PRODUCED WATER SOCIETY 2024

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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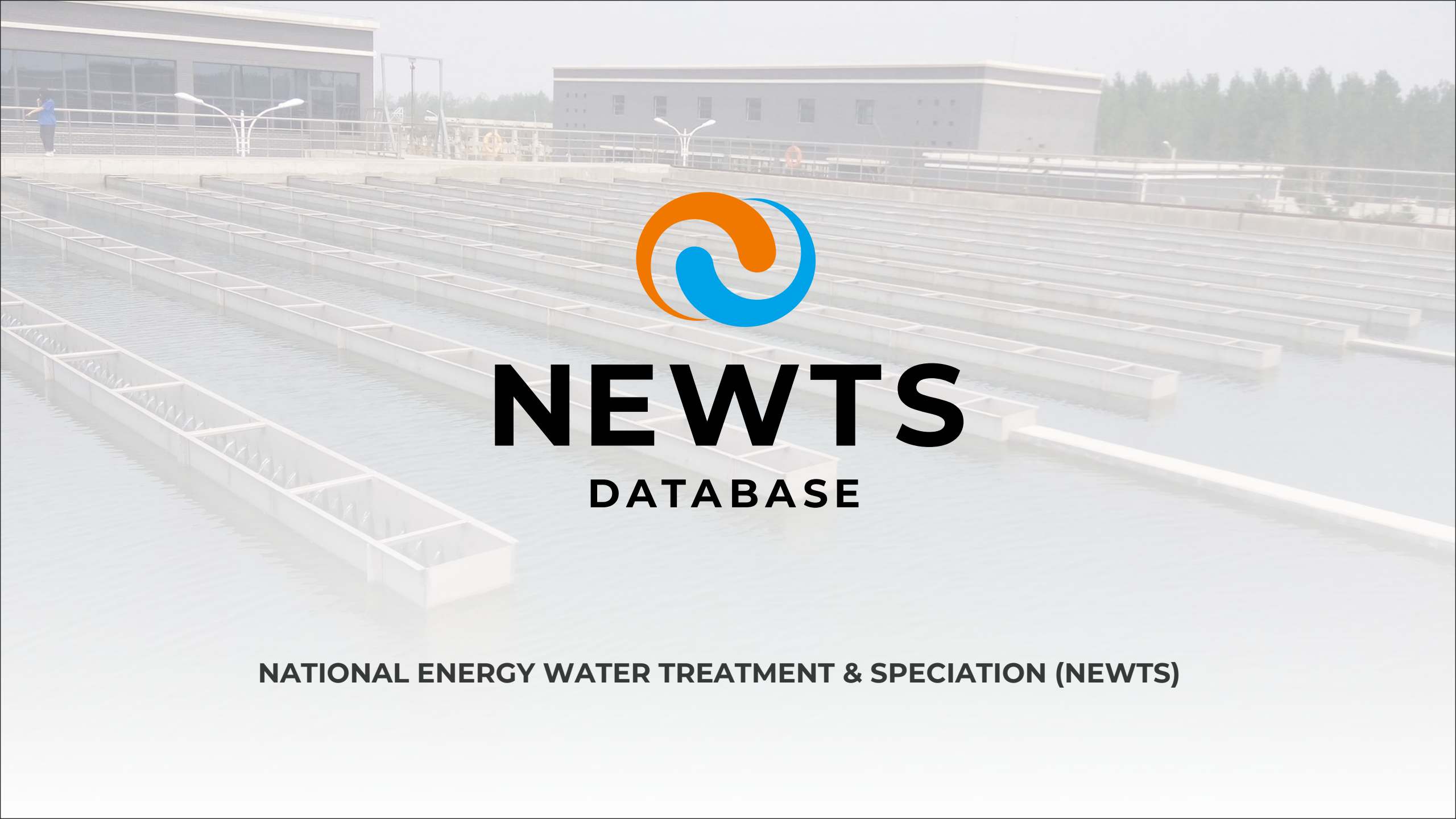
NATIONAL ENERGY TECHNOLOGY LABORATORY



NEWTS

DATABASE

NATIONAL ENERGY WATER TREATMENT & SPECIATION (NEWTS)

PRODUCED WATER SOCIETY 2024

Authors and Contact Information

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Motivation for NEWTS Database

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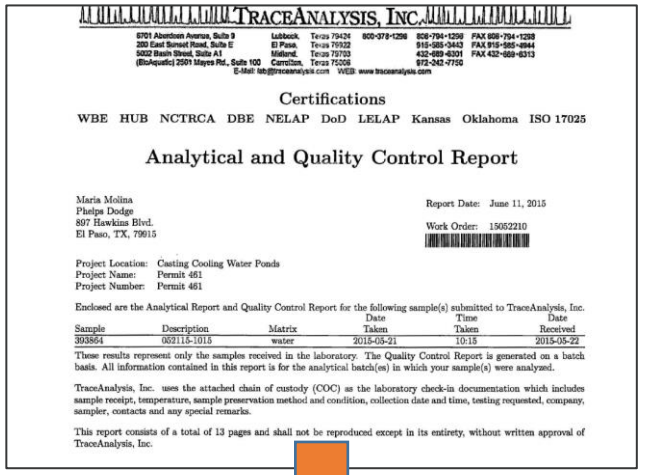
Prior state of energy-water data

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



TRACEANALYSIS, INC.

Certifications

WBE HUB NCTRCA DBE NELAP DoD LELAP Kansas Oklahoma ISO 17025

Analytical and Quality Control Report

Maria Molina
Phelps Dodge
897 Hawkins Blvd.
El Paso, TX, 79915

Report Date: June 11, 2015
Work Order: 15052210

Project Location: Casting Cooling Water Ponds
Project Name: Permit 461
Project Number: Permit 461

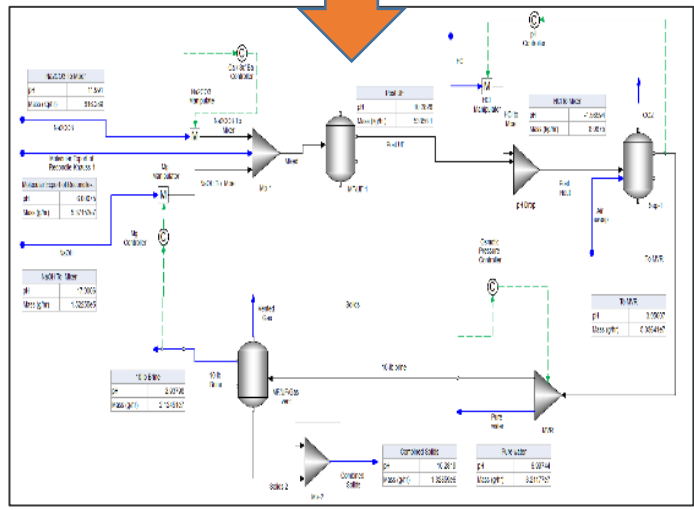
Enclosed are the Analytical Report and Quality Control Report for the following sample(s) submitted to TraceAnalysis, Inc.

Sample	Description	Matrix	Date Taken	Time Taken	Date Received
393864	002115-1015	water	2015-05-21	10:15	2015-05-22

These results represent only the samples received in the laboratory. The Quality Control Report is generated on a batch basis. All information contained in this report is for the analytical batch(es) in which your sample(s) were analyzed.

TraceAnalysis, Inc. uses the attached chain of custody (COC) as the laboratory check-in documentation which includes sample receipt, temperature, sample preservation method and condition, collection date and time, testing requested, company, sampler, contacts and any special remarks.

This report consists of a total of 13 pages and shall not be reproduced except in its entirety, without written approval of TraceAnalysis, Inc.



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

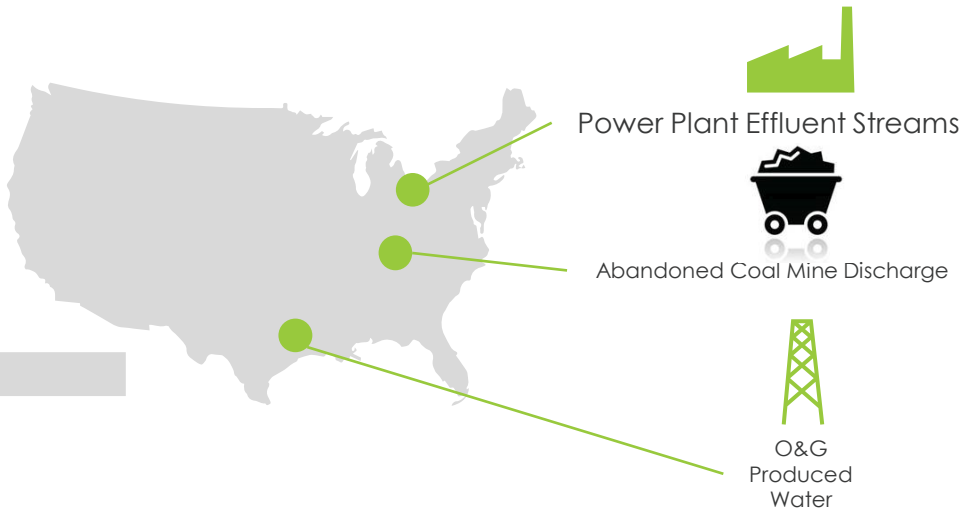
National Energy Water Treatment & Speciation Database

Leveraging NETL R&D Core Capabilities

Solution: Develop a Nationwide Energy Wastewater Data System

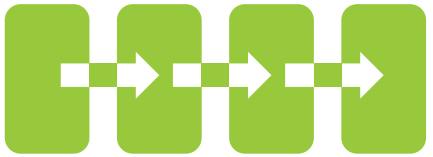
- Supplemented with thermodynamic & chemical modeling
- Includes **waste streams** such as:
  - USGS oil & gas produced water
  - Energy sector effluent (FGD, etc.)
  - Acid mine drainage (OSMRE)
  - Landfill leachate
  - And more

➢ Enables **design of localized treatment**
➢ **Publicly Available Data** hosted & displayed through **NETL's EDX**, and a custom visualization dashboard



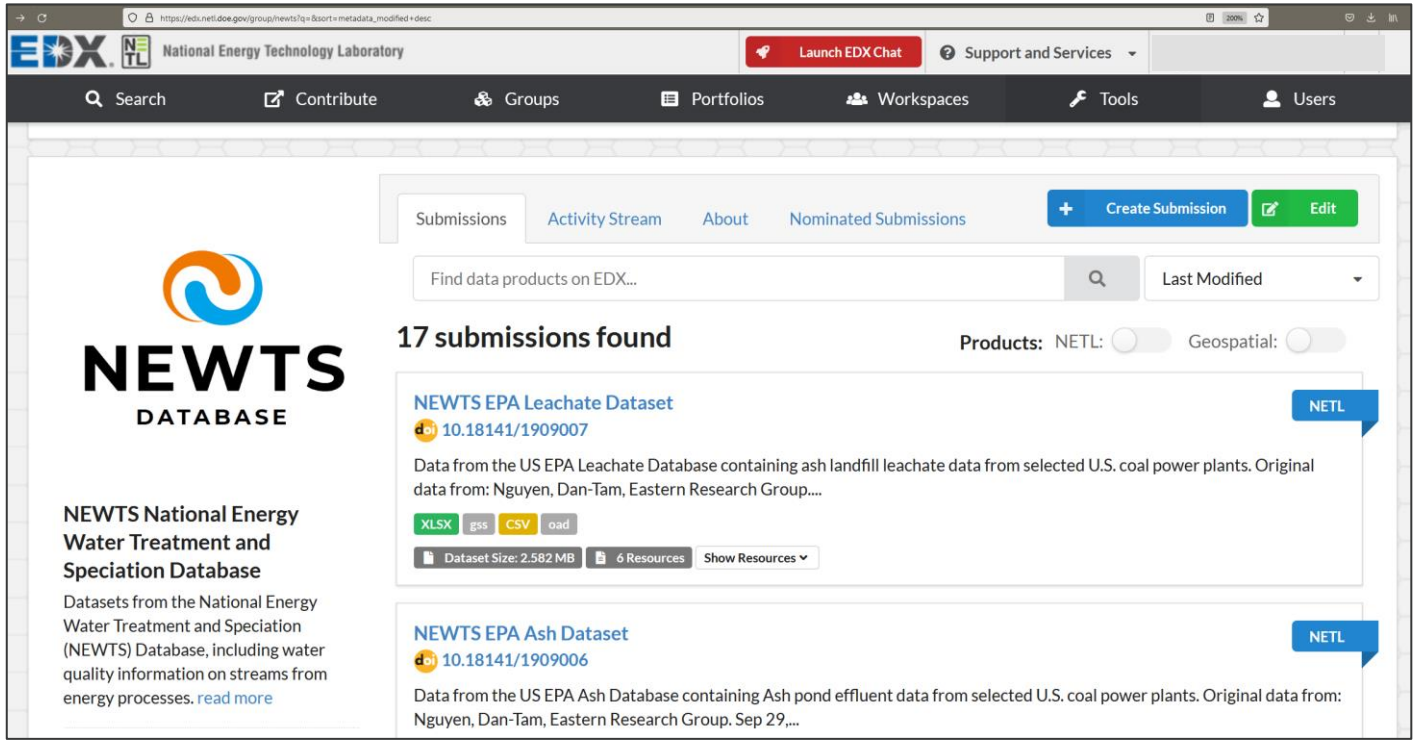
Assess localized composition values, scaling potential, osmotic pressure, estimated flow rates, temporal information

Add water quality attributes using thermodynamic and aqueous chemistry modeling, and fill information across spatial and data gaps



Enabling researchers & industry to tailor treatment steps to localized needs

NEWTS Public Group on EDX

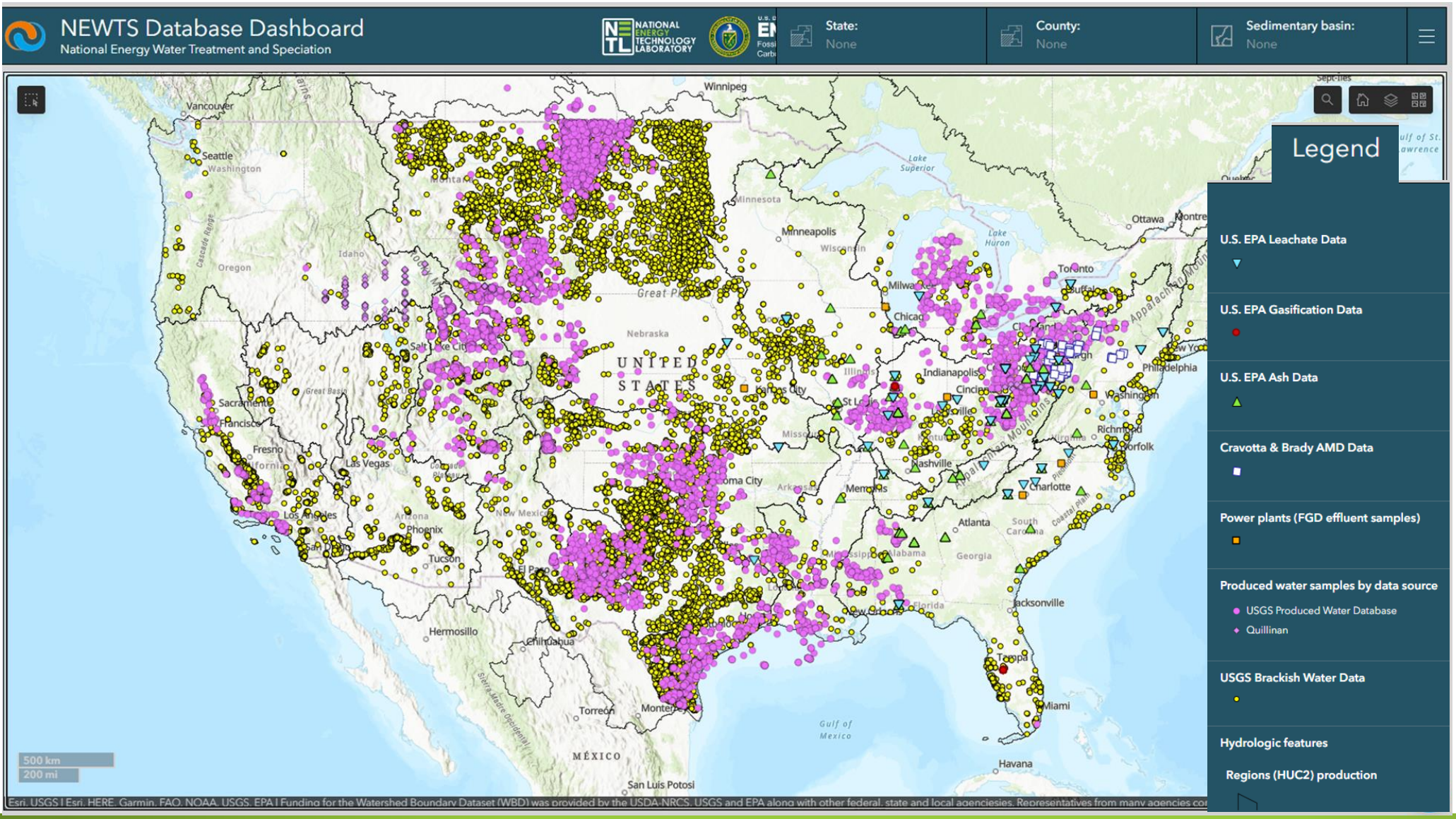


- NEWTS Data Catalog
- Overview Video
- Training Videos

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



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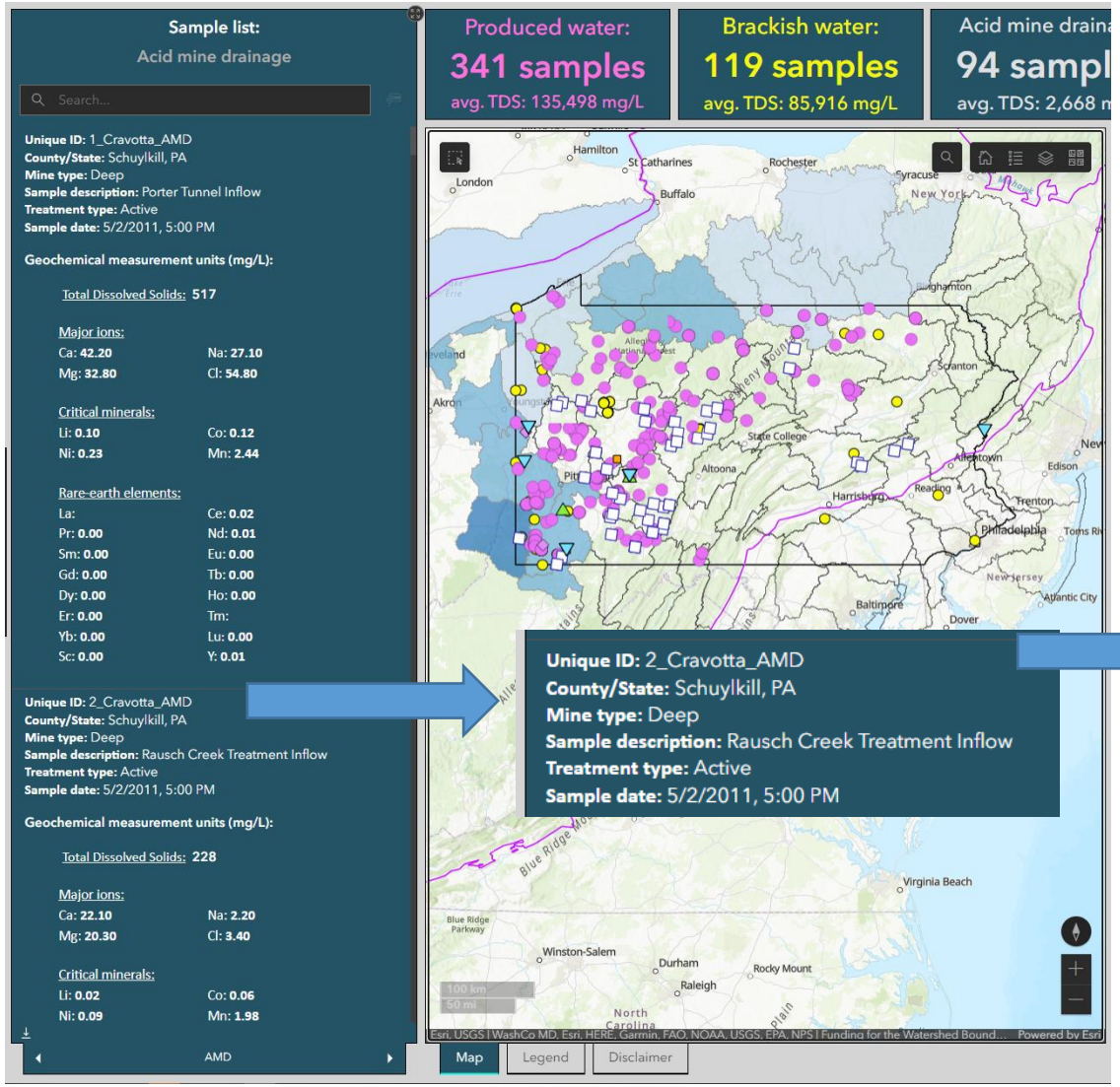
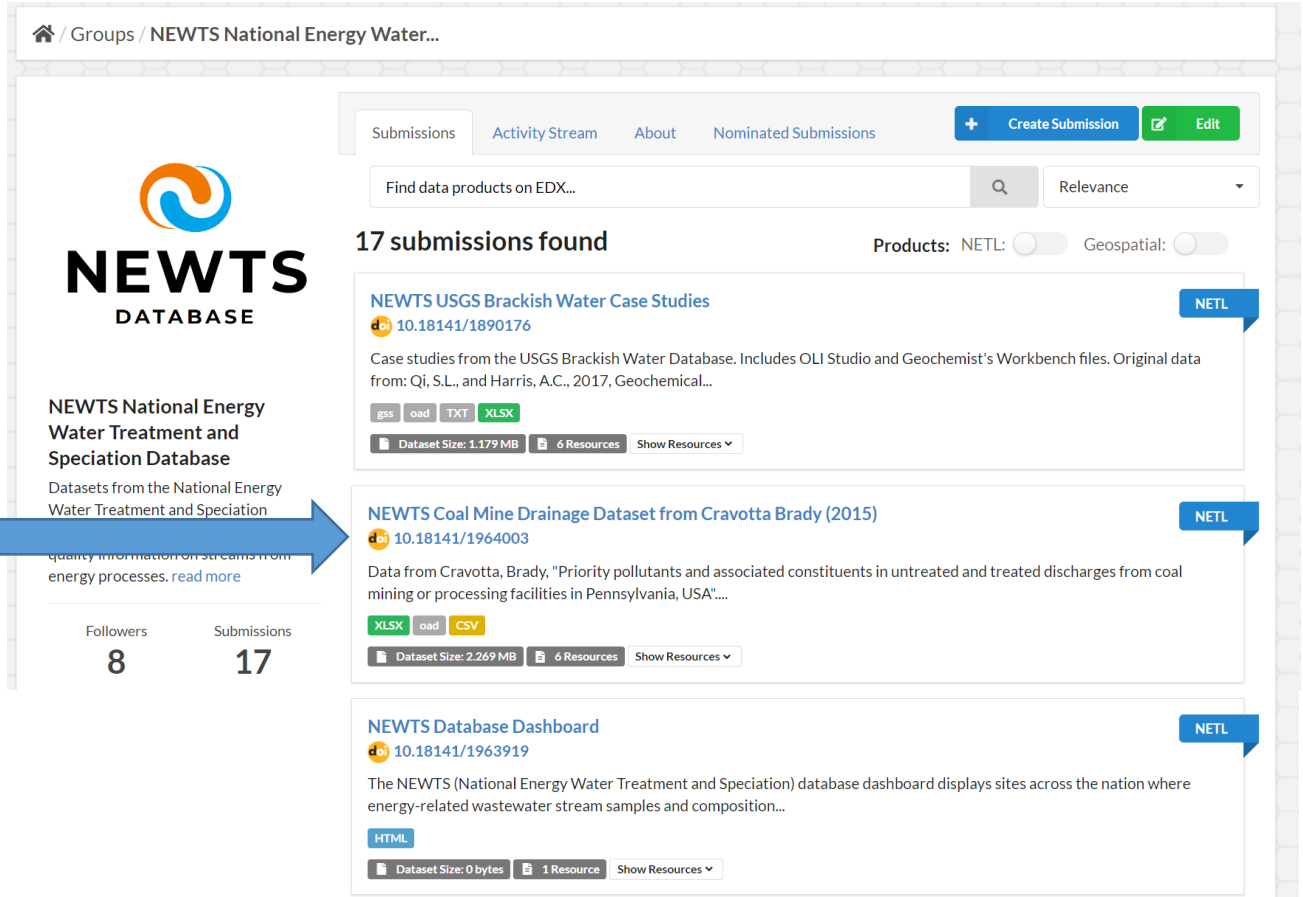
NEWTS Dashboard

Enables data visualization, exploration, and download

Connecting NEWTS Dashboard to the Database

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





Connecting NEWTS Dashboard to the Database

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

NEWTS Coal Mine Drainage Dataset from Cravotta Brady (2015)

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 co
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	View Info or Download
cb-pa-amd_pbs-job-8-inflow_id-num-25.oad	License Not Specified	View Info or Download
cravotta_oli_input_data_only.csv	License Not Specified	View Info or Download
cb-pa-amd_consol-renton-mine-inflow_id_num-39.oad	License Not Specified	View Info or Download
oli-template-for-cravotta-brady-2015.oad	License Not Specified	View Info or Download

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					1_Cravotta_AMD	2_Cravotta_AMD
ID_Num					1	2
SNAME		Descriptio	Redox State			flow Rausch Creek Trea
MINE_NUM		Some Mines have multiple Streams			1	2
STAID		Station identifier used by USG			4.03619E+14	4.03748E+14
Lon_dd					40.60056	40.62994
Lat_dd					-76.50583	-76.55399
Mine_Type					Deep	Deep
					Active	Active
					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	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)(s	Chromium	Cr_Total (	3	mg/L of CrO(OH)	2.62E-03	
GaO(OH)(s	Gallium	Ga_Total	3	mg/L of GaO(OH)	1.62E-04	5.89E-05
In(OH)3	Indium	In_Total	3	mg/L of $In(OH)_3$	1.30E-05	1.44E-06
Ru(OH)4	Ruthenium		4	mg/L of $Ru(OH)_4$		
SiO2	Silica		4	mg/L of SiO_2	2.46E+01	1.81E+01
SnO2	Tin		4	mg/L of SnO_2		
ThO2	Thorium	Th_T	4	mg/L of ThO_2	4.09E-04	4.89E-05
TiO2	Titanium		4	mg/L of TiO_2	3.50E-03	2.00E-03
ZrO2	Zirconium		4	mg/L of ZrO_2	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 UO_3	1.61E-03	3.05E-04
C6H5OH	Phenol		organic	mg/L of C_6H_5OH	3.00E-04	
O2	Oxygen		0	mg/L of O_2	10.6	10.7
NH4+1	Ammonium		-3	mg/L of NH_4^+	1.54E-01	1.29E-01
Ag+1	Silver		1	mg/L of Ag^+		
Cs+1	Cesium	Cs	1	mg/L of Cs^+	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 Ba^{2+}	2.05E-02	2.91E-02
Ca+2	Calcium		2	mg/L of Ca^{2+}	4.22E+01	2.21E+01

Original Data_Totals Only | Convert mgperL | mgperL Values | Transpose | Input to OLI | Charge Balance | Redox Species Summary

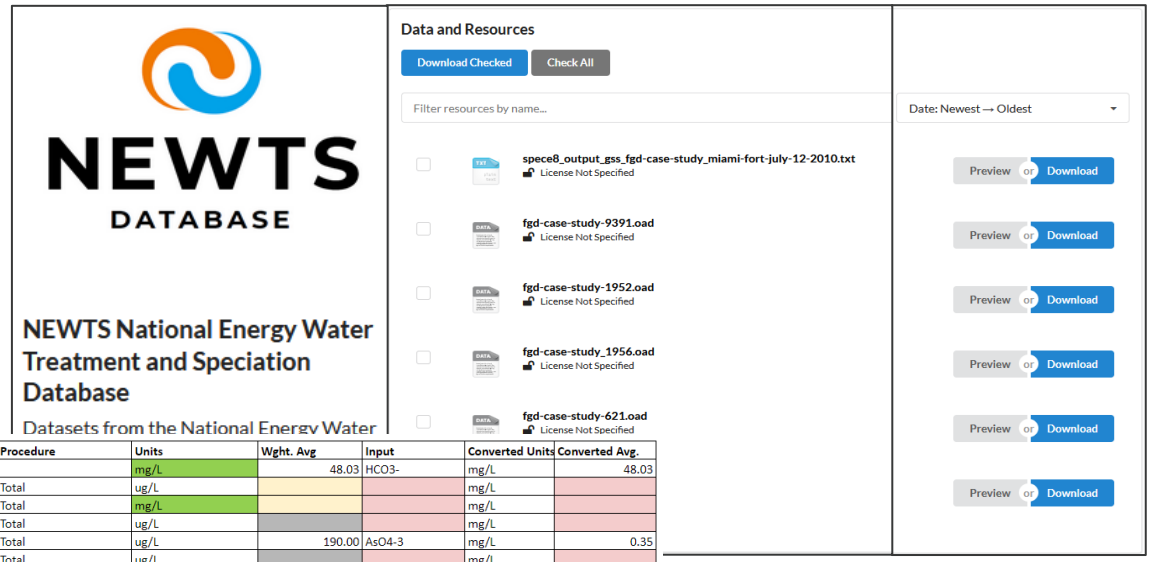
Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment

NATIONAL ENERGY TECHNOLOGY LABORATORY

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



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 Den	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

NAWI National Alliance for Water Innovation

Software include:

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

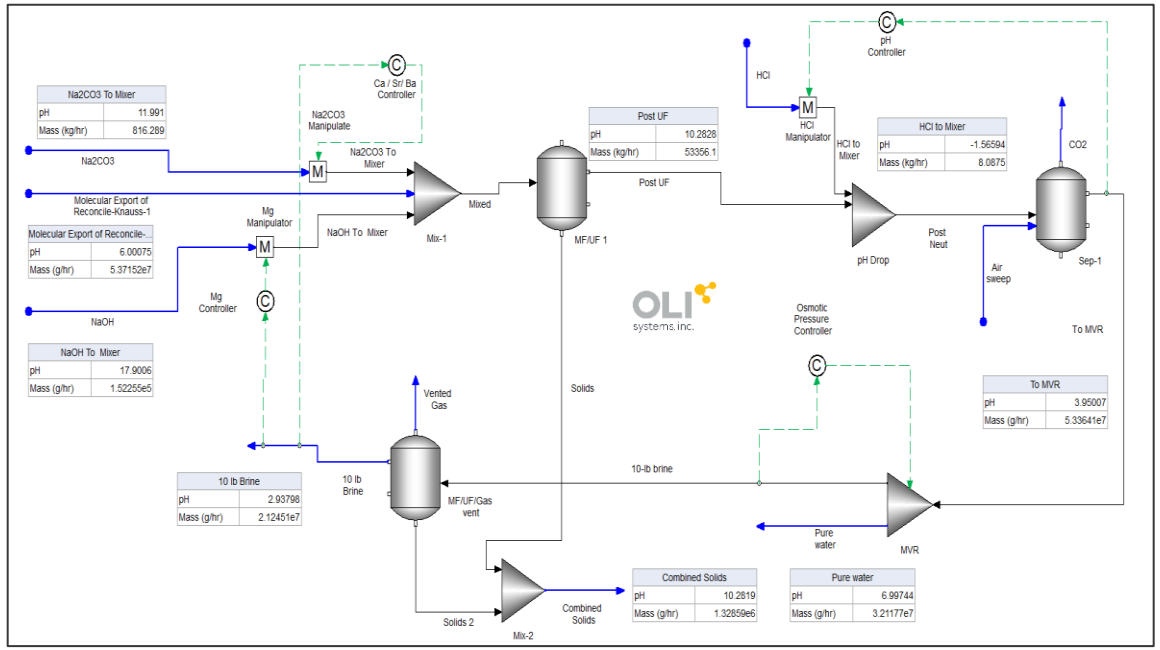
OLI systems, inc.

THE Geochemist's WORKBENCH

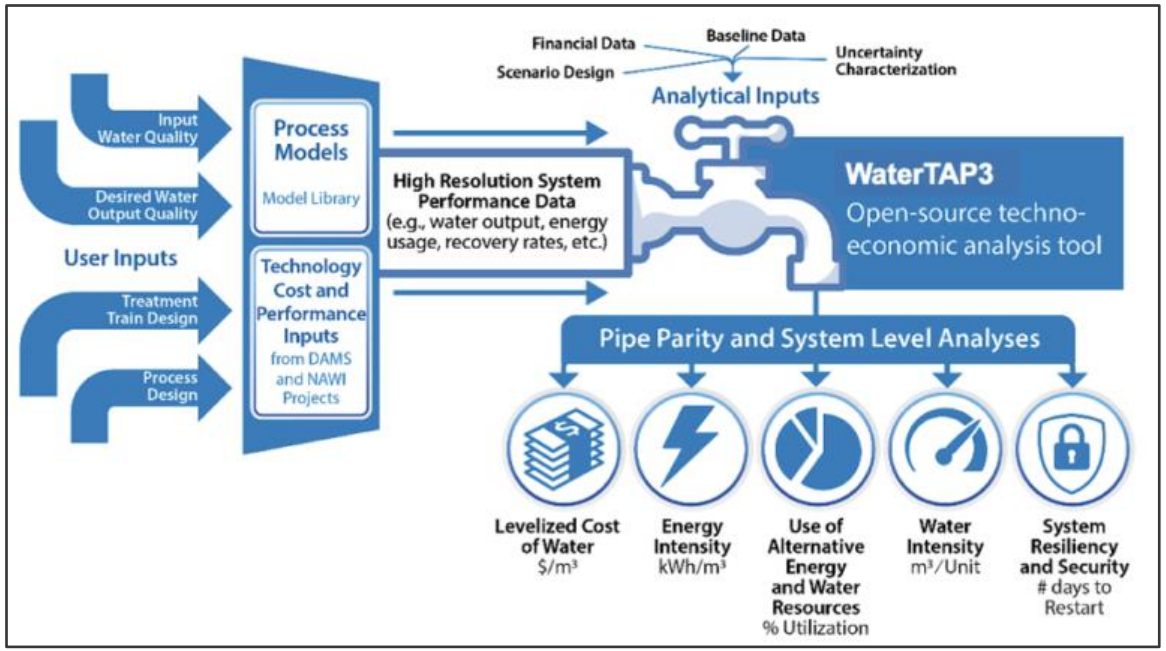
WAVE Water Treatment Design Software

Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment



Input Water Stream



Input Water Quality

OLI systems, inc.

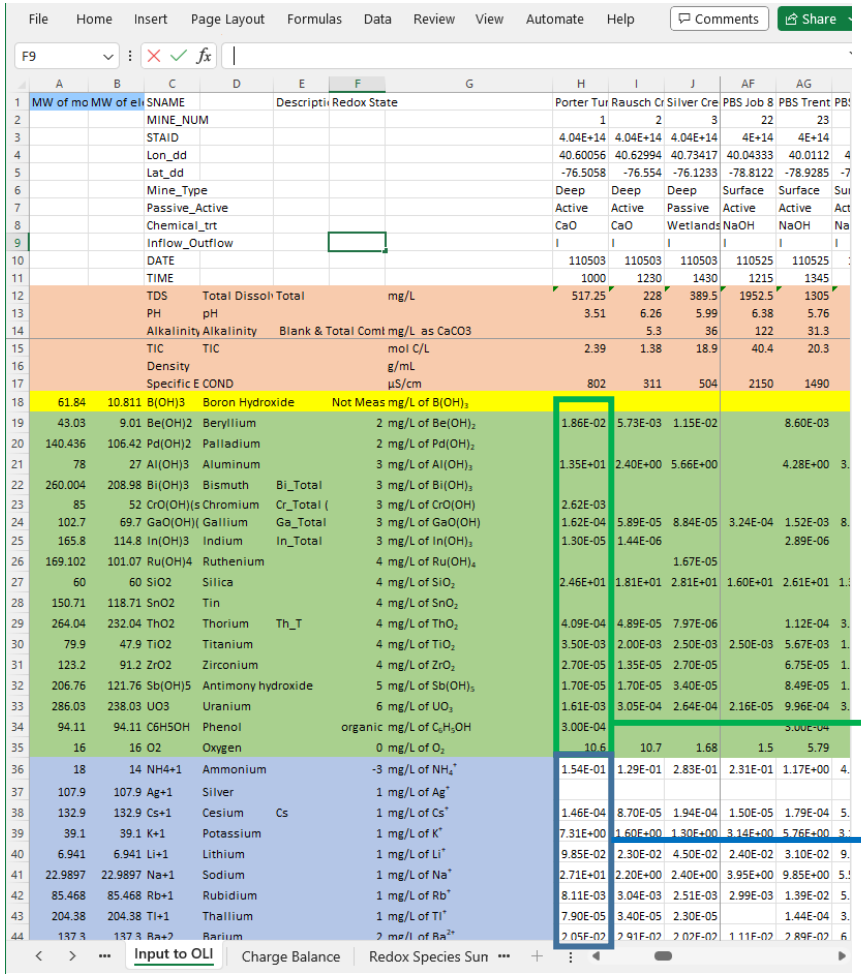
THE Geochemist's WORKBENCH

WAVE Water Treatment Design Software

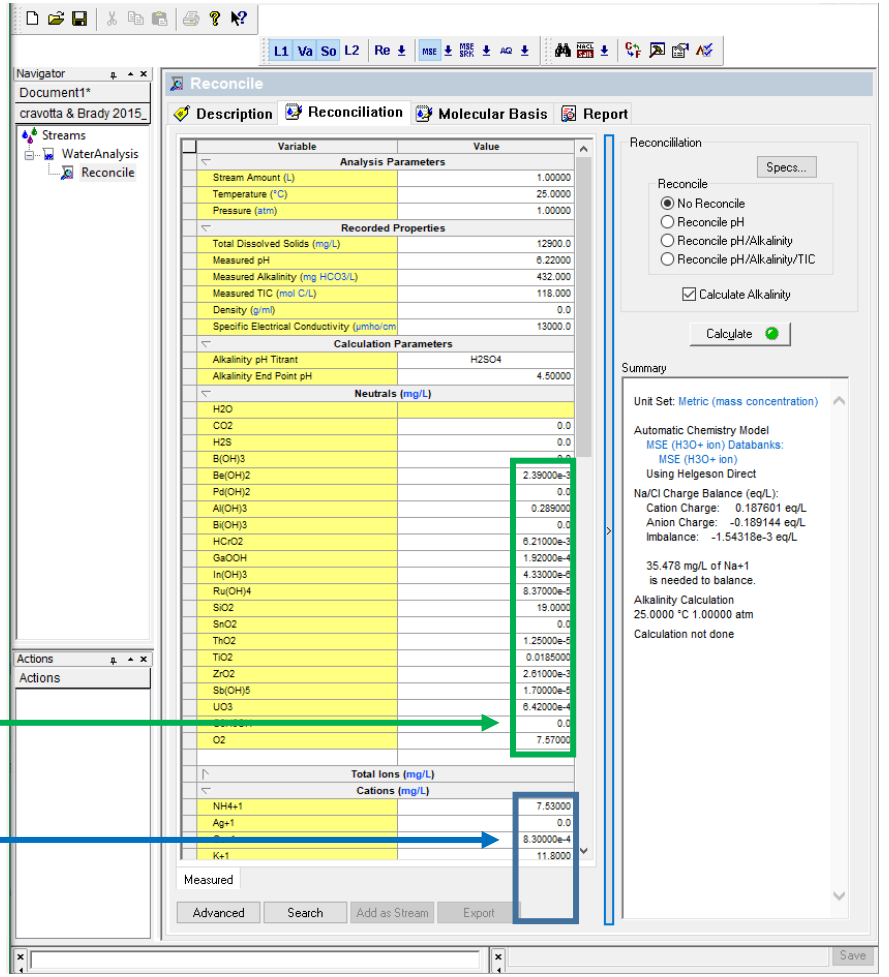
NAWI National Alliance for Water Innovation

Ease of Input into Aqueous Chemistry Software

OLI Studio example

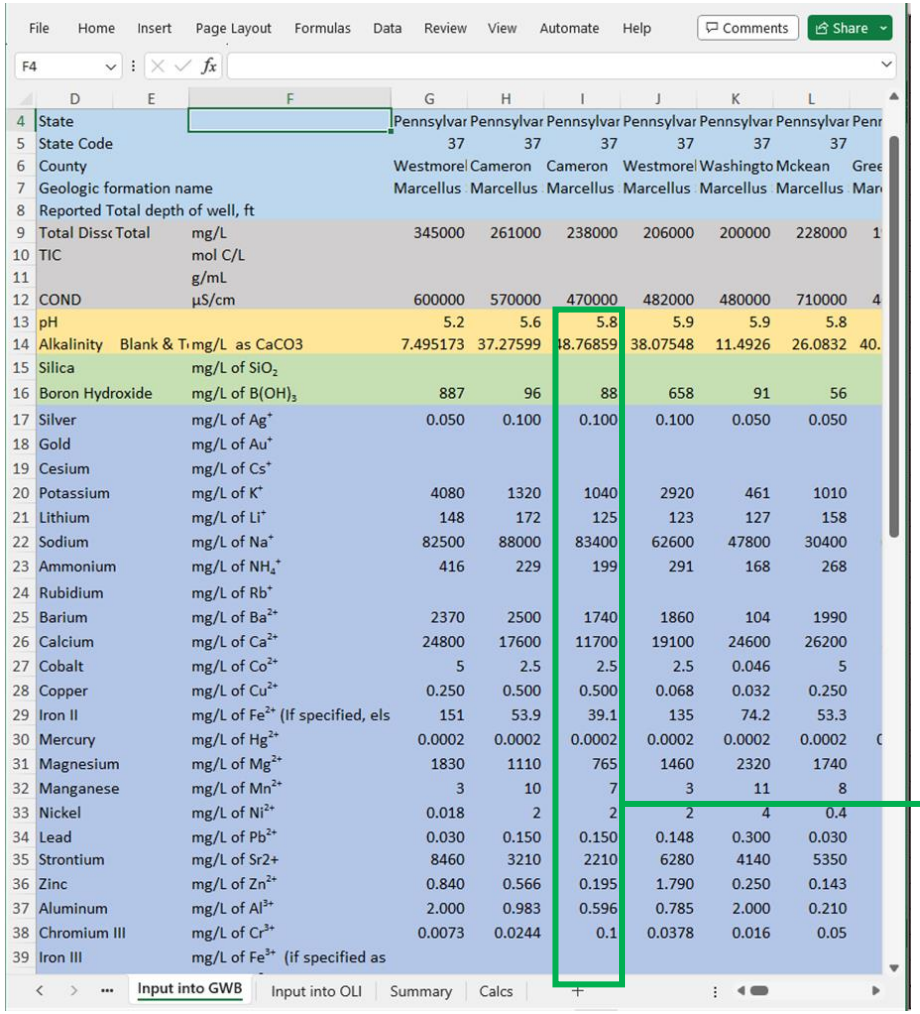


- Templates have been created so that water stream compositions can be easily input into OLI Studio and GWB Geochemist's Spreadsheet (GSS)



Ease of Input into Aqueous Chemistry Software

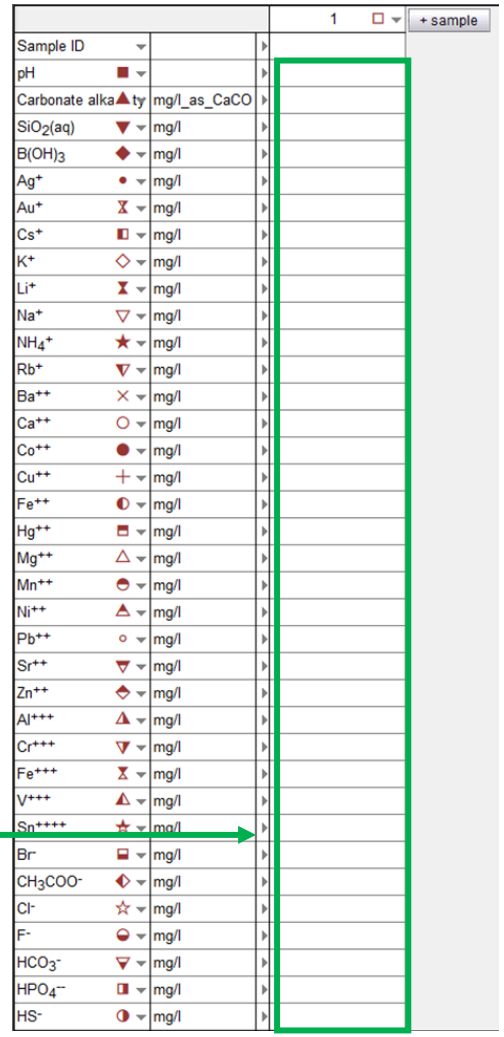
Geochemist's Workbench example



	D	E	F	G	H	I	J	K	L
4	State			Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar
5	State Code			37	37	37	37	37	37
6	County			Westmore	Cameron	Cameron	Westmore	Washingto	Mckean
7	Geologic formation name			Marcellus	Marcellus	Marcellus	Marcellus	Marcellus	Marcellus
8	Reported Total depth of well, ft								
9	Total Diss	Total	mg/L	345000	261000	238000	206000	200000	228000
10	TIC		mol C/L						
11			g/mL						
12	COND		µS/cm	600000	570000	470000	482000	480000	710000
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	48.76859	38.07548	11.4926	26.0832
15	Silica		mg/L of SiO_2						
16	Boron Hydroxide		mg/L of $B(OH)_3$	887	96	88	658	91	56
17	Silver		mg/L of Ag^+	0.050	0.100	0.100	0.100	0.050	0.050
18	Gold		mg/L of Au^+						
19	Cesium		mg/L of Cs^+						
20	Potassium		mg/L of K^+	4080	1320	1040	2920	461	1010
21	Lithium		mg/L of Li^+	148	172	125	123	127	158
22	Sodium		mg/L of Na^+	82500	88000	83400	62600	47800	30400
23	Ammonium		mg/L of NH_4^+	416	229	199	291	168	268
24	Rubidium		mg/L of Rb^+						
25	Barium		mg/L of Ba^{2+}	2370	2500	1740	1860	104	1990
26	Calcium		mg/L of Ca^{2+}	24800	17600	11700	19100	24600	26200
27	Cobalt		mg/L of Co^{2+}	5	2.5	2.5	2.5	0.046	5
28	Copper		mg/L of Cu^{2+}	0.250	0.500	0.500	0.068	0.032	0.250
29	Iron II		mg/L of Fe^{2+} (If specified, els	151	53.9	39.1	135	74.2	53.3
30	Mercury		mg/L of Hg^{2+}	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
31	Magnesium		mg/L of Mg^{2+}	1830	1110	765	1460	2320	1740
32	Manganese		mg/L of Mn^{2+}	3	10	7	3	11	8
33	Nickel		mg/L of Ni^{2+}	0.018	2	2	2	4	0.4
34	Lead		mg/L of Pb^{2+}	0.030	0.150	0.150	0.148	0.300	0.030
35	Strontium		mg/L of Sr2+	8460	3210	2210	6280	4140	5350
36	Zinc		mg/L of Zn^{2+}	0.840	0.566	0.195	1.790	0.250	0.143
37	Aluminum		mg/L of Al^{3+}	2.000	0.983	0.596	0.785	2.000	0.210
38	Chromium III		mg/L of Cr^{3+}	0.0073	0.0244	0.1	0.0378	0.016	0.05
39	Iron III		mg/L of Fe^{3+} (if specified as						

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		1
pH		
Carbonate alkalinity	mg/l_as_CaCO	
$SiO_2(aq)$	mg/l	
$B(OH)_3$	mg/l	
Ag^+	mg/l	
Au^+	mg/l	
Cs^+	mg/l	
K^+	mg/l	
Li^+	mg/l	
Na^+	mg/l	
NH_4^+	mg/l	
Rb^+	mg/l	
Ba^{++}	mg/l	
Ca^{++}	mg/l	
Co^{++}	mg/l	
Cu^{++}	mg/l	
Fe^{++}	mg/l	
Hg^{++}	mg/l	
Mg^{++}	mg/l	
Mn^{++}	mg/l	
Ni^{++}	mg/l	
Pb^{++}	mg/l	
Sr^{++}	mg/l	
Zn^{++}	mg/l	
Al^{+++}	mg/l	
Cr^{+++}	mg/l	
Fe^{+++}	mg/l	
V^{+++}	mg/l	
Sn^{++++}	mg/l	
Br^-	mg/l	
CH_3COO^-	mg/l	
Cl^-	mg/l	
F^-	mg/l	
HCO_3^-	mg/l	
HPO_4^{--}	mg/l	
HS^-	mg/l	

+ sample

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 $CaCO_3$
Silica	Silica			mg/L of SiO_2
B(OH)3	Boron Hydroxide			mg/L of $B(OH)_3$ 441.0197022
TiO2	Titanium dioxide			mg/L of TiO_2
Sb(OH)5	Antimony hydroxide			mg/L of $Sb(OH)_5$ 0.095772536
Al(OH)3	Aluminum			mg/L of $Al(OH)_3$ 1.487777778
Be(OH)2	Beryllium			mg/L of $Be(OH)_2$ 0.003963918
CrO(OH)	Chromium			mg/L of CrO(OH) 0.016346154
Ag+1	Silver			mg/L of Ag^+ 0.0002
K+1	Potassium			mg/L of K^+
Li+1	Lithium			mg/L of Li^+
Na+1	Sodium			mg/L of Na^+
NH4+1	Ammonium			mg/L of NH_4^+
Tl+1	Thallium			mg/L of Tl^{+1} 0.00241
VO2+1	Vanadium			mg/L of VO_2^+ 0.02279466
Ba+2	Barium			mg/L of Ba^{2+} 0.408
Ca+2	Calcium			mg/L of Ca^{2+}
Cd+2	Cadmium			mg/L of Cd^{2+} 0.00277
Co+2	Cobalt			mg/L of Co^{2+} 0.022
Cu+2	Copper			mg/L of Cu^{2+} 0.016
Hg+2	Mercury			mg/L of Hg^{2+} 0.00116
Mg+2	Magnesium			mg/L of Mg^{2+}
Mn+2	Manganese			mg/L of Mn^{2+} 1.88
Ni+2	Nickel			mg/L of Ni^{2+} 0.126
Pb+2	Lead			mg/L of Pb^{2+} 0.019
Sr+2	Strontium			mg/L of Sr2+
Zn+2	Zinc			mg/L of Zn^{2+} 0.038
Fe+3	Iron			mg/L of Fe^{3+} 1.04
Mo+3	Molybdenum			mg/L of Mo^{3+} 0.0449
Sn+4	Tin			mg/L of Sn^{4+}
Br-1	Bromide			mg/L of Br^-
Cl-1	Chloride			mg/L of Cl^- 4300
F-1	Fluoride			mg/L of F^- 9.4
CN-1	Cyanide			mg/L of CN^-
NO3-1	Nitrate			mg/L of NO_3^-
CrO4-2	Chromate			mg/L of CrO_4^{2-}
SO4-2	Sulfate			mg/L of SO_4^{2-} 1200
SO3-2	Sulfite			mg/L of SO_3^{2-}
SeO4-2	Selenate			mg/L of SeO_4^{2-}
SeO3-2	Selenite			mg/L of SeO_3^{2-}
AsO4-3	Arsenic(V) Tetraoxid			mg/L of AsO_4^{3-}
PO4-3	Phospate			mg/L of PO_4^{3-}

OLI Studio Output Report

Scaling Tendencies

Row Filter Applied: Values > 1.0e-4

Solids	Post-Scale Q/K	Pre-Scale Q/K
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

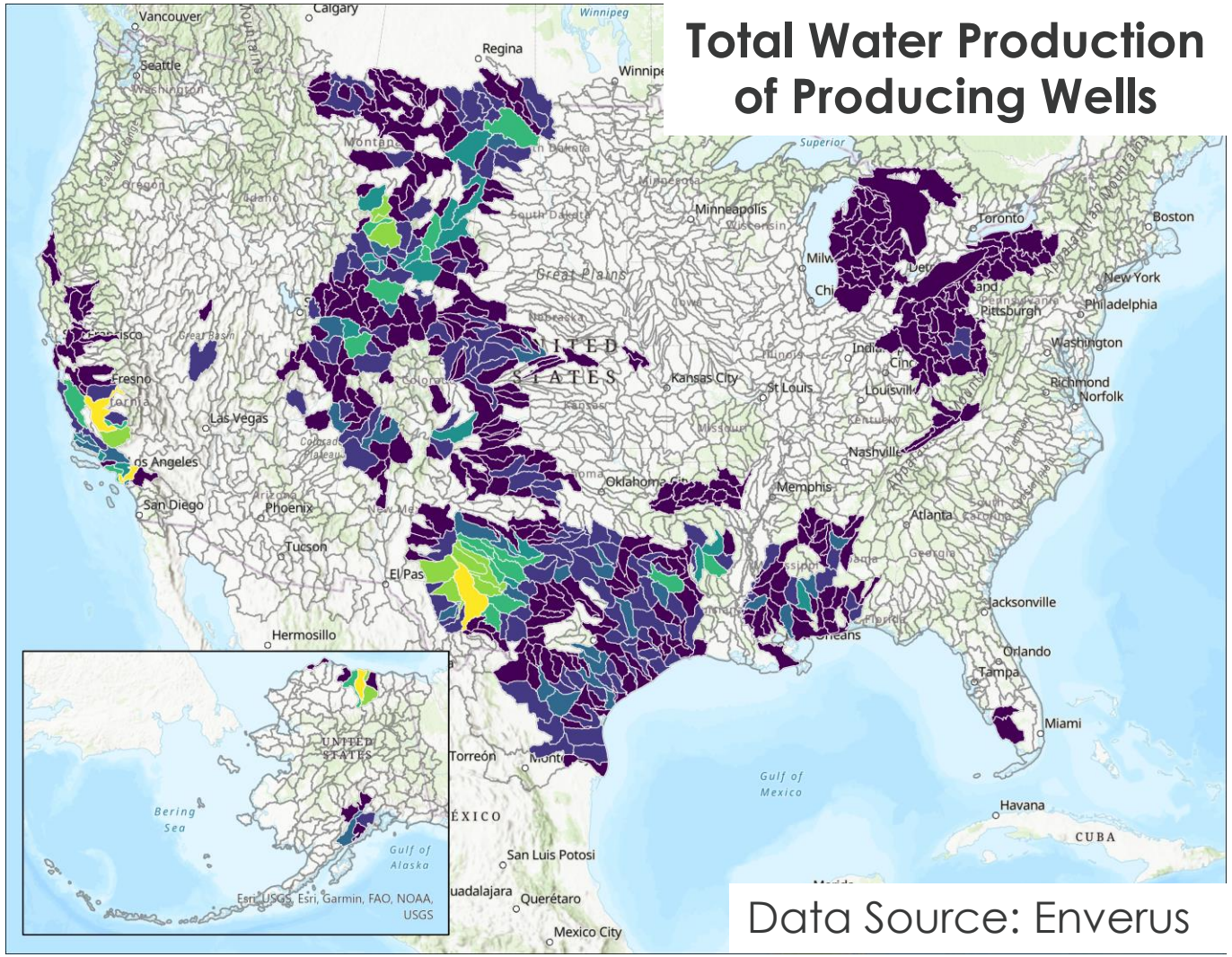
Integrating water volume data

- 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

Millions of Barrels of Water

- < 100
- 100 – 500
- 500 – 1,000
- 1,000 – 2,000
- 2,000 – 5,000
- 5,000 – 10,000
- 10,000 – 21,370

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, https://doi.org/10.5066/F72F7KK1.	https://doi.org/10.5066/F72F
1	EPA FGD Effluent Database	epa-fgd-effluent_all-tabs.xlsx	Nguyen, Dan-Tam, Eastern Research Group. Sep 29, 2015. Analytical Database for the Steam Electric Rulemaking - DCN SE05359.	https://www.regulations.gov/c OW-2009-0819-5640

- 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

NEWTS EPA Leachate Case Studies

doi 10.18141/1909011

License(s):

License Not Specified

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

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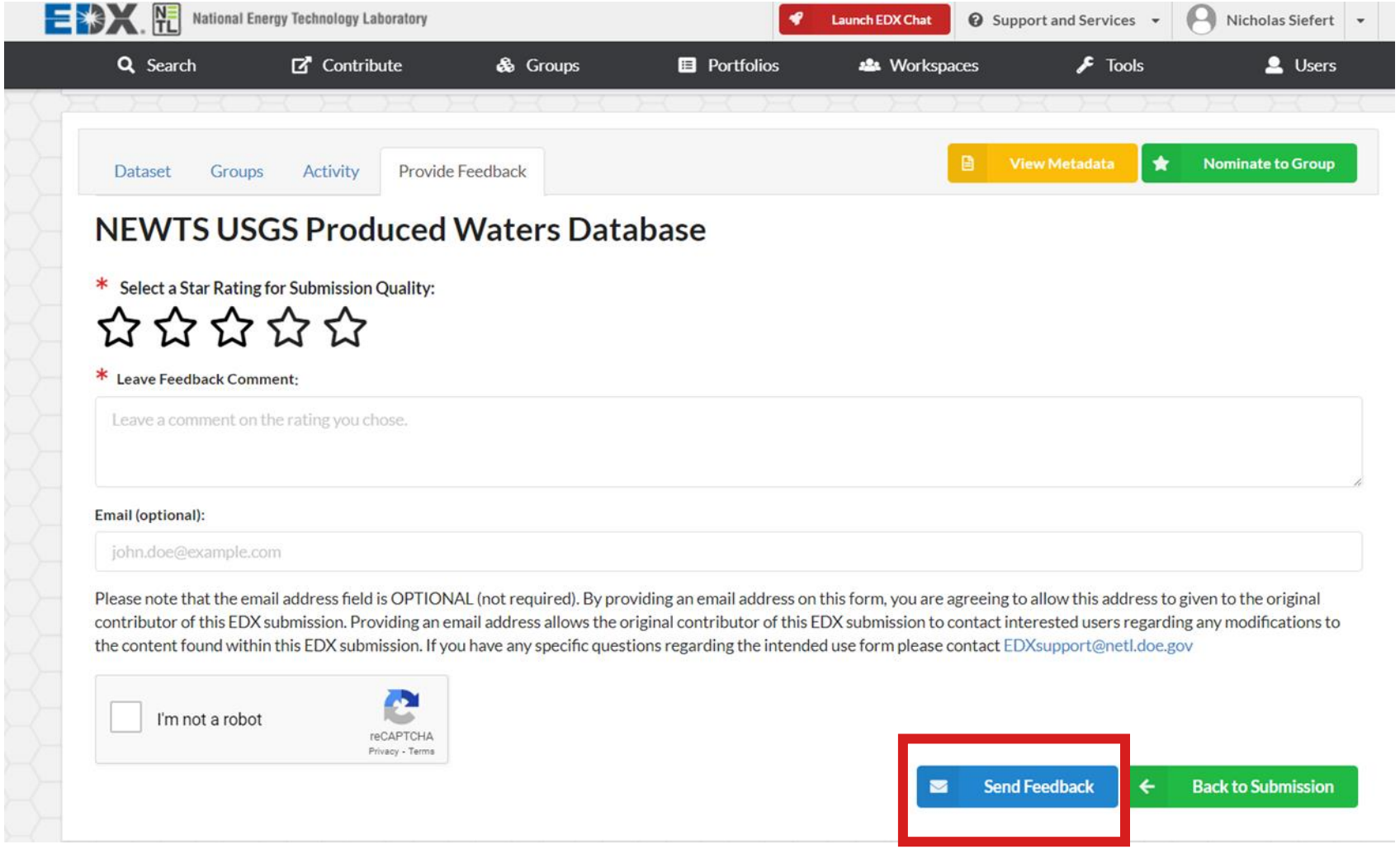
Citation (Click to Copy)

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

Providing Feedback

- Preferred option: Comments on submissions can be sent through the EDX site

- Or reach out to dataset authors listed for each resource



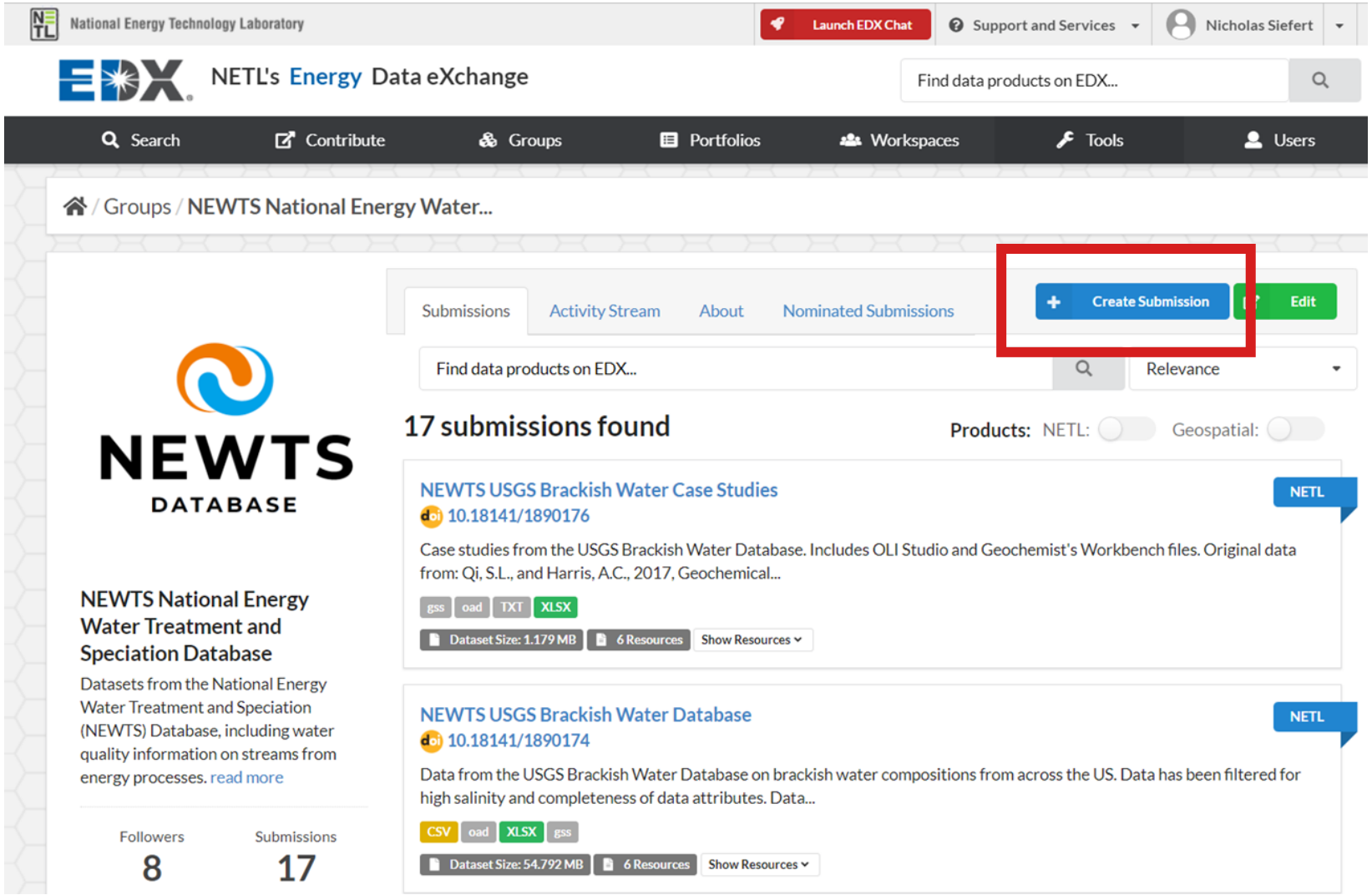
Creating your own data submission

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



PRODUCED WATER SOCIETY 2024

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PRODUCED WATER SOCIETY 2024

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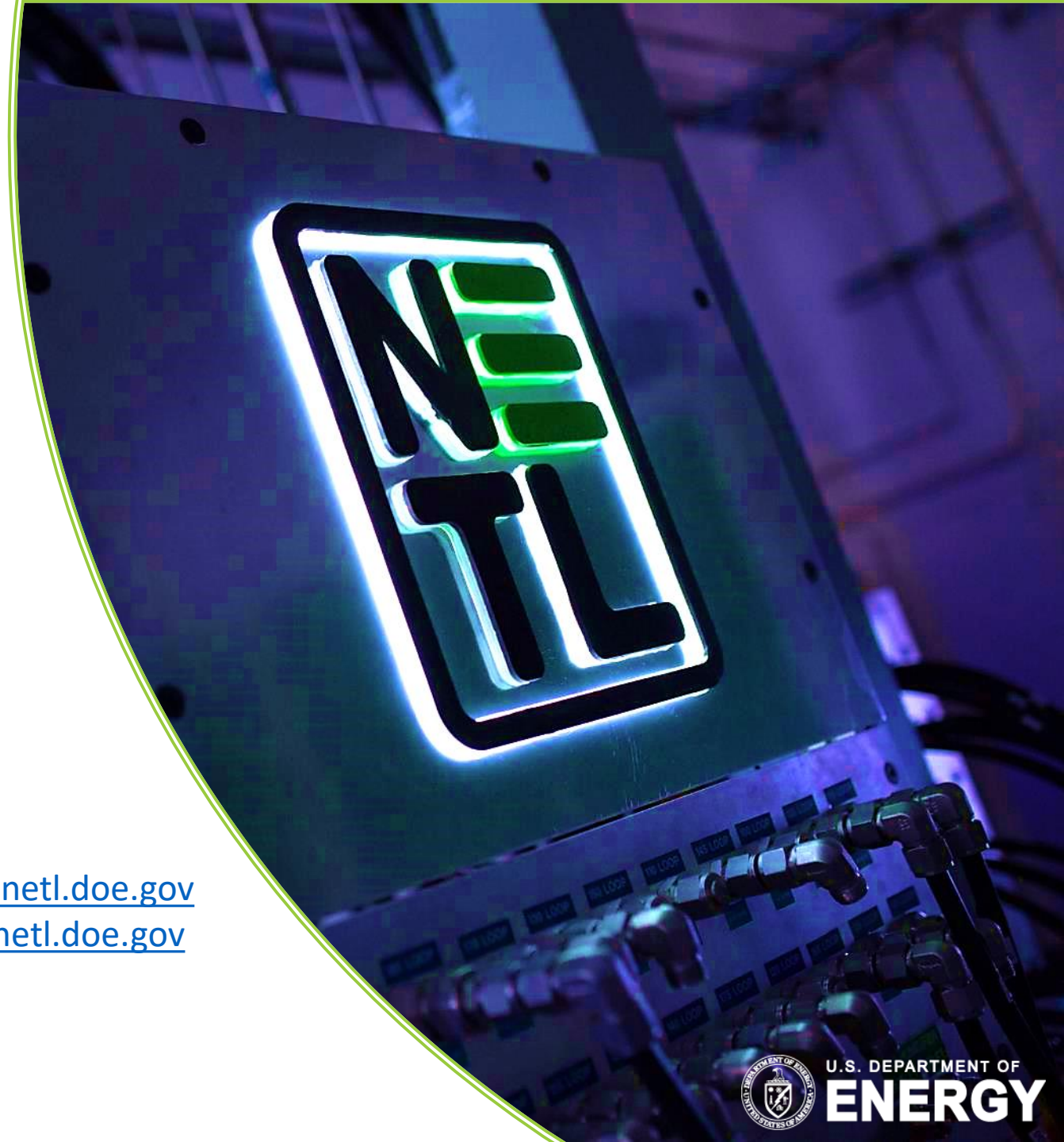
NEWTS DATABASE



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