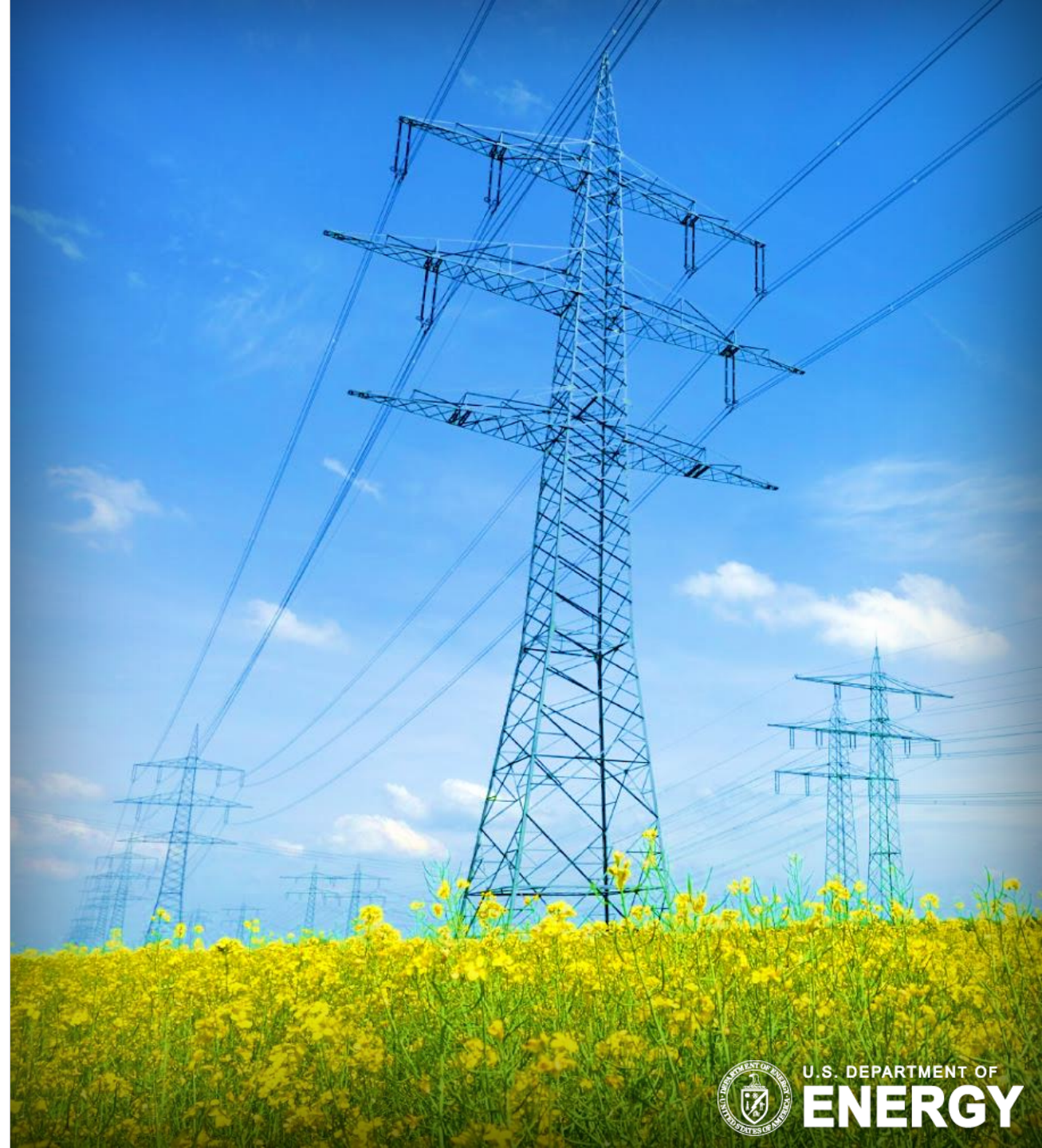
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U.S. DEPARTMENT OF  
**ENERGY**





# **NEWTS**

## **DATABASE**

**NATIONAL ENERGY WATER TREATMENT & SPECIATION (NEWTS)**

# Authors and Contact Information

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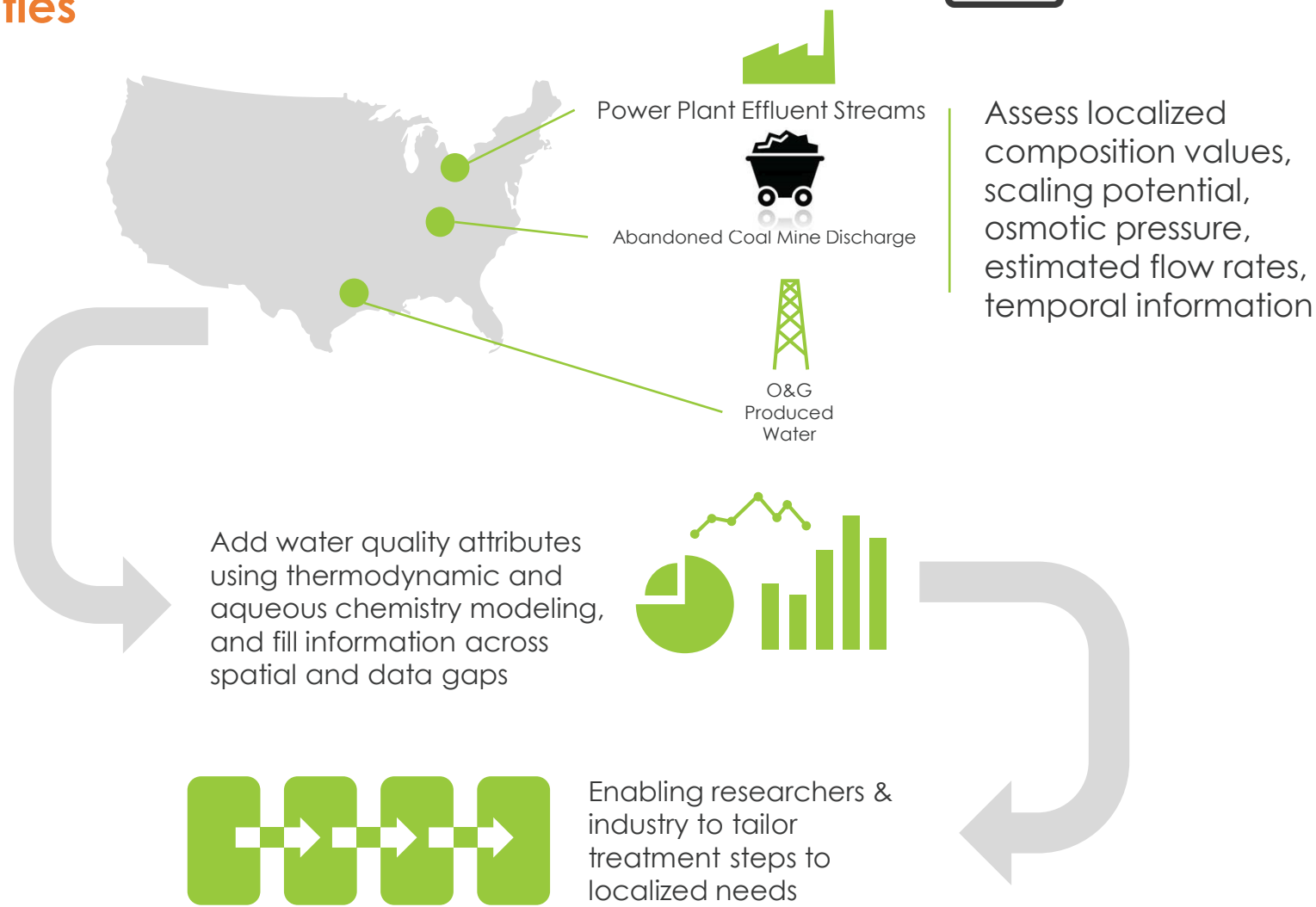


# National Energy Water Treatment & Speciation Database

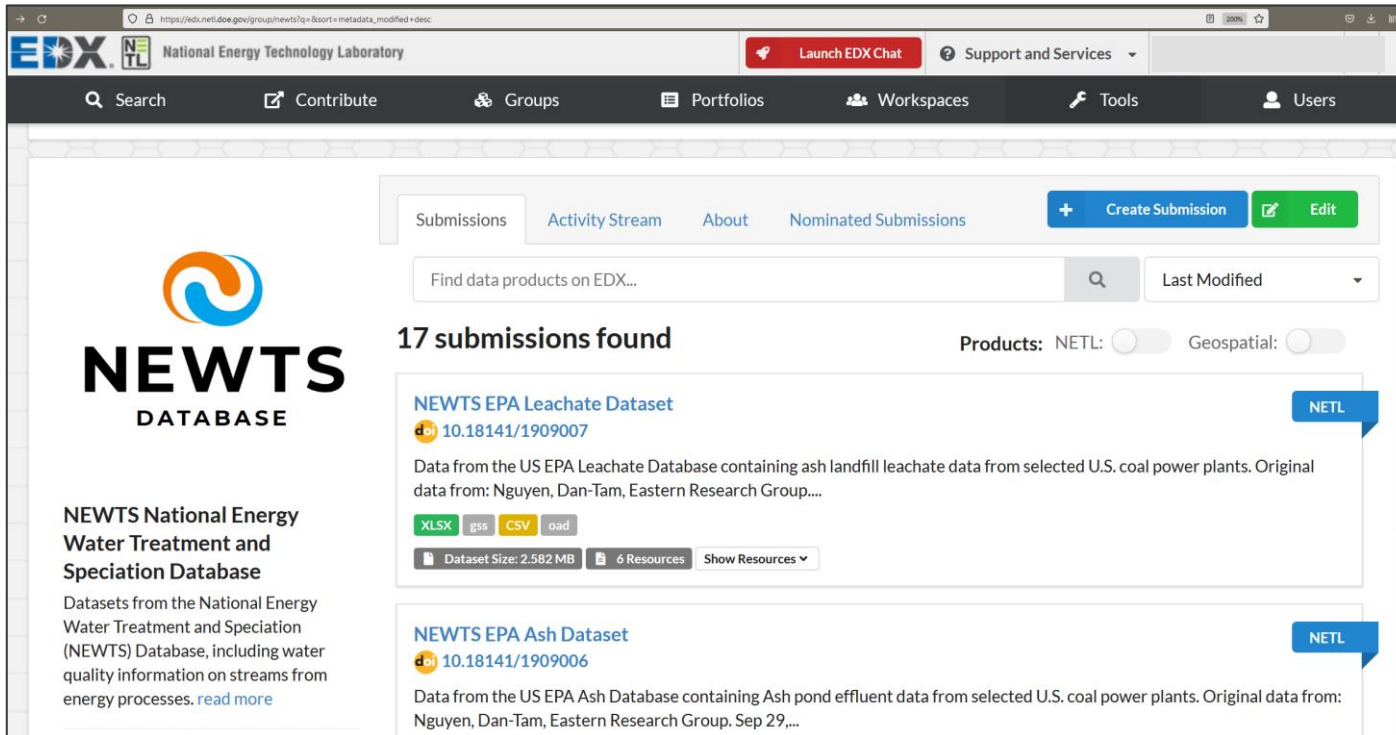
## Leveraging NETL R&D Core Capabilities

### 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,...



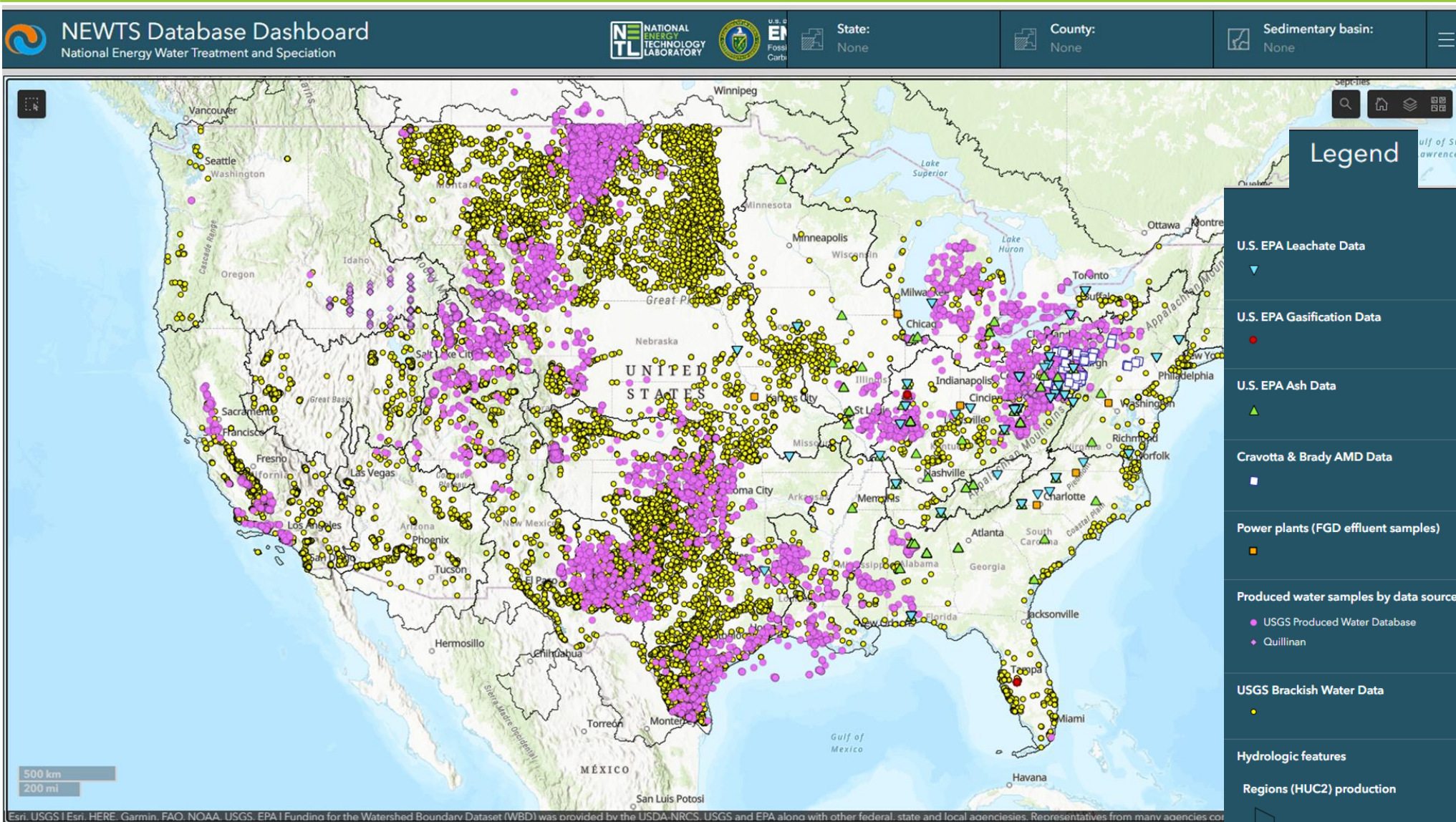
- NEWTS Data Catalog
- [Overview Video](#)
- Training Videos

<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

# 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

**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**

Groups / NEWTS National Energy Water...

Submissions Activity Stream About Nominated Submissions

Find data products on EDX...

17 submissions found

Products: NETL: ☒ Geospatial: ☐

**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...  
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"...  
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...  
Dataset Size: 0 bytes 1 Resource Show Resources

**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

# 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_Cravotta_AMD	
SNAME	Descriptio Redox State	1		2		3	
MINE_NUM	Some Mines have multiple Streams	1		2		3	
STAD	Station identifier used by USGS	4.03619E+14		4.03748E+14		4.03748E+14	
Lon_dd		40.60056		40.62994		40.62994	
Lat_dd		-76.50583		-76.55399		-76.55399	
Mine_Type		Deep		Deep		Deep	
Passive		Active		Active		Active	
CaO		CaO		CaO		CaO	
Inflow_Outflow		110503		110503		110503	
DATE		1000		1230		1230	
TIME							
Alkalinity	Alkalinity	Blank & Total Comb	mg/L as CaCO3			5.3	
TIC	TIC		mol C/L	2.39		1.38	
Density			g/mL				
Specific El COND			μS/cm	802		311	
B(OH)3	Boron Hydroxide	Not Meas	mg/L of B(OH)3				
Be(OH)2	Beryllium	2	mg/L of Be(OH)2	1.86E-02		5.73E-03	
Pd(OH)2	Palladium	2	mg/L of Pd(OH)2				
Al(OH)3	Aluminum	3	mg/L of Al(OH)3	1.35E+01		2.40E+00	
Bi(OH)3	Bismuth	Bi_Total	3	mg/L of Bi(OH)3			
CrO(OH)3	Chromium	Cr_Total	3	2.62E-03			
GaO(OH)3	Gallium	Ga_Total	3	1.62E-04		5.89E-05	
In(OH)3	Indium	In_Total	3	1.30E-05		1.44E-06	
Ru(OH)4	Ruthenium	4	mg/L of Ru(OH)4				
SiO2	Silica	4	mg/L of SiO2	2.46E+01		1.81E+01	
SnO2	Tin	4	mg/L of SnO2				
ThO2	Thorium	Th_T	4	4.09E-04		4.89E-05	
TiO2	Titanium	4	mg/L of TiO2	3.50E-03		2.00E-03	
ZrO2	Zirconium	4	mg/L of ZrO2	2.70E-05		1.35E-05	
Sb(OH)5	Antimony hydroxide	5	mg/L of Sb(OH)5	1.70E-05		1.70E-05	
UO3	Uranium	6	mg/L of UO3	1.61E-03		3.05E-04	
C6H5OH	Phenol	organic	mg/L of C6H5OH	3.00E-04			
O2	Oxygen	0	mg/L of O2	10.6		10.7	
NH4+1	Ammonium	-3	mg/L of NH4+	1.54E-01		1.29E-01	
Ag+1	Silver	1	mg/L of Ag+				
Cs+1	Cesium	Cs	1	1.46E-04		8.70E-05	
K+1	Potassium	1	mg/L of K+	7.31E+00		1.60E+00	
Li+1	Lithium	1	mg/L of Li+	9.85E-02		2.30E-02	
Na+1	Sodium	1	mg/L of Na+	2.71E+01		2.20E+00	
Rb+1	Rubidium	1	mg/L of Rb+	8.11E-03		3.04E-03	
Tl+1	Thallium	1	mg/L of Tl+	7.90E-05		3.40E-05	
Ba+2	Barium	2	mg/L of Ba2+	2.05E-02		2.91E-02	
Ca+2	Calcium	2	mg/L of Ca2+	4.22E+01		2.21E+01	
Co+2	Cobalt	2	mg/L of Co2+	8.05E-04		2.10E-04	
Cr+6	Chromium	6	mg/L of Cr6+	2.10E-04		2.10E-04	
Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
Mg+2	Magnesium	2	mg/L of Mg2+	2.10E-04		2.10E-04	
Mn+2	Manganese	2	mg/L of Mn2+	2.10E-04		2.10E-04	
Ni+2	Nickel	2	mg/L of Ni2+	2.10E-04		2.10E-04	
Pb+2	Lead	2	mg/L of Pb2+	2.10E-04		2.10E-04	
Se+4	Selenium	4	mg/L of Se4+	2.10E-04		2.10E-04	
Te+4	Tellurium	4	mg/L of Te4+	2.10E-04		2.10E-04	
Zn+2	Zinc	2	mg/L of Zn2+	2.10E-04		2.10E-04	
As+3	Arsenic	3	mg/L of As3+	2.10E-04		2.10E-04	
Br-1	Bromine	-1	mg/L of Br-	2.10E-04		2.10E-04	
I-1	Iodine	-1	mg/L of I-	2.10E-04		2.10E-04	
Mo+6	Molybdenum	6	mg/L of Mo6+	2.10E-04		2.10E-04	
Cr+6	Chromium	6	mg/L of Cr6+	2.10E-04		2.10E-04	
Co+2	Cobalt	2	mg/L of Co2+	2.10E-04		2.10E-04	
Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
Mg+2	Magnesium	2	mg/L of Mg2+	2.10E-04		2.10E-04	
Mn+2	Manganese	2	mg/L of Mn2+	2.10E-04		2.10E-04	
Ni+2	Nickel	2	mg/L of Ni2+	2.10E-04		2.10E-04	
Pb+2	Lead	2	mg/L of Pb2+	2.10E-04		2.10E-04	
Se+4	Selenium	4	mg/L of Se4+	2.10E-04		2.10E-04	
Te+4	Tellurium	4	mg/L of Te4+	2.10E-04		2.10E-04	
Zn+2	Zinc	2	mg/L of Zn2+	2.10E-04		2.10E-04	
As+3	Arsenic	3	mg/L of As3+	2.10E-04		2.10E-04	
Br-1	Bromine	-1	mg/L of Br-	2.10E-04		2.10E-04	
I-1	Iodine	-1	mg/L of I-	2.10E-04		2.10E-04	
Mo+6	Molybdenum	6	mg/L of Mo6+	2.10E-04		2.10E-04	
Cr+6	Chromium	6	mg/L of Cr6+	2.10E-04		2.10E-04	
Co+2	Cobalt	2	mg/L of Co2+	2.10E-04		2.10E-04	
Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
Mg+2	Magnesium	2	mg/L of Mg2+	2.10E-04		2.10E-04	
Mn+2	Manganese	2	mg/L of Mn2+	2.10E-04		2.10E-04	
Ni+2	Nickel	2	mg/L of Ni2+	2.10E-04		2.10E-04	
Pb+2	Lead	2	mg/L of Pb2+	2.10E-04		2.10E-04	
Se+4	Selenium	4	mg/L of Se4+	2.10E-04		2.10E-04	
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As+3	Arsenic	3	mg/L of As3+	2.10E-04		2.10E-04	
Br-1	Bromine	-1	mg/L of Br-	2.10E-04		2.10E-04	
I-1	Iodine	-1	mg/L of I-	2.10E-04		2.10E-04	
Mo+6	Molybdenum	6	mg/L of Mo6+	2.10E-04		2.10E-04	
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Co+2	Cobalt	2	mg/L of Co2+	2.10E-04		2.10E-04	
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Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
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Pb+2	Lead	2	mg/L of Pb2+	2.10E-04		2.10E-04	
Se+4	Selenium	4	mg/L of Se4+	2.10E-04		2.10E-04	
Te+4	Tellurium	4	mg/L of Te4+	2.10E-04		2.10E-04	
Zn+2	Zinc	2	mg/L of Zn2+	2.10E-04		2.10E-04	
As+3	Arsenic	3	mg/L of As3+	2.10E-04		2.10E-04	
Br-1	Bromine	-1	mg/L of Br-	2.10E-04		2.10E-04	
I-1	Iodine	-1	mg/L of I-	2.10E-04		2.10E-04	
Mo+6	Molybdenum	6	mg/L of Mo6+	2.10E-04		2.10E-04	
Cr+6	Chromium	6	mg/L of Cr6+	2.10E-04		2.10E-04	
Co+2	Cobalt	2	mg/L of Co2+	2.10E-04		2.10E-04	
Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
Mg+2	Magnesium	2	mg/L of Mg2+	2.10E-04		2.10E-04	
Mn+2	Manganese	2	mg/L of Mn2+	2.10E-04		2.10E-04	
Ni+2	Nickel	2	mg/L of Ni2+	2.10E-04		2.10E-04	
Pb+2	Lead	2	mg/L of Pb2+	2.10E-04		2.10E-04	
Se+4	Selenium	4	mg/L of Se4+	2.10E-04		2.10E-04	
Te+4	Tellurium	4	mg/L of Te4+	2.10E-04		2.10E-04	
Zn+2	Zinc	2	mg/L of Zn2+	2.10E-04		2.10E-04	
As+3	Arsenic	3	mg/L of As3+	2.10E-04		2.10E-04	
Br-1	Bromine	-1	mg/L of Br-	2.10E-04		2.10E-04	
I-1	Iodine	-1	mg/L of I-	2.10E-04		2.10E-04	
Mo+6	Molybdenum	6	mg/L of Mo6+	2.10E-04		2.10E-04	
Cr+6	Chromium	6	mg/L of Cr6+	2.10E-04		2.10E-04	
Co+2	Cobalt	2	mg/L of Co2+	2.10E-04		2.10E-04	
Fe+2	Iron	2	mg/L of Fe2+	2.10E-04		2.10E-04	
Mg+2	Magnesium	2	mg/L of Mg2+	2.10E-04		2.10E-04	
Mn+2	Manganese	2	mg/L of Mn2+	2.10E-04		2.10E-04	
Ni+2	Nickel	2	mg/L of Ni2+	2.10E-04		2.10E-04	
Pb+2	Lead	2	mg/L of Pb2+	2			

# Integration with Modeling Software

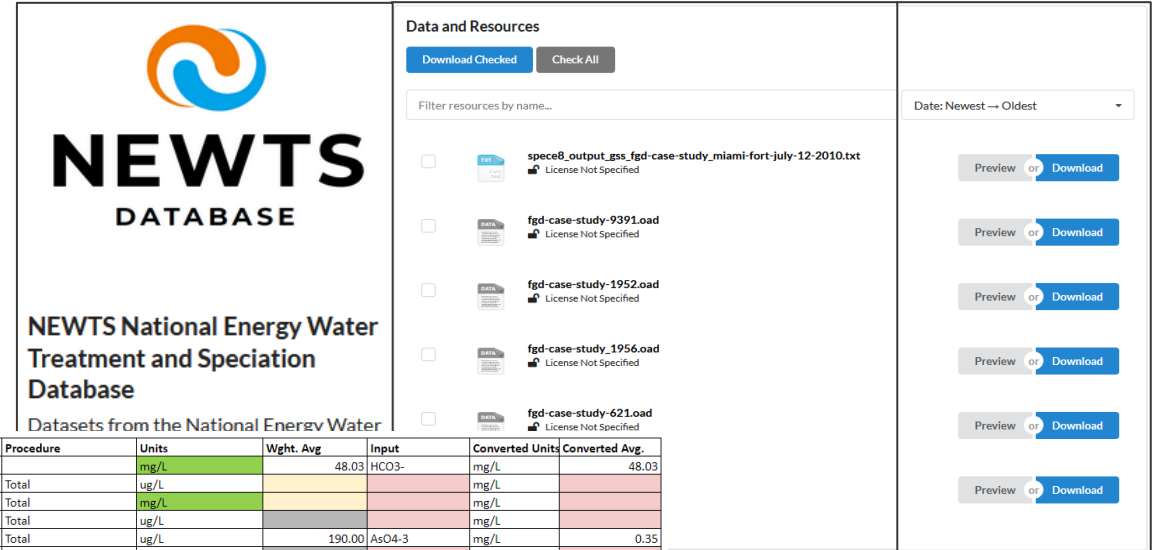
Leveraging tools for filling data gaps & modeling treatment

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



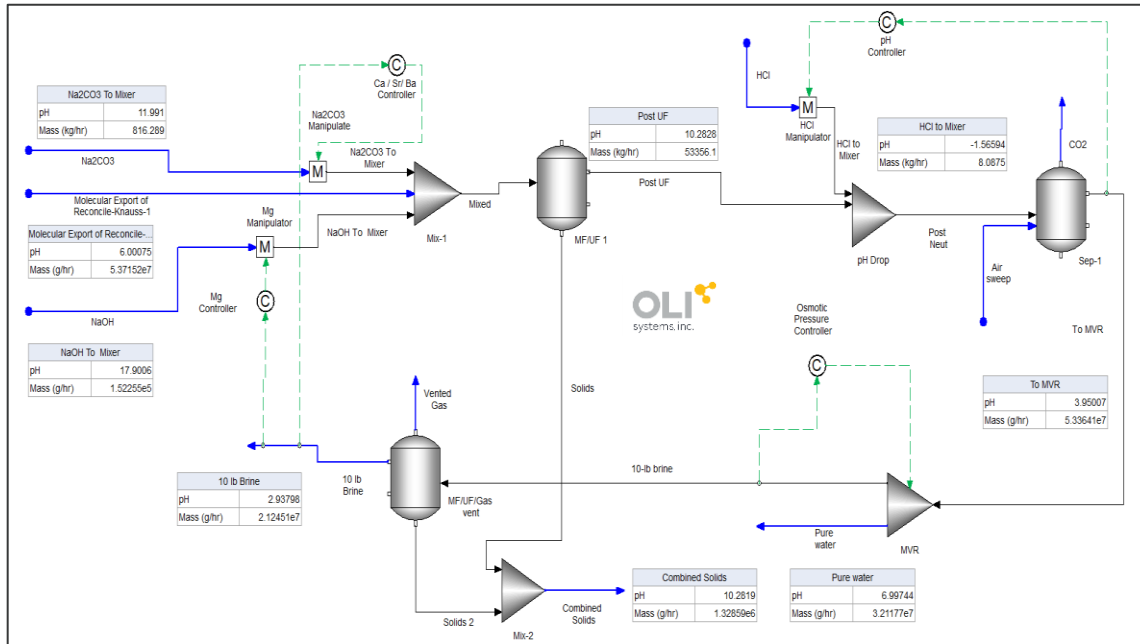
The screenshot shows the NEWTS Database interface. On the left is the NEWTS logo and text: "NEWTS National Energy Water Treatment and Speciation Database". On the right, under "Data and Resources", there are buttons for "Download Checked" and "Check All", a search bar, and a list of datasets with checkboxes and "Preview" or "Download" buttons. The datasets listed are: "spece8\_output\_gss\_fgd-case-study\_miami-fort-july-12-2010.txt", "fgd-case-study-9391.oad", "fgd-case-study-1952.oad", "fgd-case-study\_1956.oad", and "fgd-case-study-621.oad".

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

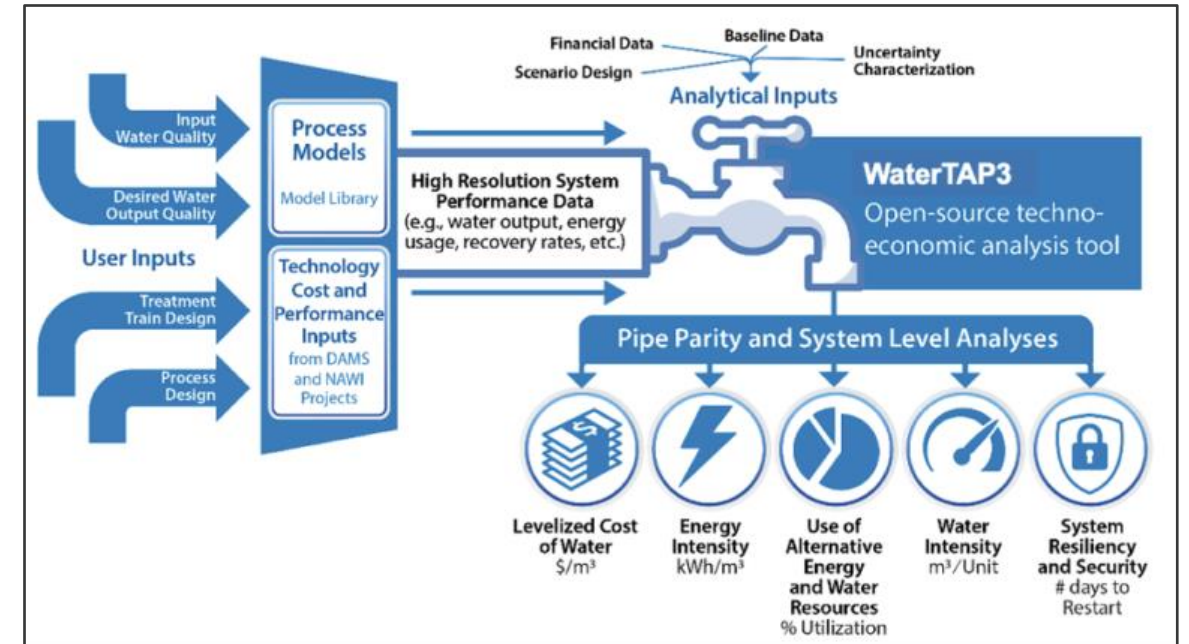


# Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment



Input Water Stream



Input Water Quality



# 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 Coml	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

Be(OH)2 2.39000E-3

Pd(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-5

Ru(OH)4 8.37000E-5

SiO2 19.0000

SnO2 0.0

ThO2 1.25000E-5

TiO2 0.0185000

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.

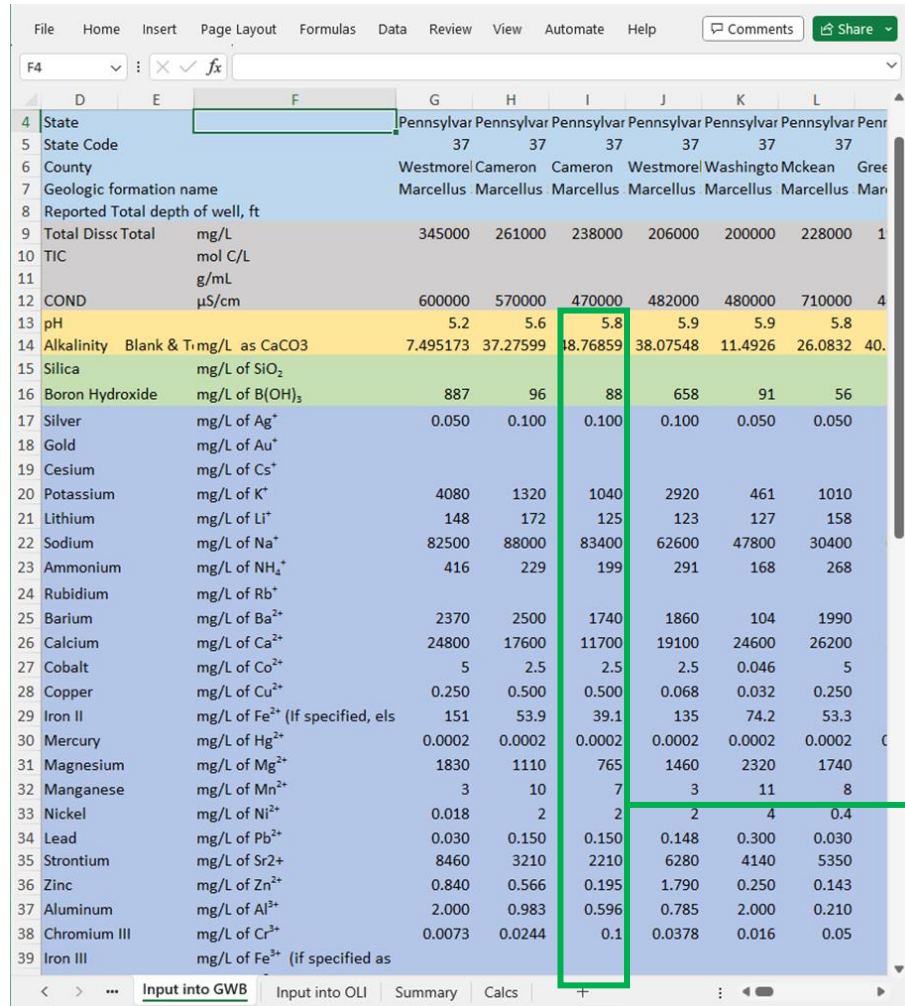
Alkalinity Calculation

25.0000 °C 1.00000 atm

Calculation not done

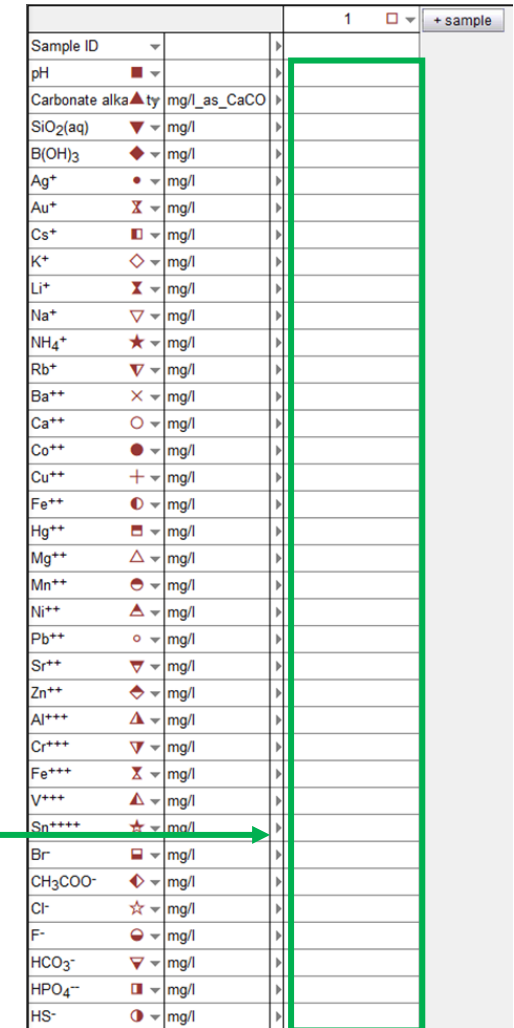
# Ease of Input into Aqueous Chemistry Software

Geochemist's Workbench example



	D	E	F	G	H	I	J	K	L
4	State		Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan	Pennsylvan
5	State Code		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	Mar
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 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)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 with others (silica) likely in the future



NATIONAL  
ENERGY  
TECHNOLOGY  
LABORATORY

- Millions of  
Barrels of Water
- 
- A vertical legend with seven color-coded squares and their corresponding ranges:
- |             |                 |
|-------------|-----------------|
| Dark purple | < 100           |
| Dark blue   | 100 – 500       |
| Medium blue | 500 – 1,000     |
| Teal        | 1,000 – 2,000   |
| Green       | 2,000 – 5,000   |
| Light green | 5,000 – 10,000  |
| Yellow      | 10,000 – 21,370 |



# 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/EPA-HQ-OW-2009-0819-5640">https://www.regulations.gov/collection/EPA-HQ-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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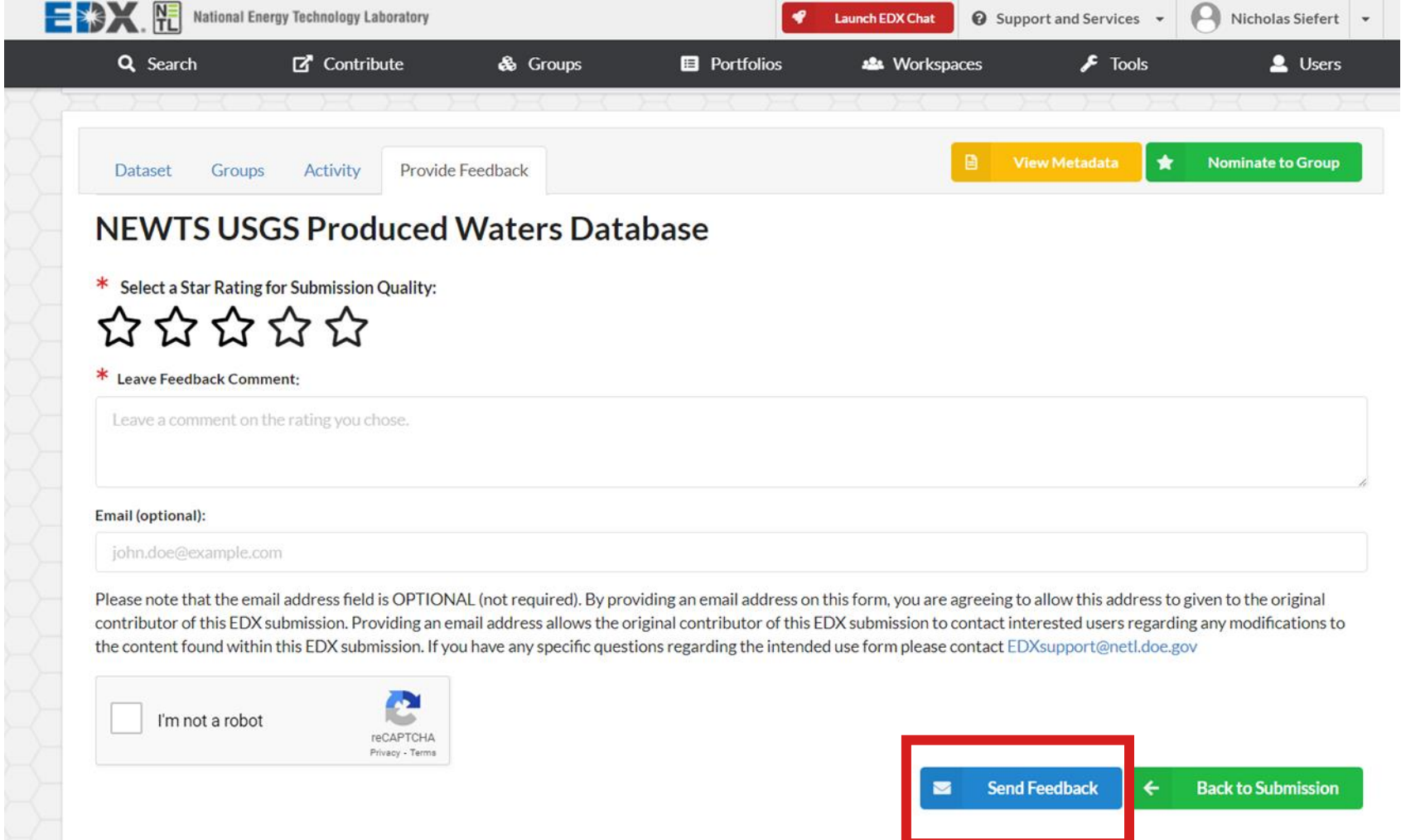
### Citation (Click to Copy)

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 EDX website interface. At the top, there's a navigation bar with 'EDX' and 'National Energy Technology Laboratory' logos, a 'Launch EDX Chat' button, and a 'Support and Services' dropdown. Below this is a secondary navigation bar with links for 'Search', 'Contribute', 'Groups', 'Portfolios', 'Workspaces', 'Tools', and 'Users'. The main content area has tabs for 'Dataset', 'Groups', 'Activity', and 'Provide Feedback'. The 'Provide Feedback' tab is active, showing a form for the 'NEWTS USGS Produced Waters Database'. The form includes a star rating section with five stars, a text area for a comment, an optional email field, and a reCAPTCHA security check. At the bottom right, there are two buttons: 'Send Feedback' (highlighted with a red box) and 'Back to Submission'.

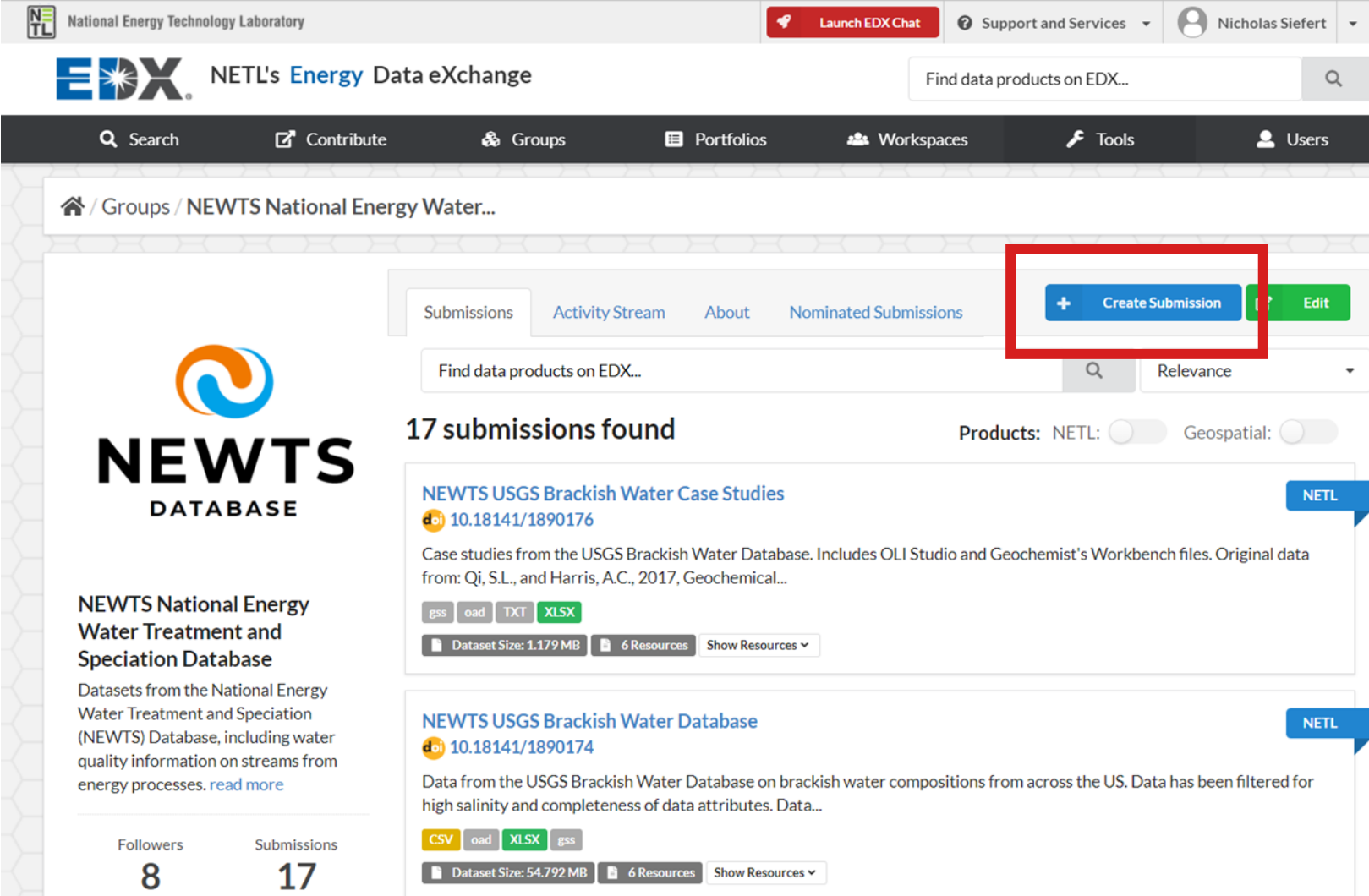
# Creating your own data submission

## 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

## 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..." group. On the left, there's a sidebar with the "NEWTS DATABASE" logo and 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". The main content area has tabs for "Submissions", "Activity Stream", "About", and "Nominated Submissions". A "Create Submission" button is highlighted with a red box. Below the tabs is a search bar and a "Relevance" dropdown. It shows "17 submissions found". Two dataset entries are visible: "NEWTS USGS Brackish Water Case Studies" and "NEWTS USGS Brackish Water Database". Each entry includes a DOI, a description, file format tags (e.g., gss, oad, TXT, XLSX), dataset size, and number of resources.

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