National Energy Water Treatment and Speciation (NEWTS) Database & Dashboard

ASME Power Conference 2024
Technical Presentation#119098

NEWTS Team: ***Nicholas Siefert***, Madison Wenzlick, Rachel Yesenchak, Burt Thomas, Lucy Romeo, Devon Justman, Justin Mackey, Zineb Belarbi, Isabelle Pfander, Kathryn Smith

NATIONAL ENERGY TECHNOLOGY LABORATORY

NEWTS DATABASE

Acknowledgment:

NATIONAL ENERGY TECHNOLOGY LABORATORY

We thank the Department of Energy's Office of Fossil Energy & Carbon Management (DOE/FECM) for their support of this research.

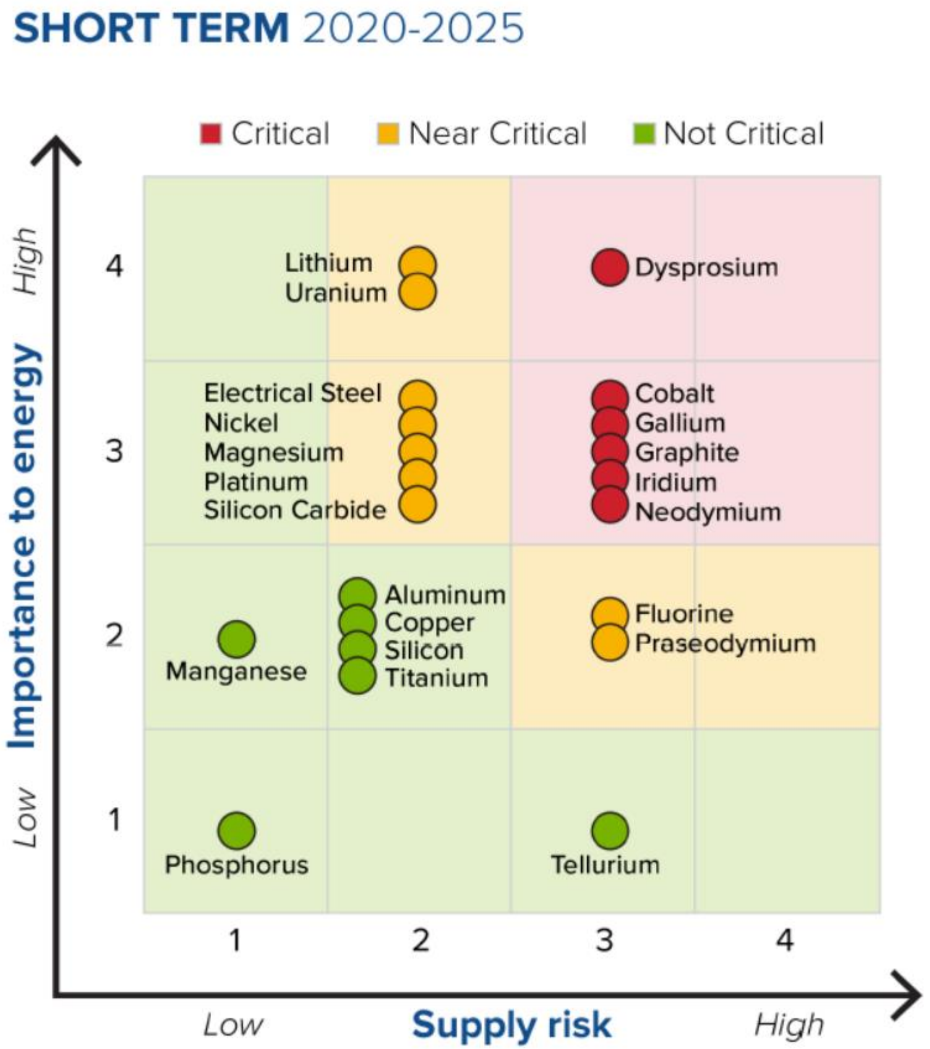
HQ Project Manager: Hichem Hadjeres

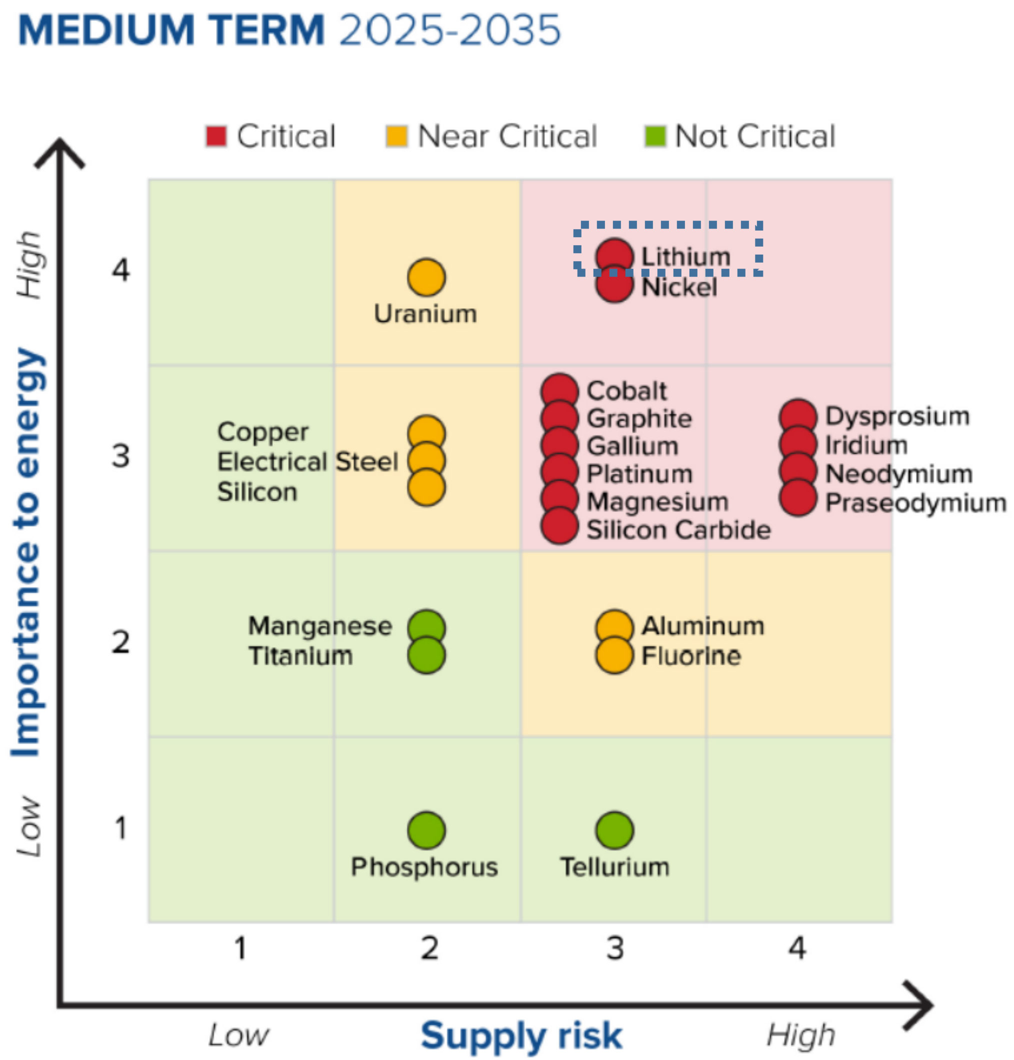
Advanced Remediation Technologies Division: Vanessa Nunez-Lopez

Technology Manager: John Rogers

Motivation: DOE 2023 Critical Materials Assessment

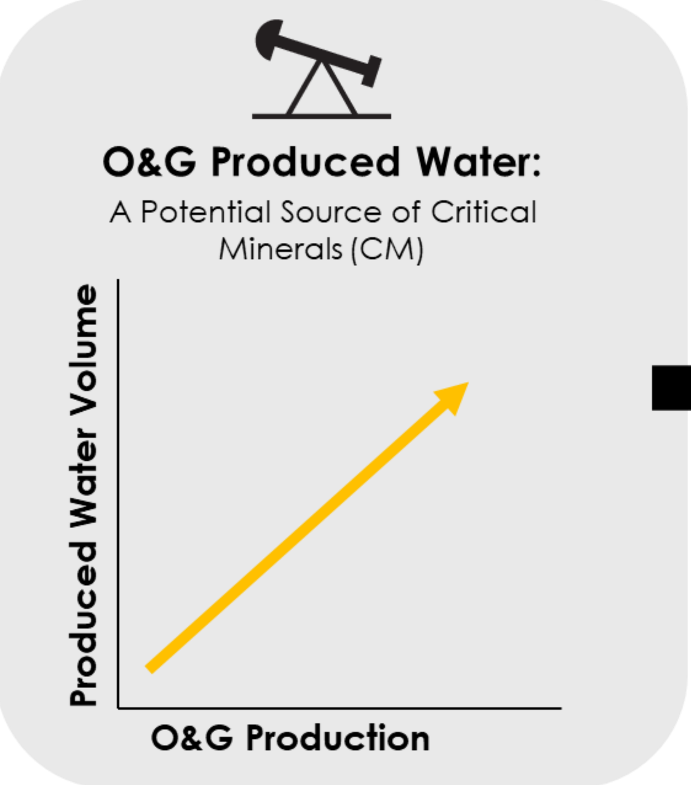
Short and Mid Term Demand & Risk for Critical Materials

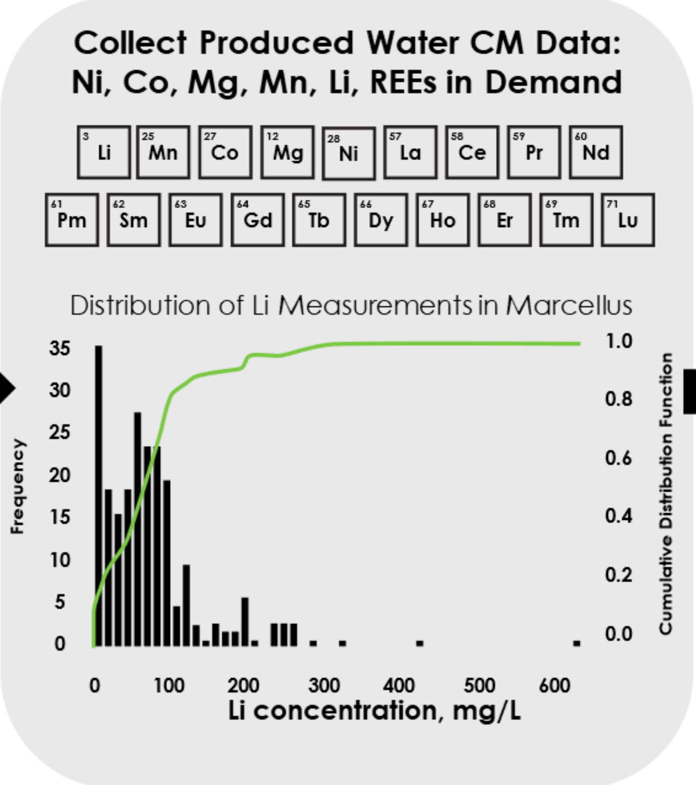


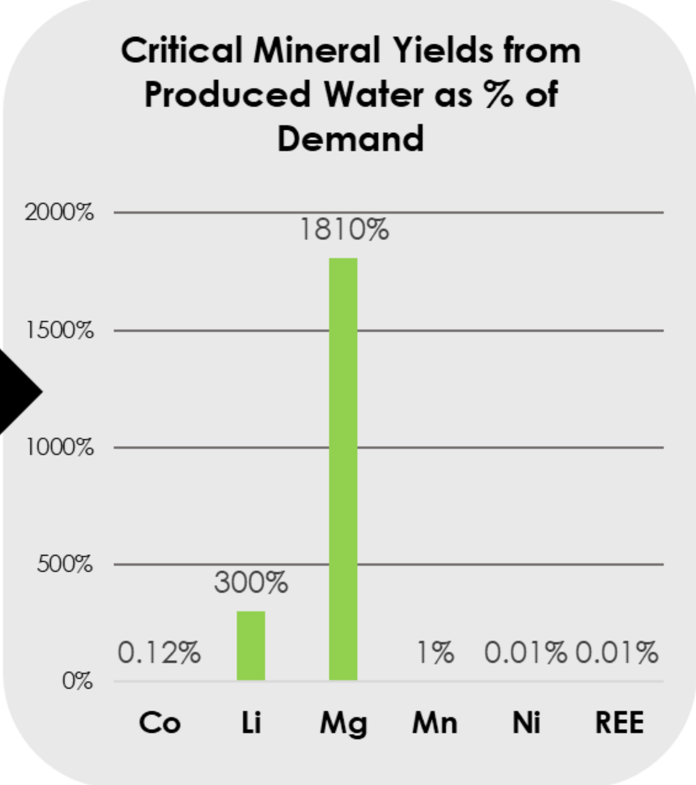


[2023 Critical Materials Assessment (energy.gov)](energy.gov)

Critical mineral source potential from oil & gas produced waters in the United States







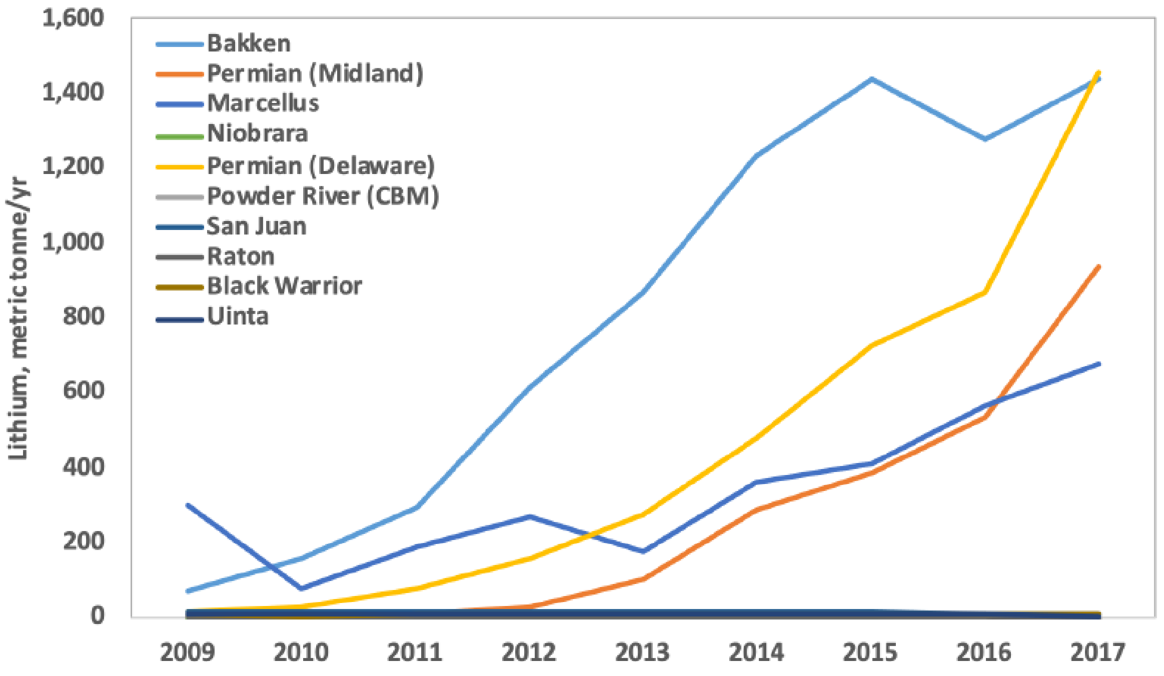
Key finding: Lithium in US PW can meet 300% of current "USGS estimated" U.S. lithium demand

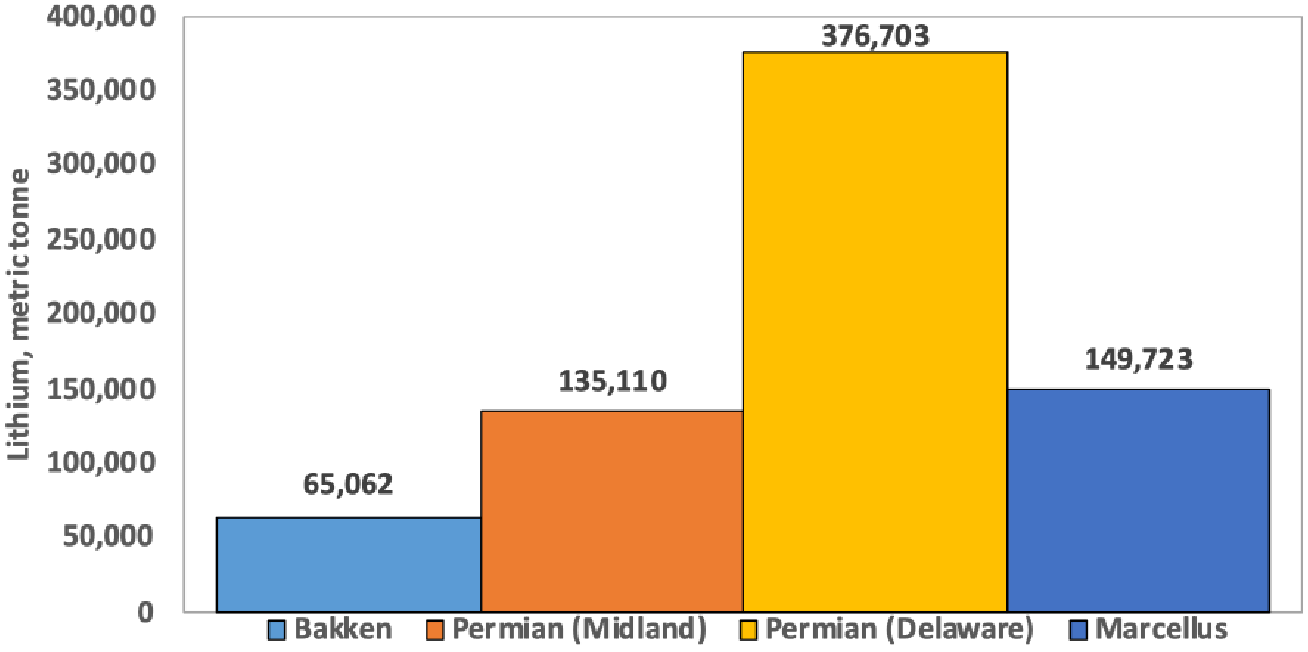
Critical mineral source potential from oil & gas produced waters in the United States
Kathryn H. Smith, Justin E. Mackey, Madison Wenzlick, Burt Thomas, Nicholas S. Siefert
Science of The Total Environment, Volume 929, 15 June 2024, 172573

NEWTS DATABASE

Lithium Resource Assessment

Permian Basin and Marcellus Shale have largest resource potentials





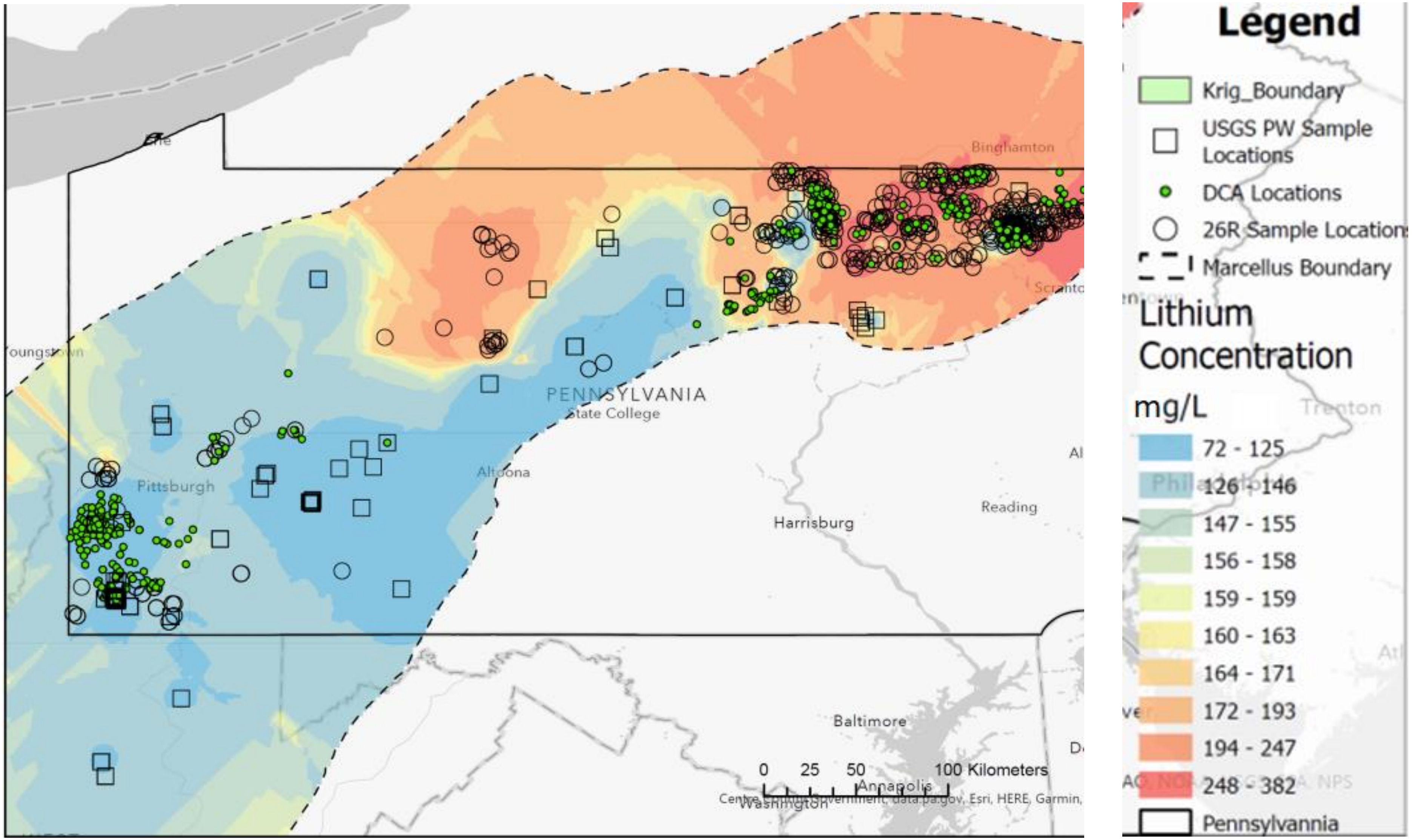
Concentration of Li is ~10 times higher in Marcellus than Permian Basin

Fig.1 Time series of Lithium resource potential calculated from PW volumes presented by Scanlon et al. 2020 and average Li concentration from from USGS PW database (Blondes et al. 2018)

Fig.2. Projected Lithium resource potential calculated from projected remaining PW volumes (Scanlon et al. 2020) and average Li concentration in each formation

Lithium Concentrations in Marcellus Shale

NATIONAL ENERGY TECHNOLOGY LABORATORY



[Lithium geochemistry and regional production decline curves of Marcellus Shale produced water - Submissions - EDX (doe.gov)]

Figure 1. Map of study area showing the Marcellus shale extent, well locations using in decline curve analysis (DCA), PW samples used in this study, and previous USGS sample locations.

PA DEP 26r Reports contain full compositional analysis of produced water. To be uploaded to EDX.

NEWTS

DATABASE

NATIONAL ENERGY WATER TREATMENT & SPECIATION (NEWTS)

National Energy Water Treatment & Speciation Database

NATIONAL ENERGY TECHNOLOGY LABORATORY

Leveraging NETL R&D Core Capabilities

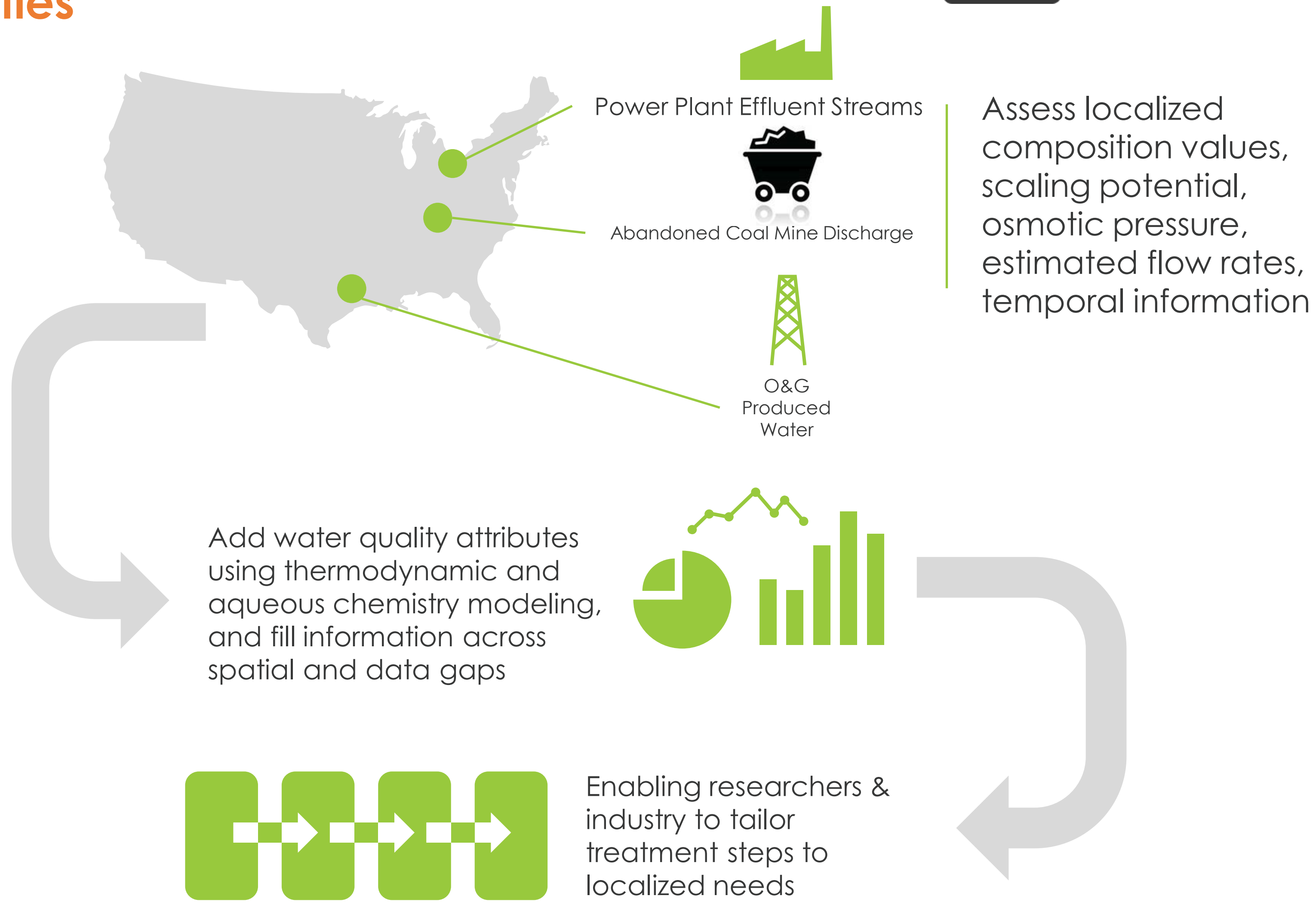
Solution: Develop a Nationwide Energy Wastewater Data System

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

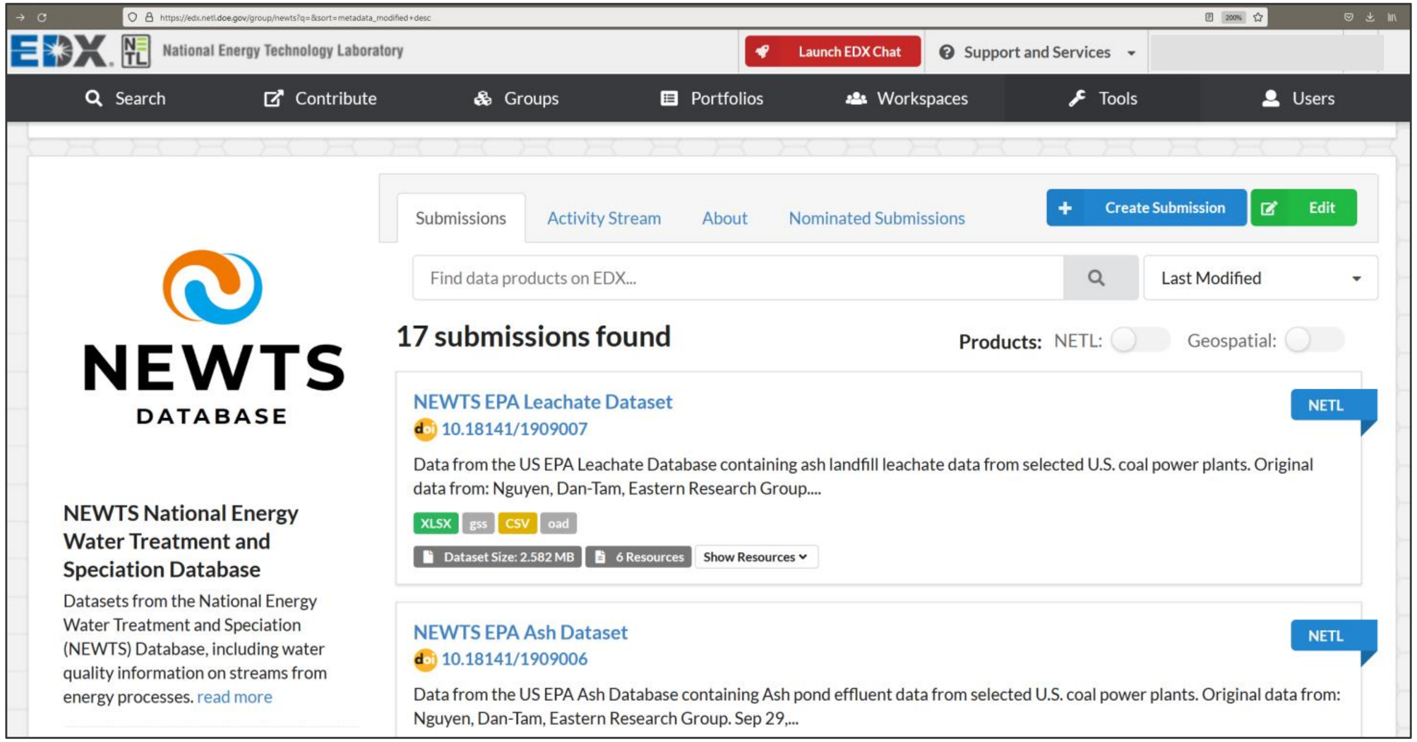
➢ Enables **design of localized treatment**

➢ **Publicly Available Data** hosted & displayed through **NETL's EDX®**, and a custom **visualization dashboard**

EDX™ Energy Data exchange



NEWTS Public Group on EDX

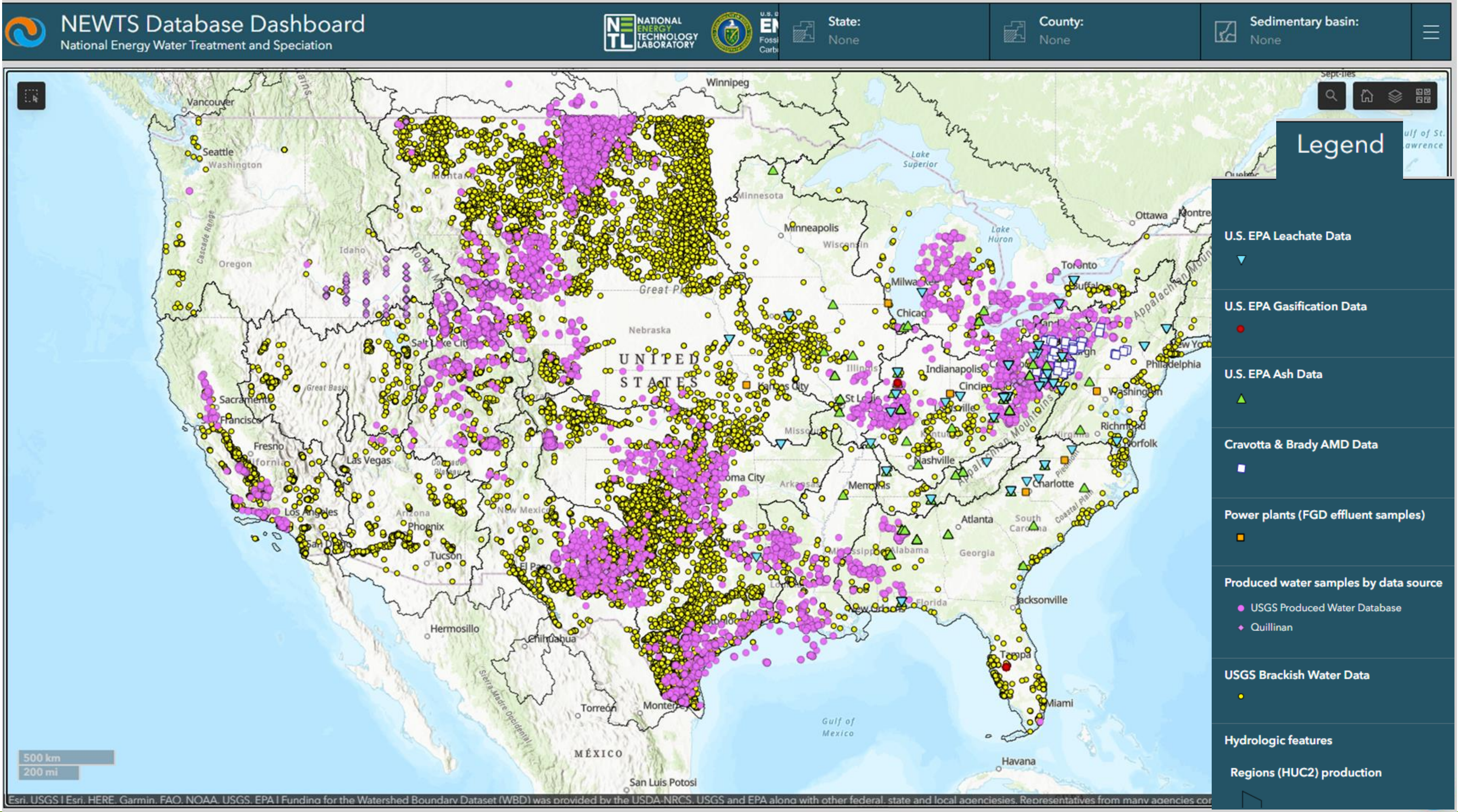


- Original data as well as each step along NEWTS standard formatting for input into OLI & GWB
- Templates for direct input into OLI Studio & Geochemist's WorkBench
- Case studies

- NEWTS Data Catalog
- [Overview Video]
- Training Videos

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

NEWTS Federal Level Dashboard



NEWTS Dashboard

Enables data visualization, exploration, and download

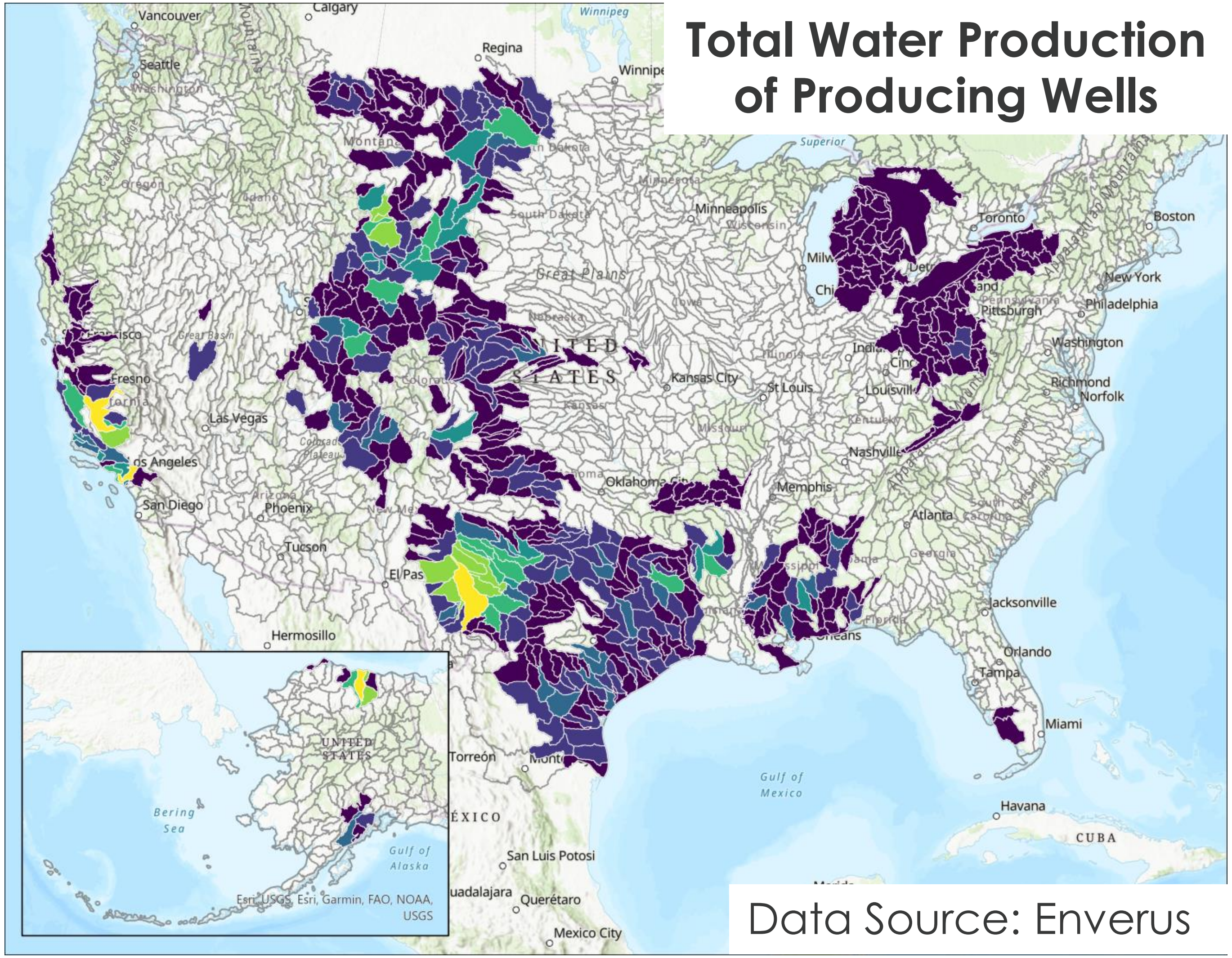
Integrating Water Volume Data

- 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

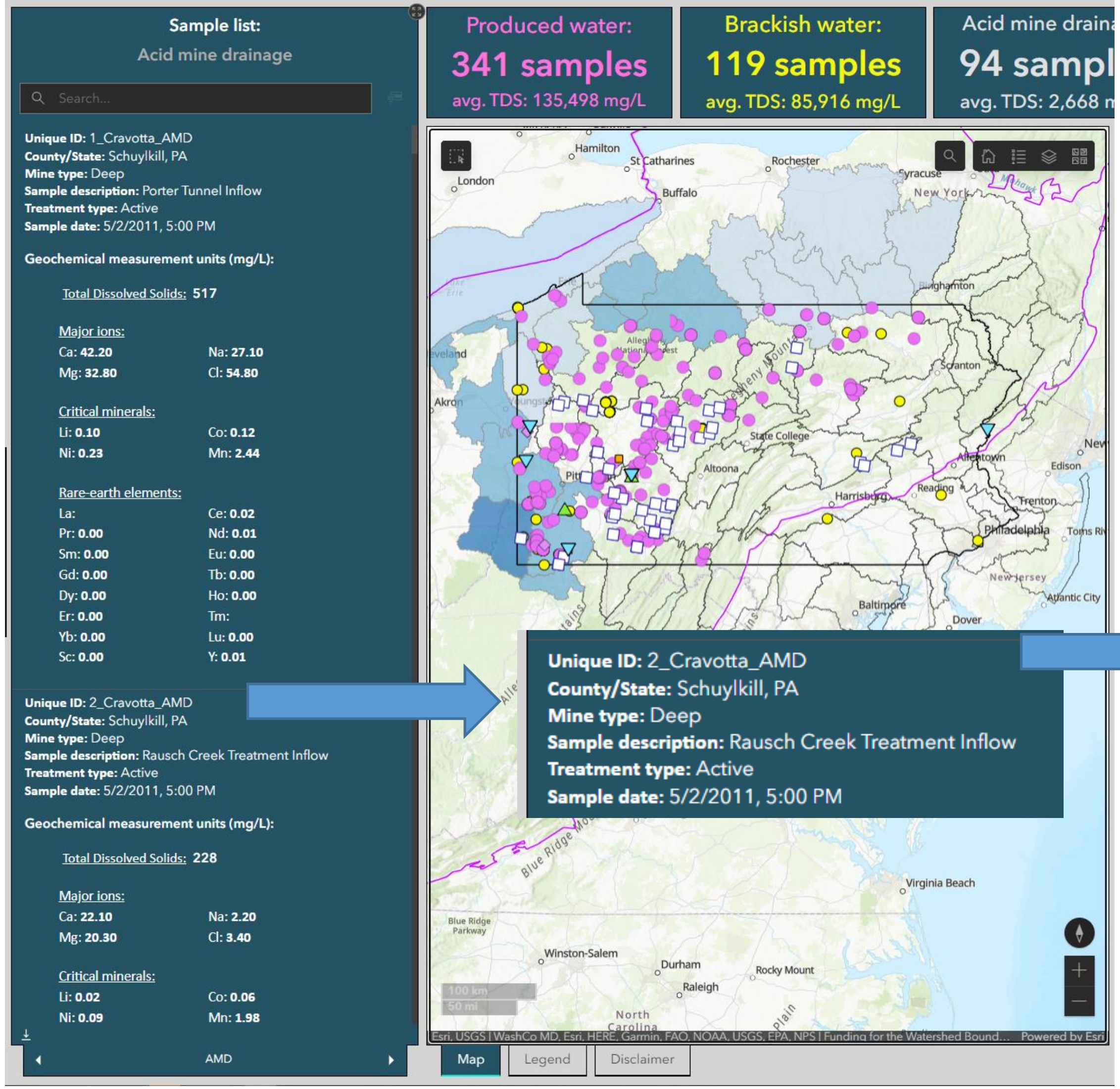
Total Water Production of Producing Wells

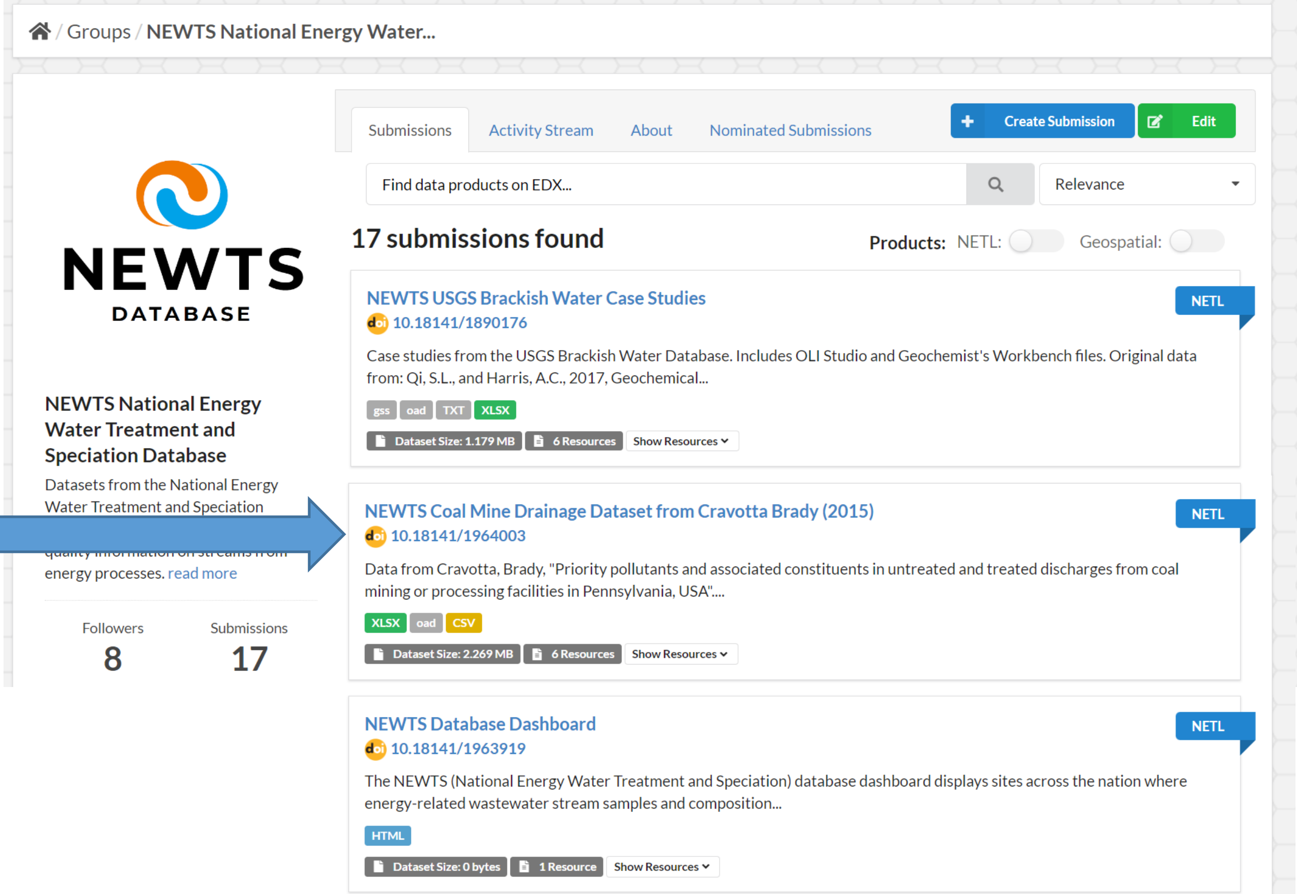


Data Source: Enverus

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

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

- 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	3_
ID_Num					1	2	
SNAME		Descriptio	Redox State		flow	Rausch Creek Trea	Si
MINE_NUM		Some Mines have multiple Streams			1	2	
STAID		Station identifier used by US			4.03619E+14	4.03748E+14	
Lon_dd					40.60056	40.62994	
Lat_dd					-76.50583	-76.55399	-
Mine_Type					Deep	Deep	D
Pas					Active	Active	P
					CaO	CaO	W
Inflow_Outflow					I	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	1
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	5
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)(	Gallium	Ga_Total	3	mg/L of GaO(OH)	1.62E-04	5.89E-05	8
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 $Ru(OH)_4$			1
SiO2	Silica		4	mg/L of SiO_2	2.46E+01	1.81E+01	2
SnO2	Tin		4	mg/L of SnO_2			
ThO2	Thorium	Th_T	4	mg/L of ThO_2	4.09E-04	4.89E-05	7
TiO2	Titanium		4	mg/L of TiO_2	3.50E-03	2.00E-03	2
ZrO2	Zirconium		4	mg/L of ZrO_2	2.70E-05	1.35E-05	2
Sb(OH)5	Antimony hydroxide		5	mg/L of $Sb(OH)_5$	1.70E-05	1.70E-05	3
UO3	Uranium		6	mg/L of UO_3	1.61E-03	3.05E-04	2
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	2
Ag+1	Silver		1	mg/L of Ag^+			
Cs+1	Cesium	Cs	1	mg/L of Cs^+	1.46E-04	8.70E-05	1
K+1	Potassium		1	mg/L of K^+	7.31E+00	1.60E+00	1
Li+1	Lithium		1	mg/L of Li^+	9.85E-02	2.30E-02	4
Na+1	Sodium		1	mg/L of Na^+	2.71E+01	2.20E+00	2
Rb+1	Rubidium		1	mg/L of Rb^+	8.11E-03	3.04E-03	2
Tl+1	Thallium		1	mg/L of Tl^+	7.90E-05	3.40E-05	2
Ba+2	Barium		2	mg/L of Ba^{2+}	2.05E-02	2.91E-02	2
Ca+2	Calcium		2	mg/L of Ca^{2+}	4.22E+01	2.21E+01	4

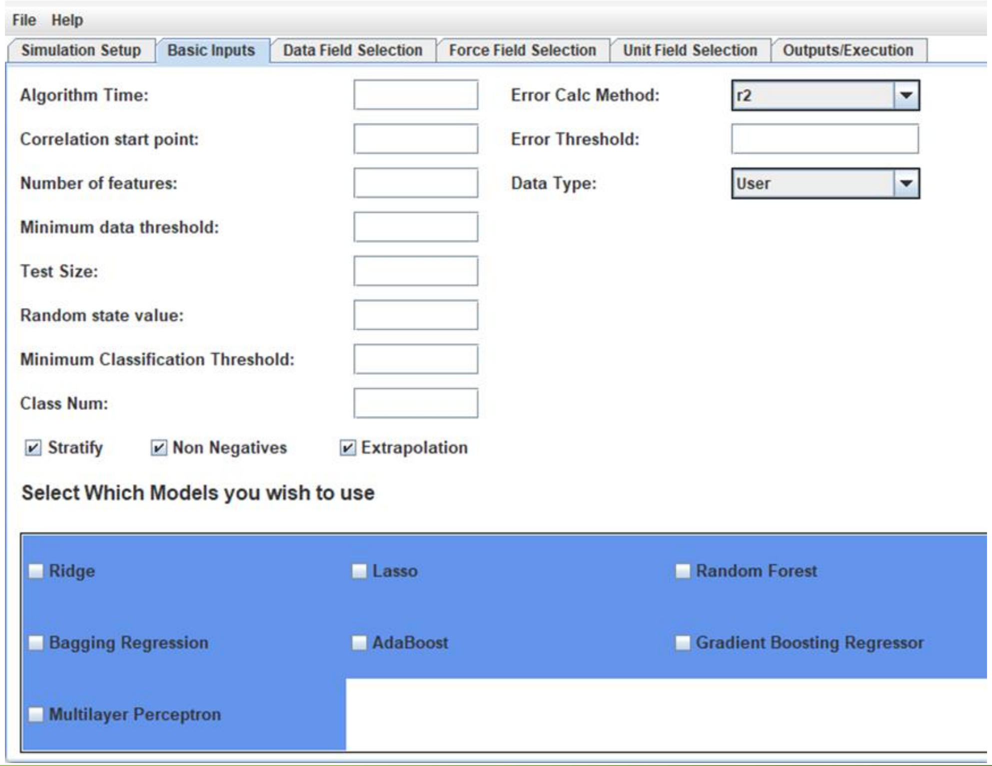
Original Data_Totals Only | Convert mgperL | mgperL Values | Transpose | Input to OLI | Charge Balance | Redox Species Summary

Machine Learning Approaches for Energy Wastewater Characterization

NATIONAL ENERGY TECHNOLOGY LABORATORY

CO-DART
CONSTITUENT DATA REPLACEMENT TOOL

- To accurately model treatment and byproduct recovery costs for energy wastewaters, we need complete composition data.
- **CoDaRT (Composition Data Replacement Tool)** was developed in python to predict missing constituents in a user's water data set using machine learning techniques.



- The tool applies machine learning algorithms to replace missing data based on user preferences for options including algorithm type, number of features, and classification variables.
- The tool can use the user's data alone or combine user data with the NEWTS datasets

U.S. DEPARTMENT OF ENERGY

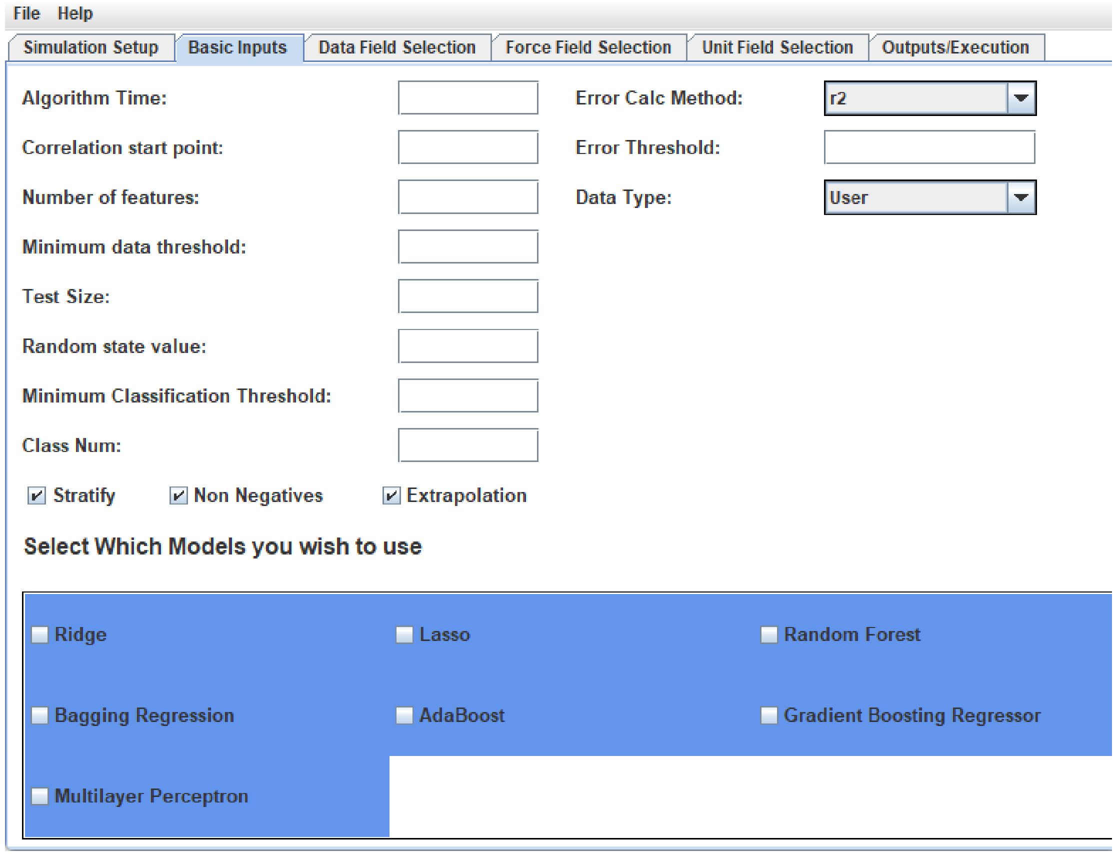
Constituent Data Replacement Tool - EDX (doe.gov)

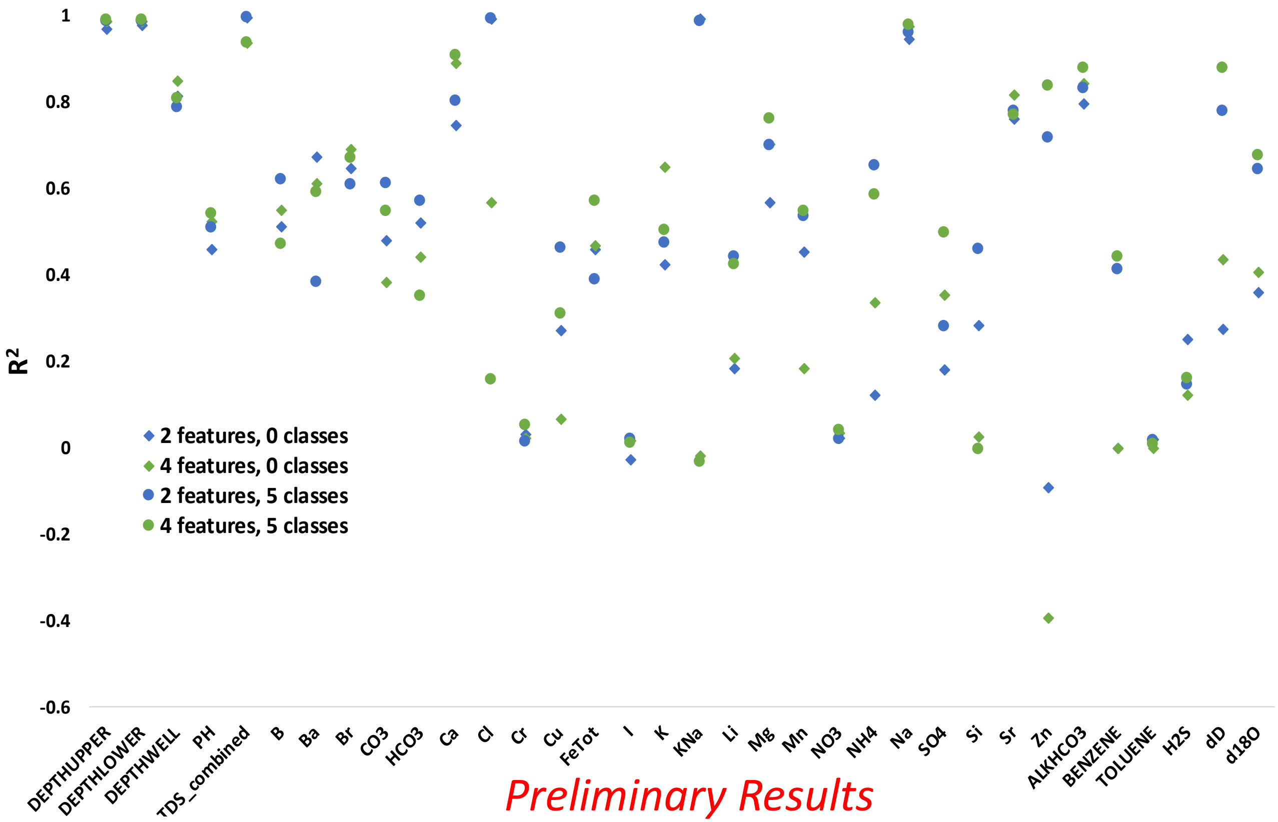
Machine Learning Approaches for Energy Wastewater Characterization

NATIONAL ENERGY TECHNOLOGY LABORATORY

Techno-Economic Modeling of Treating Energy Influent and Effluent Wastewater Streams

A graphical user interface model was built to allow users who are unfamiliar with python to use the tool.





Preliminary Results

Example data replacement performance for the NEWTS USGS Produced Water Databased for multiple feature options.

U.S. DEPARTMENT OF ENERGY

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$$

y_i = true value
$\hat{y}_i$ = predicted value
$\bar{y}$ = average value

UT Austin Archived Historical Produced Water Samples

NATIONAL ENERGY TECHNOLOGY LABORATORY

Samples stored at UT Austin, originally sampled around 1960

- ~850 Historical Produced Water samples from across the U.S.
- Cation compositions analyzed in 1960s are available at the NETL NEWTS group site on EDX
  - Rittenhouse *et al.* Historical Archived Data
- UT Austin and UTEP have analyzed ~80 samples for training AI/ML networks

Examples of intact samples with minimal or no water loss

Task 2: Machine Learning Approaches for Energy Wastewater Characterization

NATIONAL ENERGY TECHNOLOGY LABORATORY

Techno-Economic Modeling of Treating Energy Influent and Effluent Wastewater Streams

Before data replacement

Si	Sn	Sr	V	W	Cl	SO4	Br	CO3	HCO3
9	0.003	50							
8	0.012	30							
15	0	60							
8	0.003	50	0						
4	0.003	60	0						
5	0.003	50	0	0.01					
0	0	100							
3	0.003	150	0						
5	0.003	50	0	0.01					
2	0.003	300							
7	0.003	60	0	0.01					
5	0.002	80	0						
100			0.02						
500									
200			0.01						
150			0.01						
150									
150		15	0.015						
100	0.013	10	0.04						
1	0.025	900							
1	0.07	300							
1	0.01	300	0.008						
0		1000	0.01						
0		1000	0.025						
0		300							
0		300							
0		150	0.01						

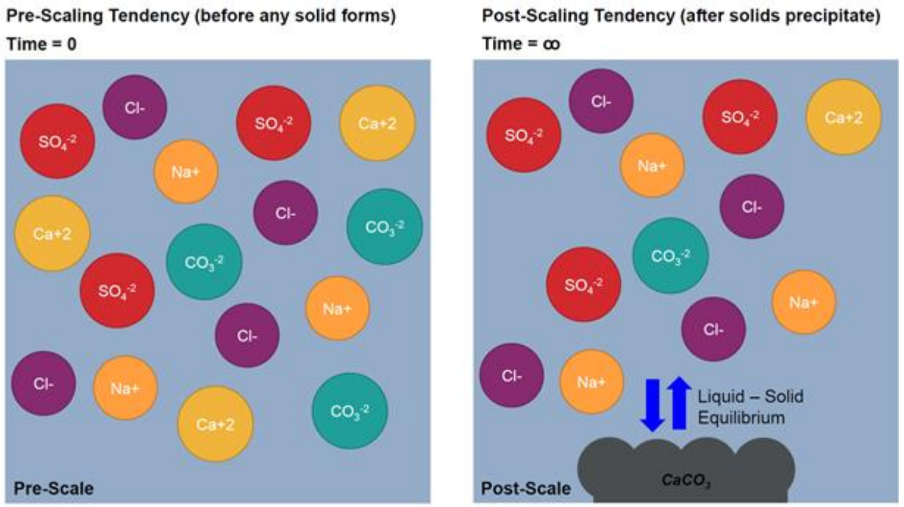
After data replacement

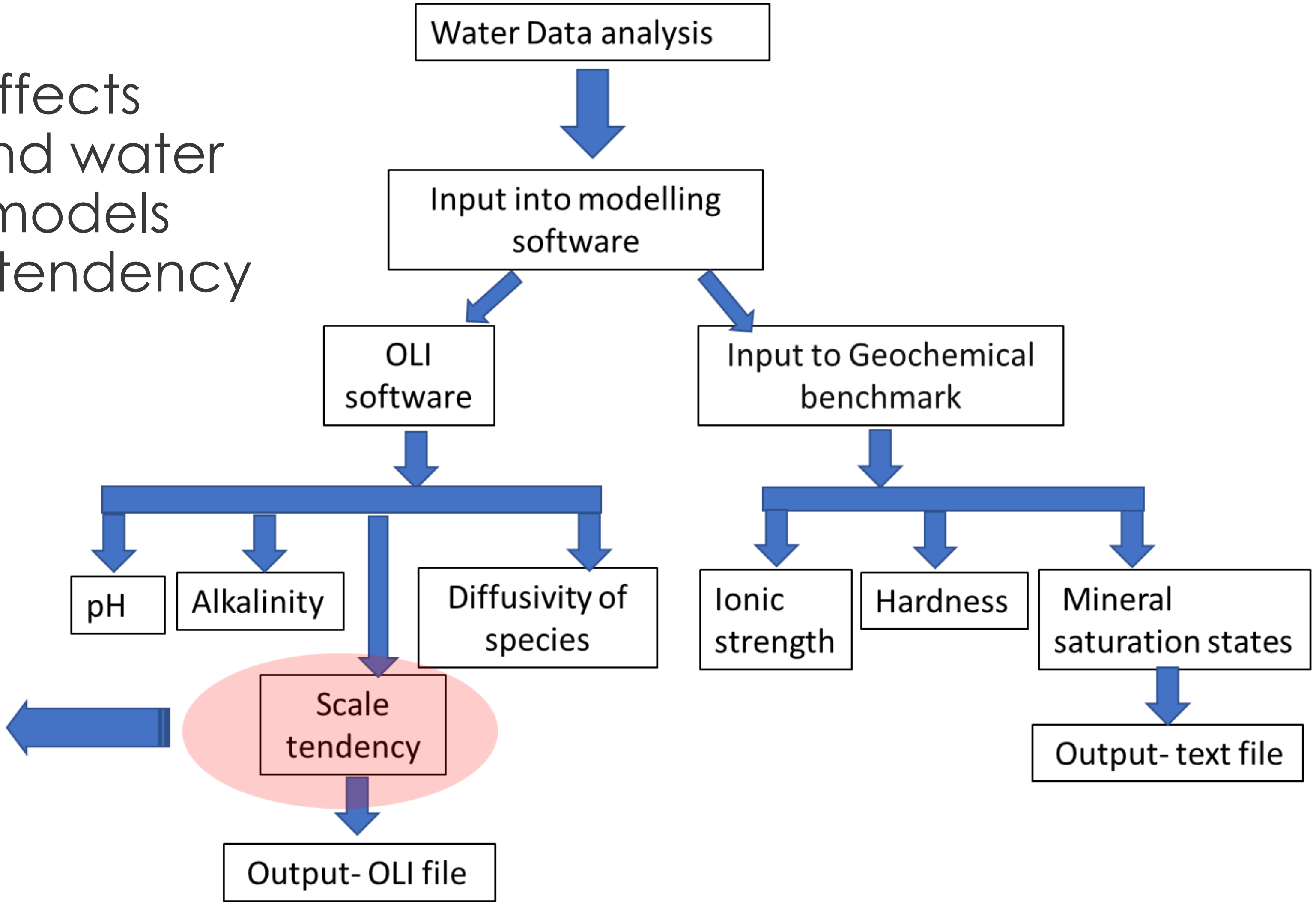
Si	Sn	Sr	V	W	Cl	SO4	Br	CO3	HCO3
9	0.003	50			72555.7	699.317	241.584		505.966
8	0.012	30			33319.8	657.754	107.375		534.926
15	0	60			36474.6	652.916	173.316		536.389
8	0.003	50	0		57912.9	681.402	209.881		567.832
4	0.003	60	0		88250	715.62	295.268		446.584
5	0.003	50	0	0.01	26524.2	645.571	102.513		507.962
0	0	100			131692	753.957	517.399		240.983
3	0.003	150	0		68915	674.23	302.664		452.968
5	0.003	50	0	0.01	36474.6	654.528	173.316		527.919
2	0.003	300			114946	703.783	441.735		330.563
7	0.003	60	0	0.01	45373.4	661.873	222.138		492.484
5	0.002	80	0		34371.4	649.69	129.355		483.481
100			0.02		669.15				
500									
200			0.01		3139.65		22.5239		
150			0.01						
150					669.15				
150		15	0.015		17107.6	640.467	70.3026		583.089
100	0.013	10	0.04		6372.5	631.419			454.124
1	0.025	900			232002	651.796	2202.49		140.296
1	0.07	300			189937	748.572	1323.28		121.017
1	0.01	300	0.008		197784	757.53	1350.12		360.498
0		1000	0.01		208301	644.625	1569.92		
0		1000	0.025		197784	644.625	1350.12		
0		300			176752	757.53	910.512		51.1679
0		300			176752	757.53	910.512		81.1031
0		150	0.01		176752	781.724	910.512		93.7455

Importance of Modeling Results

Chemistry matters

Formation of mineral scales affects water treatment processes and water quality. The thermodynamic models accurately identify the scale tendency of wastewater





Aqueous Chemistry Modeling: Case Studies

NATIONAL ENERGY TECHNOLOGY LABORATORY

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-}		

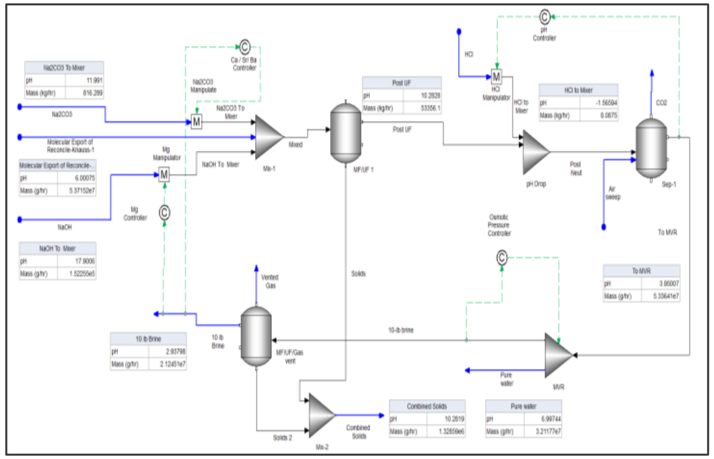
Output from OLI Studio

Scaling Tendencies

Row Filter Applied: Values > 1.0e-4

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

Becomes Input into OLI Flowsheet



Integration with Modeling Software

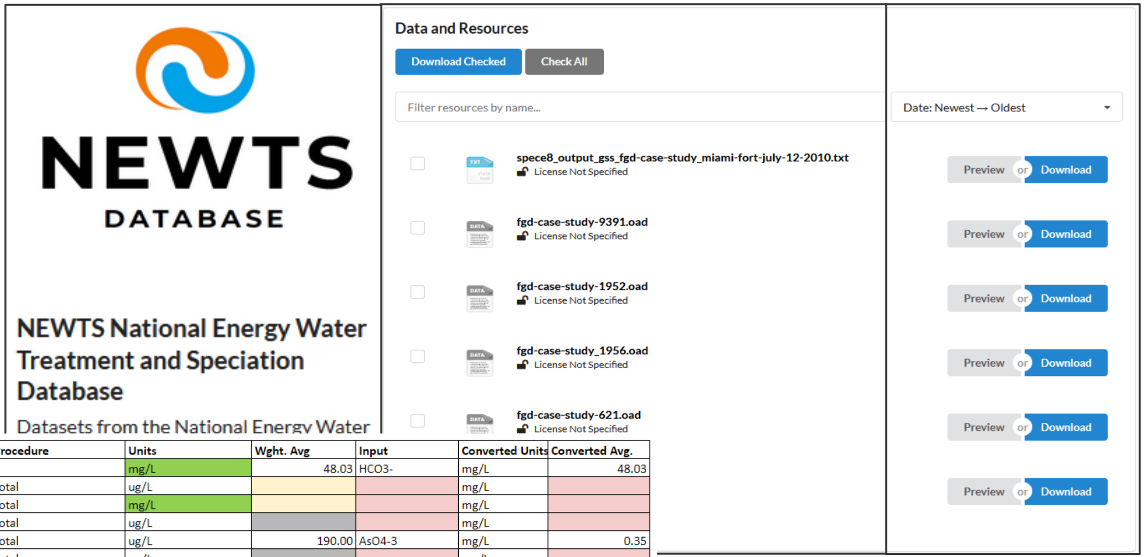
Leveraging tools for filling data gaps & modeling treatment

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:

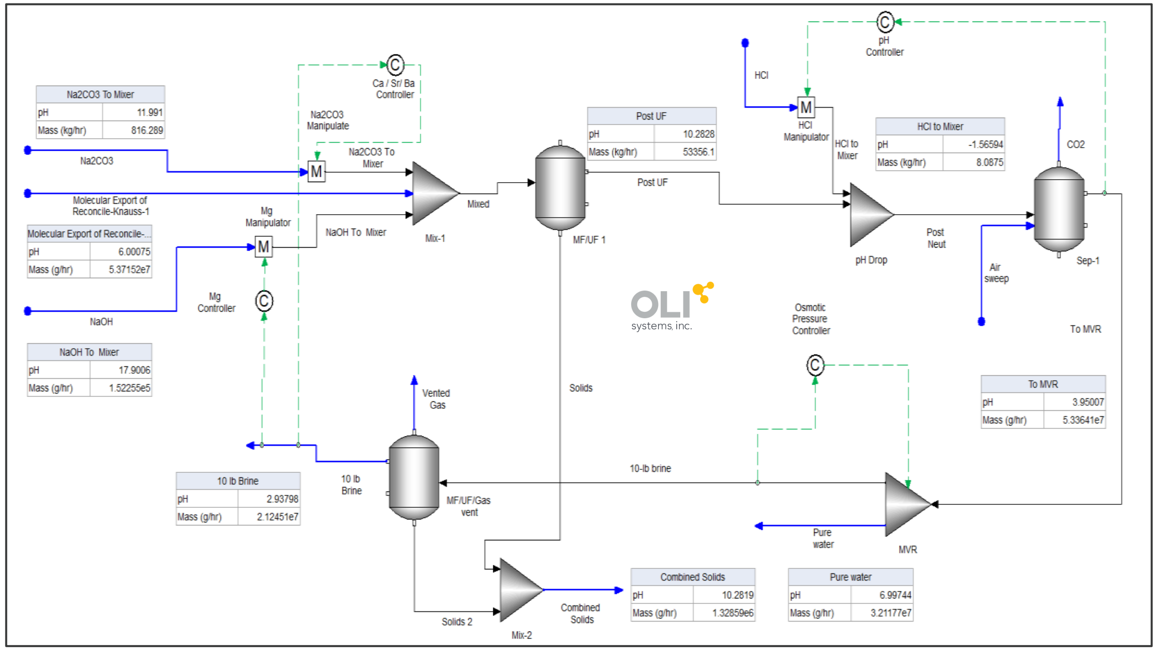
- OLI Studio
- Geochemist's Workbench
- DuPont Wave
- NAWI Water-Tap3

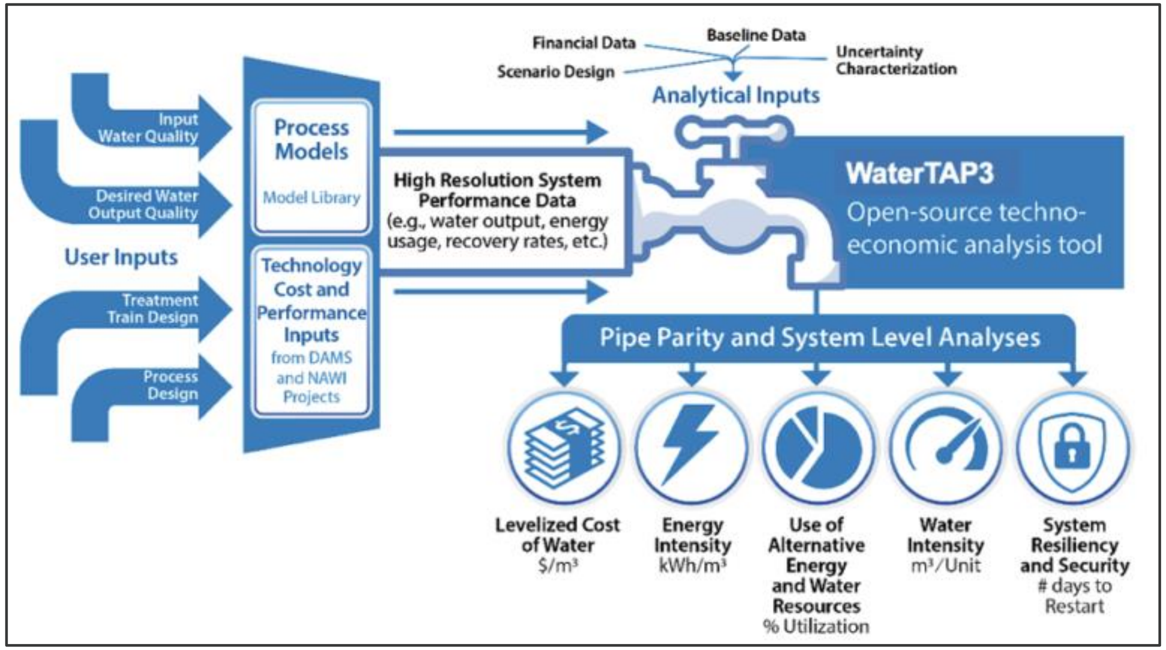


Analyte	Procedure	Units	Wght. Avg	Input	Converted Units	Converted Avg.
Alkalinity, HCO3		mg/L	48.03	HCO3-	mg/L	48.03
Aluminum	Total	ug/L			mg/L	
Ammonia as N	Total	mg/L			mg/L	
Antimony	Total	ug/L			mg/L	
Arsenic	Total	ug/L	190.00	AsO4-3	mg/L	0.35
Beryllium	Total	ug/L			mg/L	
Boron	Total	ug/L	167,106.67	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 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)3	mg/L	0.40
Cobalt	Total	ug/L		Co+2	mg/L	
Copper	Total	ug/L	158.62	Cu+2	mg/L	0.16
Lithium	Total	mg/L	290.25	Li+	mg/L	0.29
Magnesium	Total	ug/L	1,014,700.00	Mg+2	mg/L	1,014.70
Manganese	Total	ug/L			mg/L	
Mercury	Total	ng/L	89,133.33	Hg+2	mg/L	0.09

Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment





Input Water Stream

Input Water Quality

OLI systems, inc. | The Geochemist's Workbench | WAVE Water Treatment Design Software | NAWI National Alliance for Water Innovation

Case Studies publicly available on [EDX NEWTS Group]

PowerShare: Energy System Modeling EDX Group

NATIONAL ENERGY TECHNOLOGY LABORATORY

Thermal & Electrochemical Power Plant Design and Cost Estimation, Siefert (2023)

- Textbook (online already), Class lecture slides and Homework (soon to be added)
- Site will host the material to conduct and share detailed thermodynamics analysis of power plant design and/or water treatment
- Location to Share AspenPlus and OLI Flowsheet model and such as the OLI Flowsheet models
- Combined with NEWTS, makes seamless integration from water compositions to full thermodynamic analysis of water treatment design

Power Share
Energy System Modeling

NETL Resources

VISIT US AT: **www.NETL.DOE.gov**

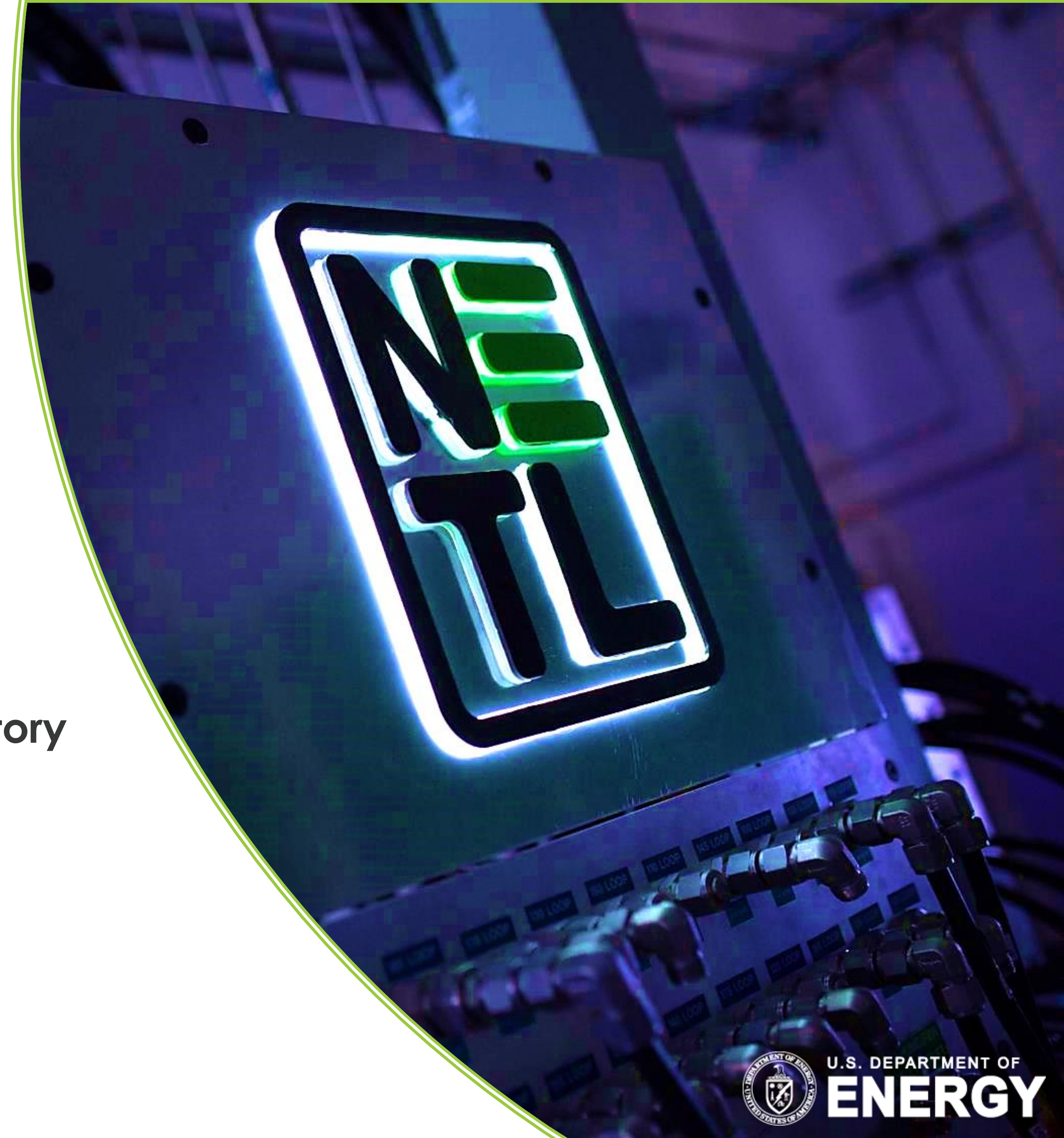
@NETL_DOE

@NETL_DOE

@NationalEnergyTechnologyLaboratory

NEWTS
DATABASE

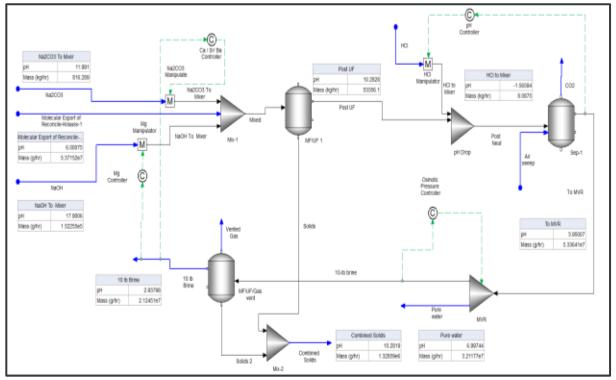
Burt.Thomas@netl.doe.gov
Nicholas.Siefert@NETL.DOE.GOV

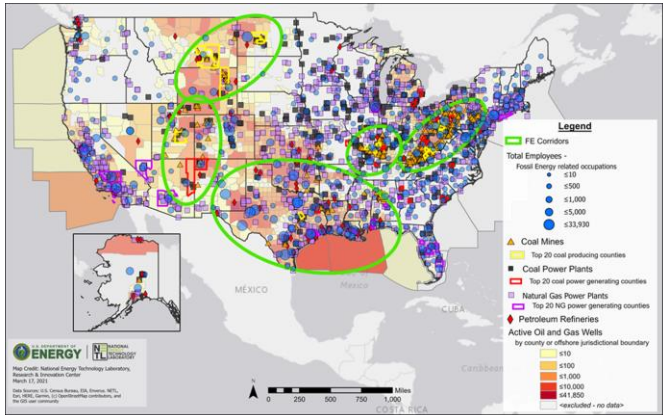


Water Data Challenges

Prior state of energy water data

- Energy process wastewater data are **disparate**, **incomplete**, and **difficult to access**
- Stored in **unusable or disparate formats**
- Regulated by different **federal and state agencies**
- Existing datasets are **not comprehensive** for energy wastewater data: most data is still **hidden** behind regulatory agency doors





These data are necessary to design **treatment technologies**

and understand cross-industry wastewater **re-use opportunities**

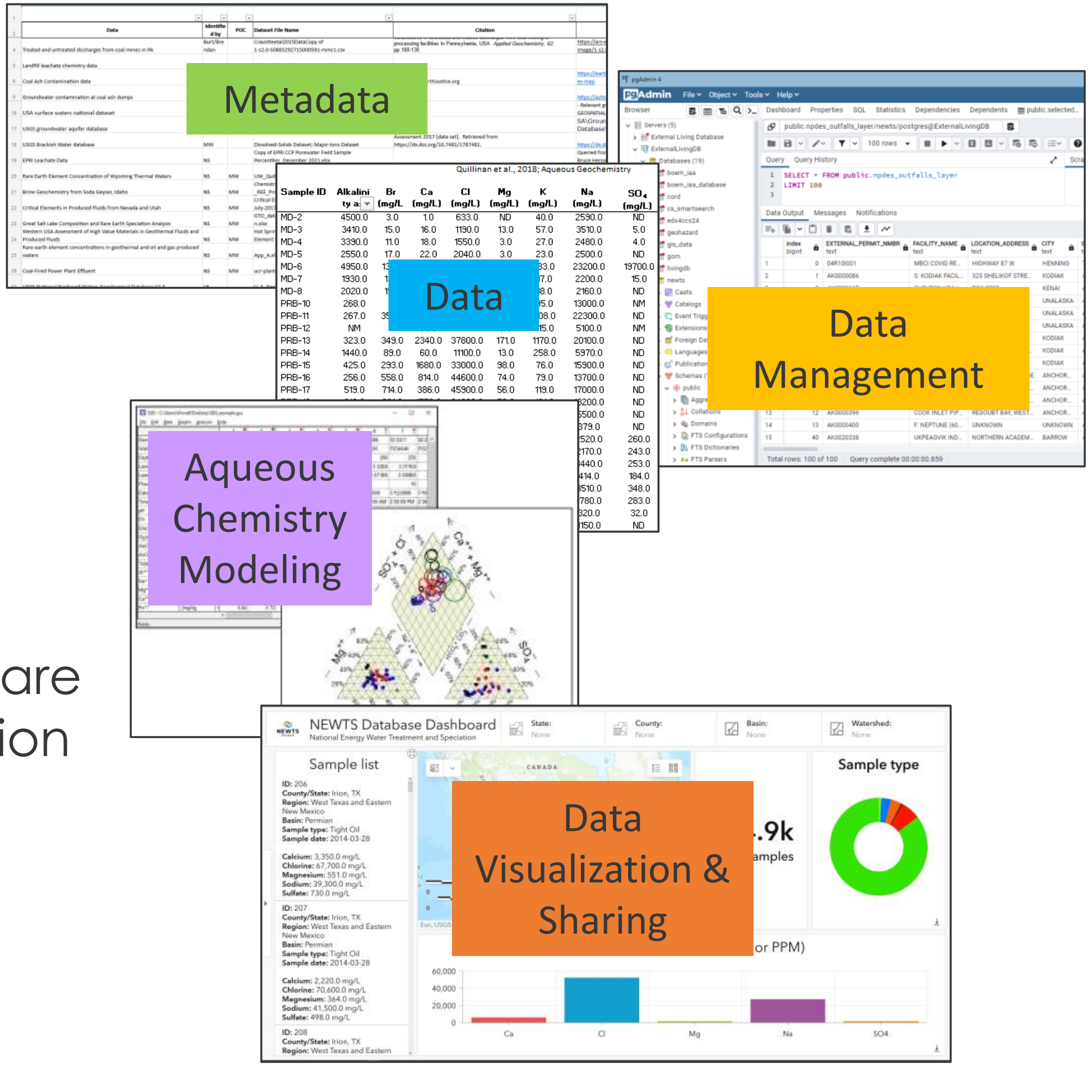
Addressing Water Data Challenges

NEWTS Data Collection & Modeling Methods

NATIONAL ENERGY TECHNOLOGY LABORATORY

Addressing these challenges through:

1) **Systematic data collection**
   - Set key words for data search & acquisition
   - Investigating federal & state data sources
   - Literature review
   - Data catalog for metadata capture
2) **Aqueous chemistry modeling of streams to supplement available data**
   - Ensure compatibility with chemistry modeling software
   - Fill in missing data & supplement reported information
3) **Presenting data through an online interactive data platform**
   - Visualization, interaction and access to data



Example Processed Data

NATIONAL ENERGY TECHNOLOGY LABORATORY

EPA FGD Effluent Dataset

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	

Raw data: one row per <u>measurement</u>

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 Treatmen	Final NPDES	FGD Wastewa	FGD
Sample Description	-	-	-	Effluent from Settling Poı	Influent to Settlir	Effluent from	Effluent from	Final NPDES	Internal point	Infl
Wastewater Classification	-	-	-	FGD Pond Effluent	FGD Purge	Comingled Wa	Bio Effluent -	Comingled W	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 $CaCO_3$							
Silica	Silica		mg/L of SiO_2							
B(OH)3	Boron Hydroxide		mg/L of $B(OH)_3$	450.743872	381.5306632	44.15917121	441.019702	4.15279253		
Ag+	Silver		mg/L of Ag^+	0.0002	0.02	0.0002	0.0002	0.0002		
K+	Potassium		mg/L of K^+							
Li+	Lithium		mg/L of Li^+							
Na+	Sodium		mg/L of Na^+							
NH4+	Ammonium		mg/L of NH_4^+							
Ba+2	Barium		mg/L of Ba^{2+}	0.31	0.579	0.201	0.169	0.045		
Ca+2	Calcium		mg/L of Ca^{2+}							
Co+2	Cobalt		mg/L of Co^{2+}	0.011	0.032	0.011	0.011	0.011		
Cu+2	Copper		mg/L of Cu^{2+}	0.016	0.074	0.016	0.016	0.016		
Hg+2	Mercury		mg/L of Hg^{2+}	0.00052	0.028	0.00011	0.00012	0.00011	0.0043	
Mg+2	Magnesium		mg/L of Mg^{2+}							
Mn+2	Manganese		mg/L of Mn^{2+}	0.846	3.5	0.245	0.592	0.154		
Ni+2	Nickel		mg/L of Ni^{2+}	0.096	0.158	0.018	0.018	0.018		
Pb+2	Lead		mg/L of Pb^{2+}	0.019	0.032	0.019	0.019	0.019		
Sr+2	Strontium		mg/L of Sr2+							
Zn+2	Zinc		mg/L of Zn^{2+}	0.049	0.259	0.038	0.038	0.038		
Al+++	Aluminum trivalent c		mg/L of Al^{3+}							
Cr+++	Chromium trivalent c		mg/L of Cr^{3+}							
Fe+3	Iron		mg/L of Fe^{3+}	0.22	40.8	0.22	0.22	0.22		
Sn+4	Tin		mg/L of 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

U.S. DEPARTMENT OF ENERGY