NETL/RIC Water Management FWP

2024 Resource Sustainability Project Review Meeting

Apr 3, 2024

Technical Portfolio Lead: Nicholas Siefert

NETL Technology Manager: John Rogers

HQ Program Manager: Hichem Hadjeres

HQ Division Director: Vanessa Núñez-López

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.

U.S. DEPARTMENT OF ENERGY | Fossil Energy and Carbon Management

DOE/FECM HQ Program Manager: Hichem Hadjeres

DOE/FECM HQ Advanced Remediation Technologies Division: Vanessa Núñez-López

NETL/TDC Technology Manager: John Rogers

Water Management for Power Systems

NATIONAL ENERGY TECHNOLOGY LABORATORY

Program Goal

The Water Management for Power Systems FWP seeks to understand the cost of treating as well as developing novel processes to treat effluent streams generated during fossil energy extraction and conversion into energy products

Tasks:	Principal Investigators
• Task#2: Guiding R&D for Treatment of Fossil Power Plant Effluent Streams	Alison Fritz, Chad Able
• Task#4: Concentrating Wastewater Effluent Streams & Resource Recovery	Nicholas Siefert, Charlotte Rutnik
• Task#5: Metrics for Water Use of Power Systems	Erik Shuster, Haleigh Heil
• Task#9: National Energy Water Treatment & Speciation (NEWTS) Database	Burt Thomas, Rachel Yesenchak

Motivation for Water Management

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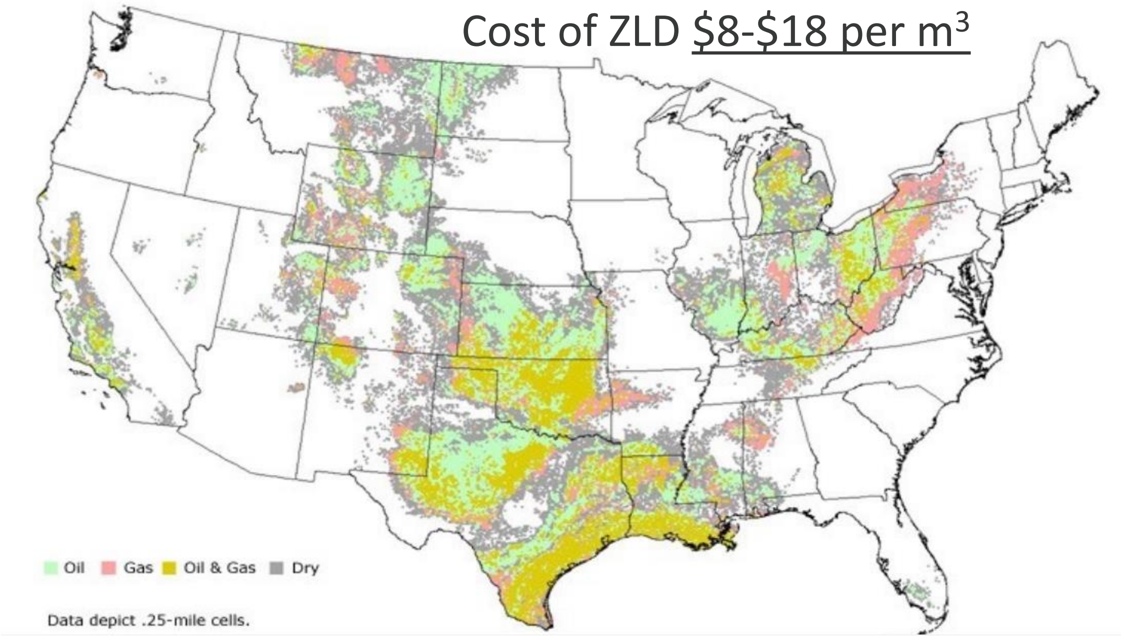
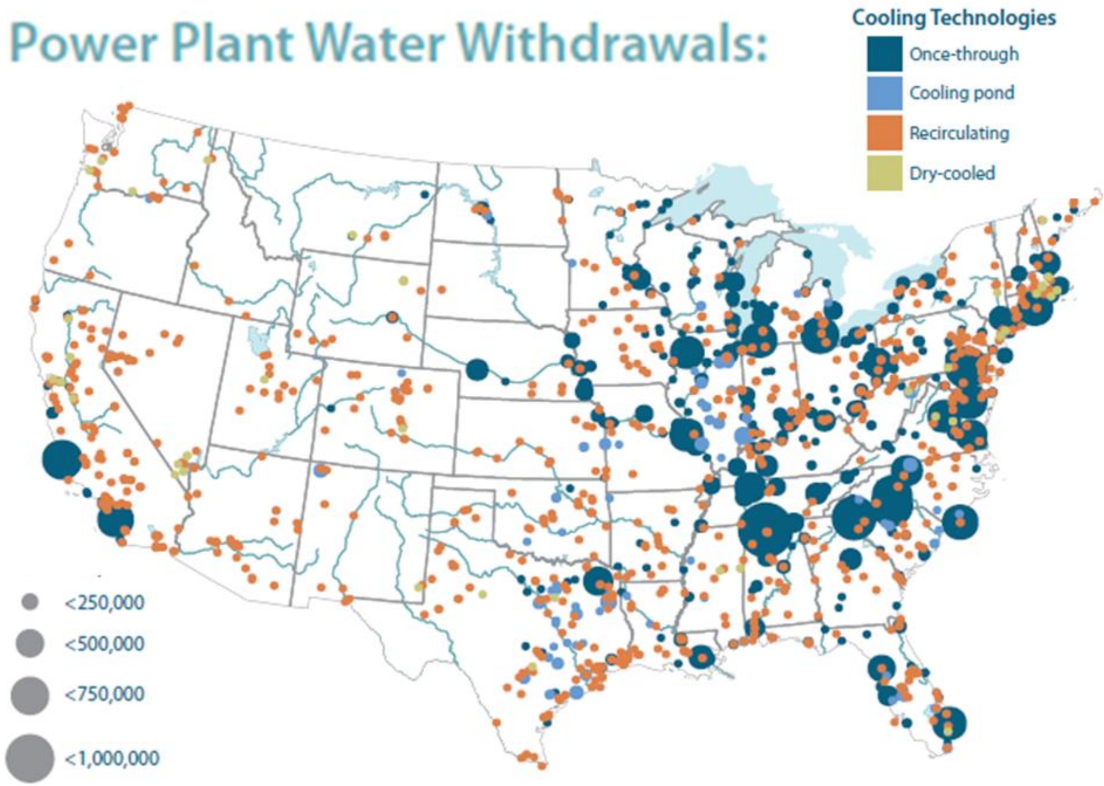
Produced Water from Oil&Gas Wells and Water Consumption at Thermal Power Plants

Distribution of Oil & Gas Wells

Cost of SWD of produced water $5-$12 per m^3

Cost of ZLD $8-$18 per m^3





US generates **4 billion** m^3 of produced water per year

2 billion m^3 of produced water reinjected for EOR

2 billion m^3 of produced water to SWD

Potential for ~**100 million tons/yr** of salt and ~10 kton/yr of Li

US power plants consume **4 billion** m^3 of fresh water per year

US consumes **50 million tons** per year of road salt

World mines ~20 kton per year of Lithium (as Li)

Task#2: Machine Learning Approaches for Energy Wastewater Characterization

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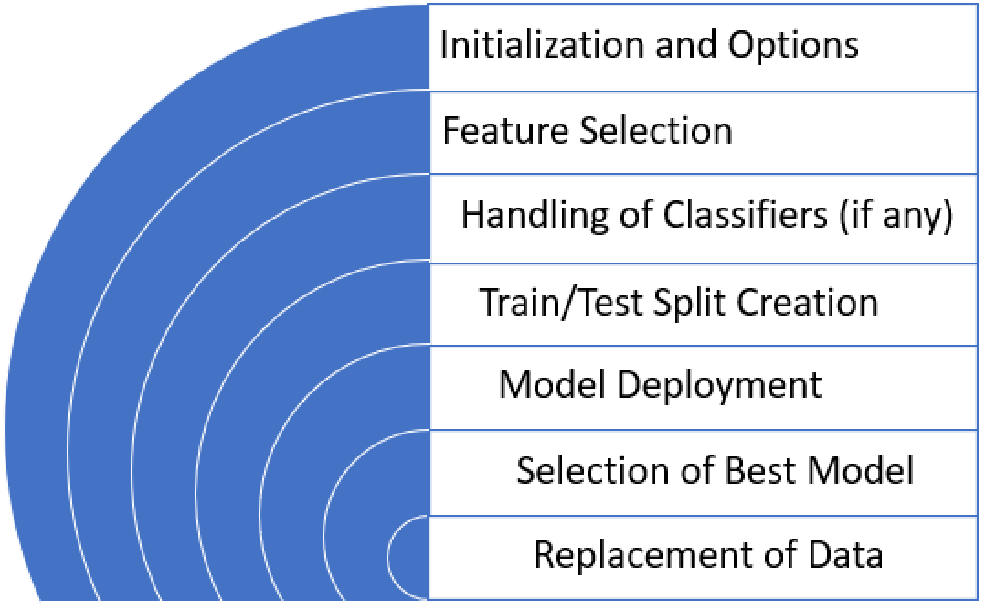
CO-DART
CONSTITUENT DATA REPLACEMENT TOOL

- To accurately model treatment and byproduct recovery costs for energy wastewaters, we need complete composition data.
- **CoDaRT (Constituent 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
- The tool can use the user's data alone or combine user data with publicly-available NEWTS datasets.
- <u>Will be made available in FY24 for public download via EDX</u>

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NETL PI: Alison Fritz, Systems Analysis PI: Chad Able

Task 2: Machine Learning Approaches for Energy Wastewater Characterization

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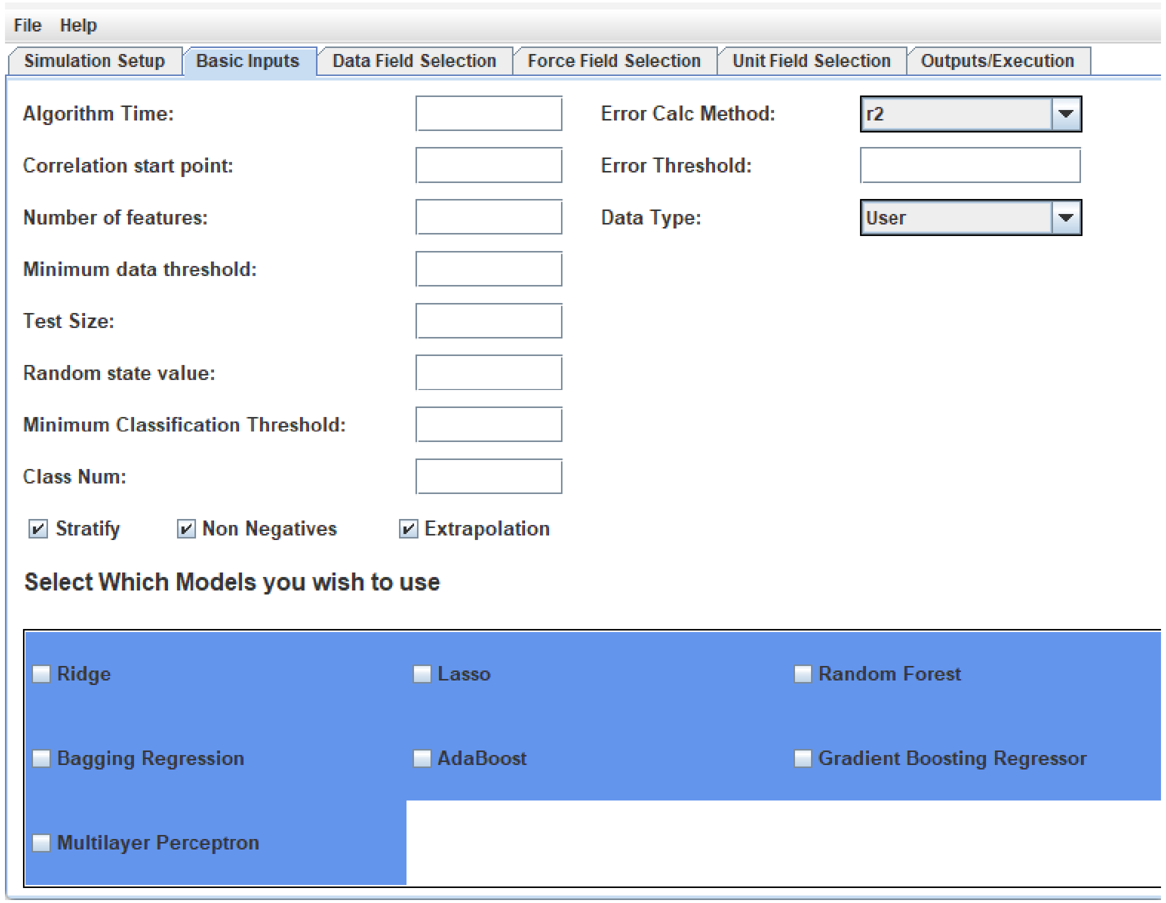
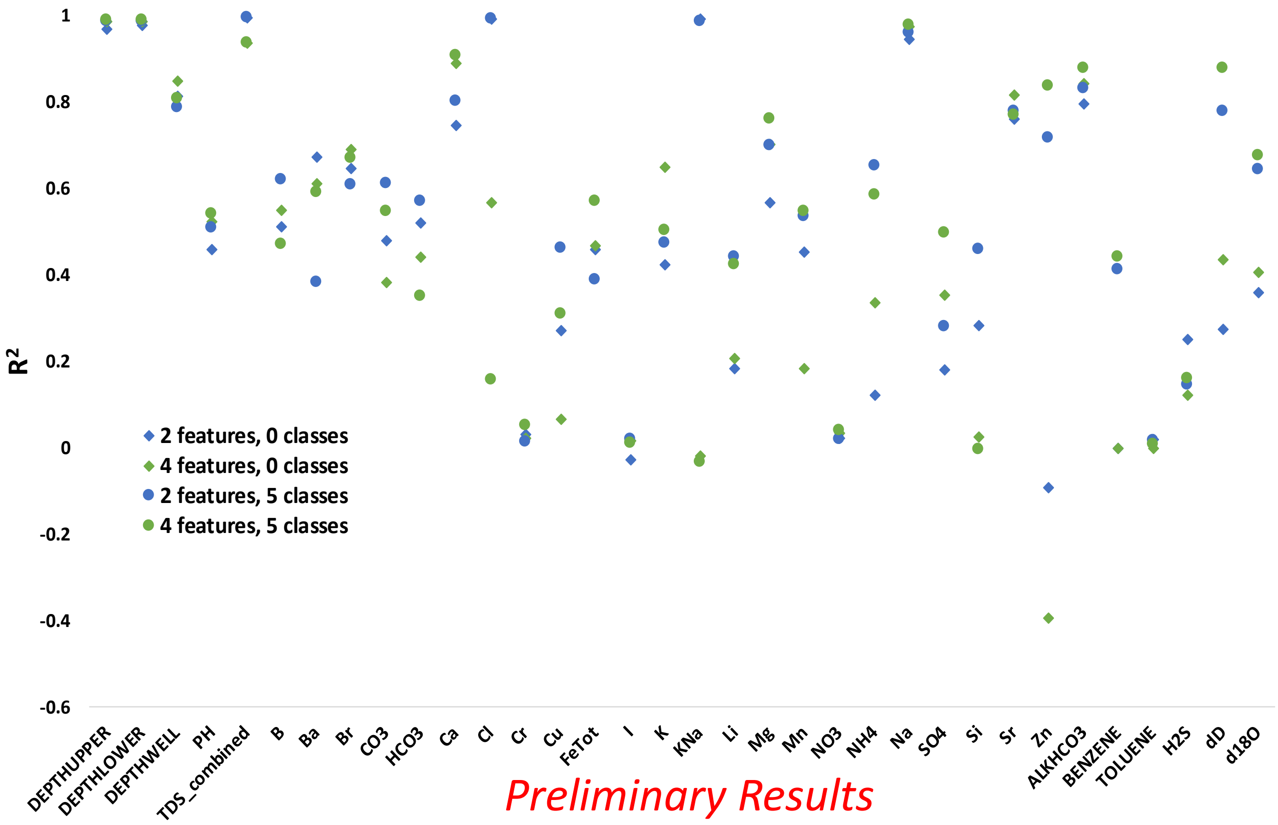
CO-DART GUI





Example data replacement performance for the NEWTS USGS Produced Water Database.

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

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

Task 2: Machine Learning Approaches for Energy Wastewater Characterization

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

Example using: Rittenhouse et al. 1960s Historical Archived Produced Water Dataset - Submissions - EDX (doe.gov)

Task#2: Local treatment needs and critical mineral market size for combustion residual leachate

NATIONAL ENERGY TECHNOLOGY LABORATORY

Assessment of combustion residual leachate: Local treatment needs and CM recovery

Resources, Conservation & Recycling 205 (2024) 107535

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Resources, Conservation & Recycling

journal homepage: www.elsevier.com/locate/resconrec

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Full length article

Assessment of combustion residual leachate: Local treatment needs and critical mineral recovery

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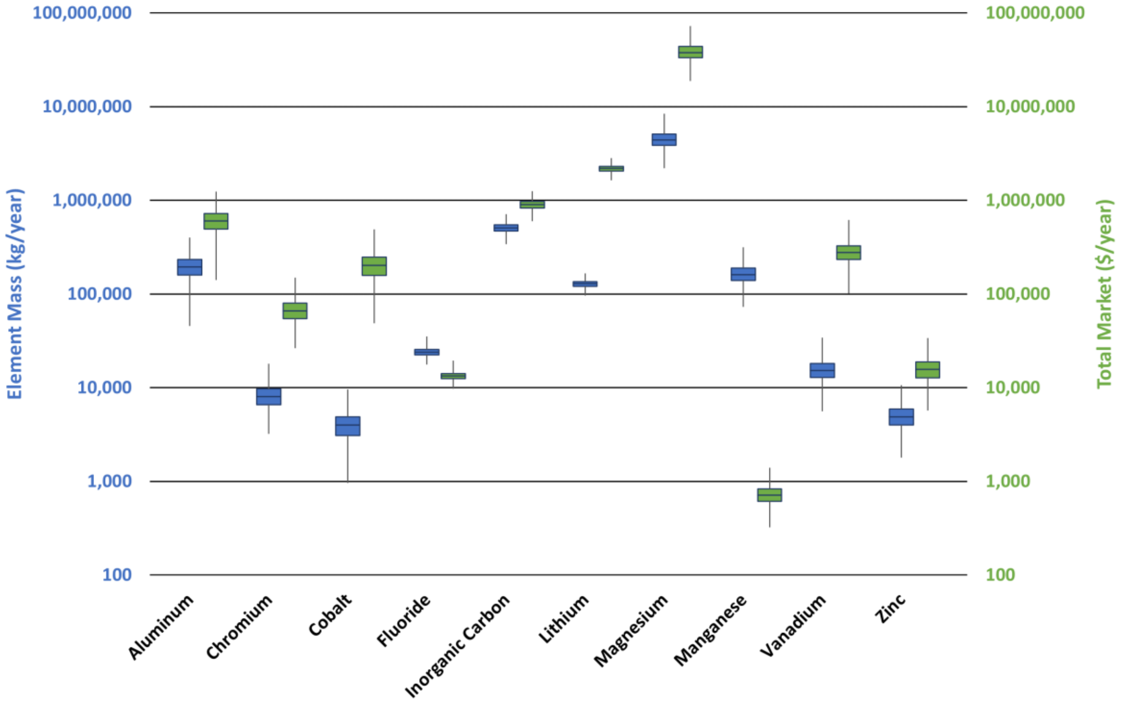
ARTICLE INFO

Keywords:
Coal ash
Combustion residual leachate
Ash pond
Effluent limitation guidelines
Landfill
Surface impoundment
Critical minerals

ABSTRACT

Combustion residual leachate from landfills and impoundments at coal-fired power plants represents a large volume of wastewater with variable treatment requirements prior to discharge. Treatment to meet these requirements can be costly, but simultaneously creates an opportunity to co-extract critical minerals. This work first characterizes the treatment needs by developing composite regional standards for 14 contaminants across the United States (U.S). We then assess data on leachate composition and present the total mineral mass and total market size that can be recovered during treatment. Magnesium has the largest total mineral mass and largest market size and can be extracted using commercially available technology. The average simulated value of this magnesium is $38 million from landfill leachate and $660 million from impoundment leachate. This would account for 9 % and 150 %, respectively, of U.S. annual consumption of magnesium.

https://doi.org/10.1016/j.resconrec.2024.107535



Recoverable Elements in Landfill Leachate, in Terms of Element and Total Market

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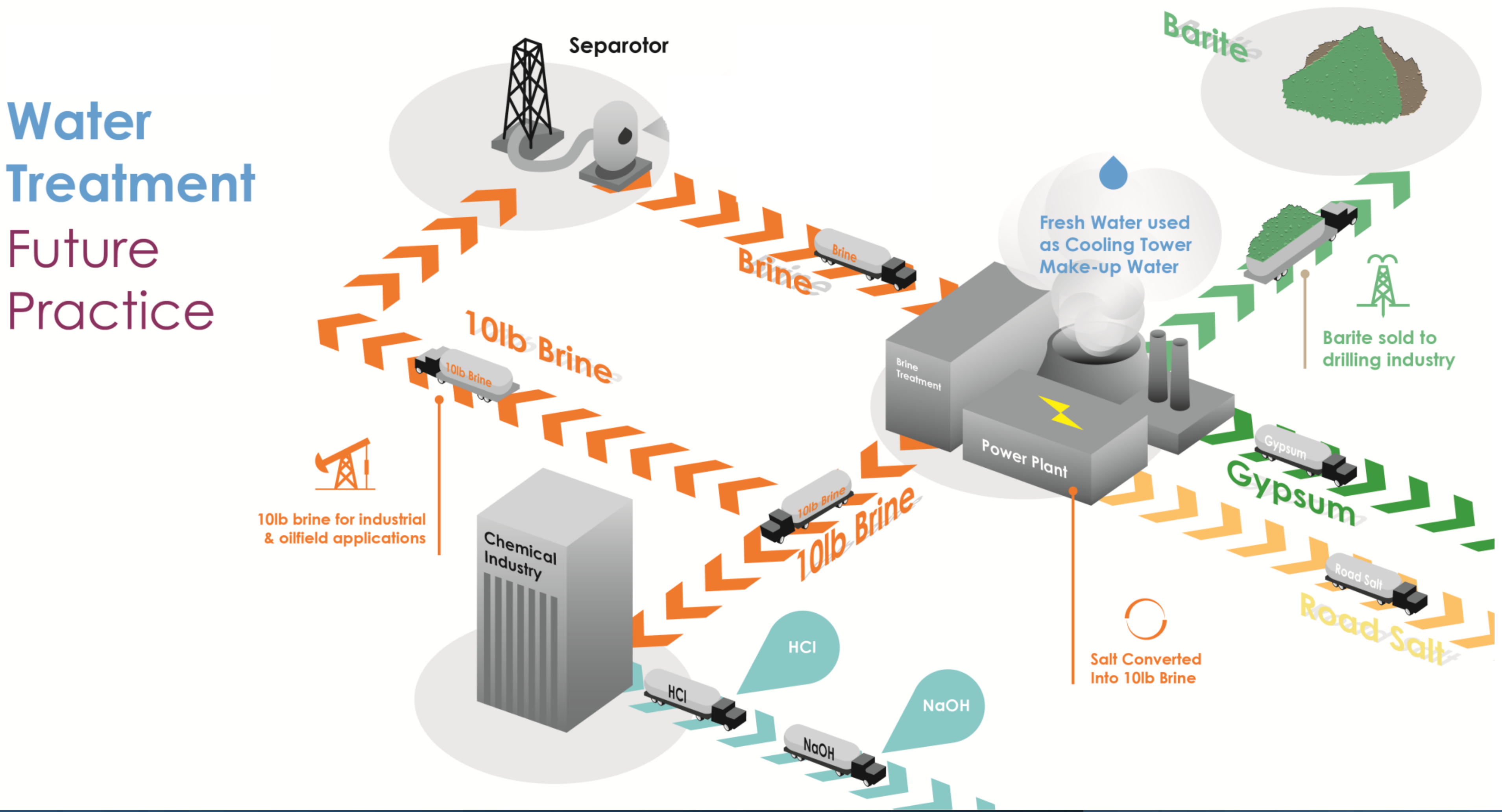
NETL PI: Alison Fritz, Systems Analysis PI: Chad Able



Task#4: Concentrating Wastewater Effluent Streams & Resource Recovery

Nicholas Siefert (NETL, PI)
Marcus Poyer(LRST)
Charlotte Rutnik (LRST)
Lance Lin (WVU)

Synergies between PW and FGD Effluent

- Appalachian produced water is high in divalent cations (Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+})
- Power plant FGD effluent is rich in sulfate (SO_4^{2-})
  - Potential to make up to 0.4 million tons per year of Barite (~$70 M/yr)
- Produced water has reducing species (NH_4^+, Fe^{2+}, $C_2H_3O_2^-$)
  - FGD biological treatment reactor need these reducing species
- Power plant FGD effluent has oxidizing species that need to be reduced NO_3^-, NO_2^-, SeO_4^{2-}, SeO_3^{2-}, CrO_4^{2-}
- Synergies make PW&FGD co-treatment advantageous

Mineral Commodity Summaries 2024 (usgs.gov)

Pilot-Scale Testing at WVU (Summer 2023)

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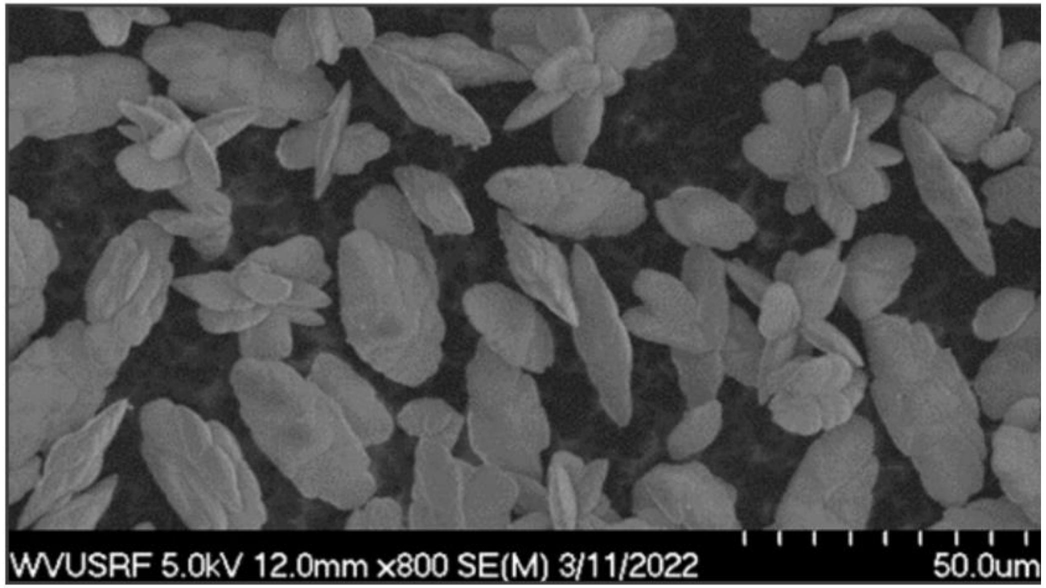


PW & FGD Effluent Treatment Process Flow Diagram

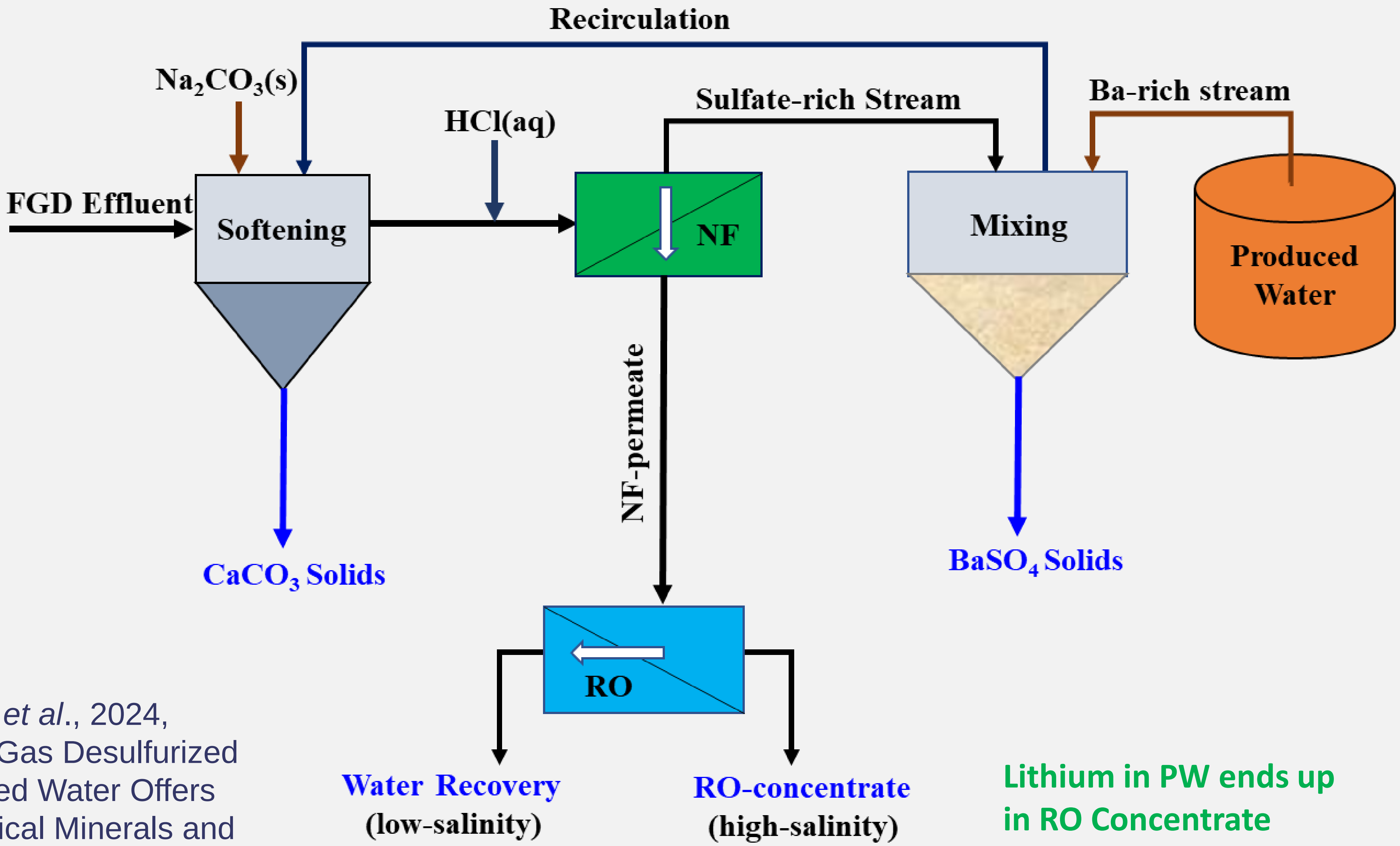
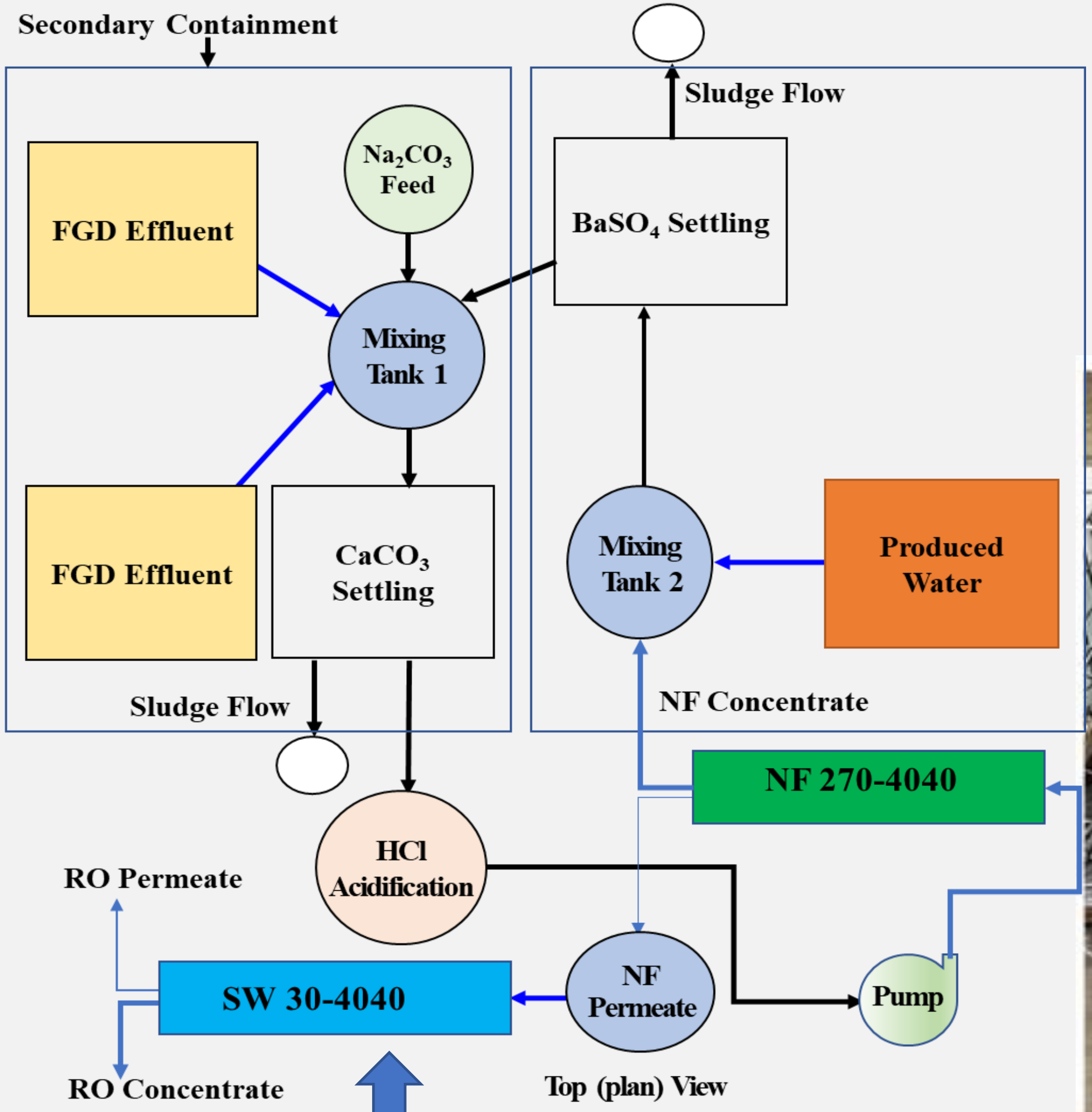


Figure from: Ahmed *et al*., 2024, "Co-managing Flue Gas Desulfurized Effluent and Produced Water Offers Opportunities of Critical Minerals and Water Recovery, *under review*.

Lithium in PW ends up in RO Concentrate

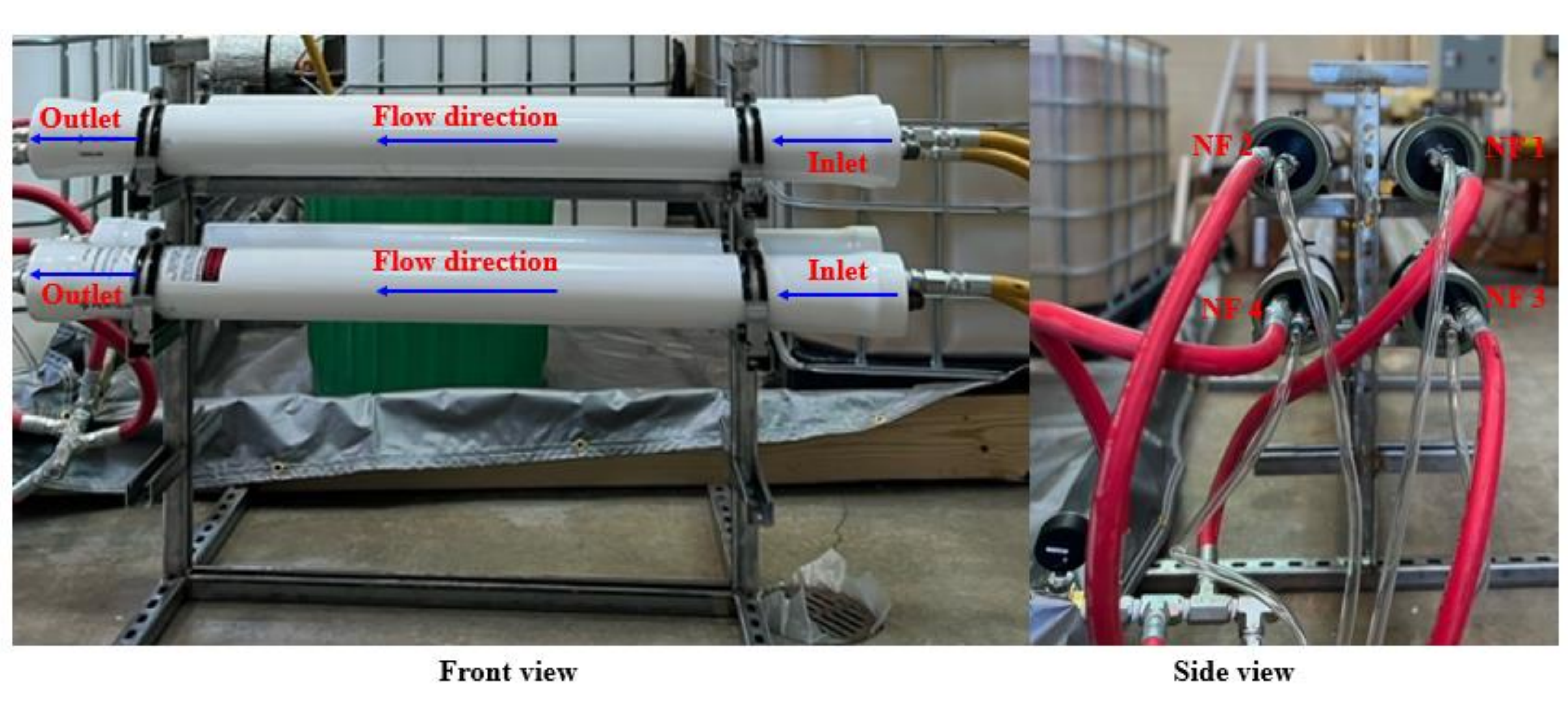
Pilot-scale Co-treatment of FGD Effluent and PW



Schematic

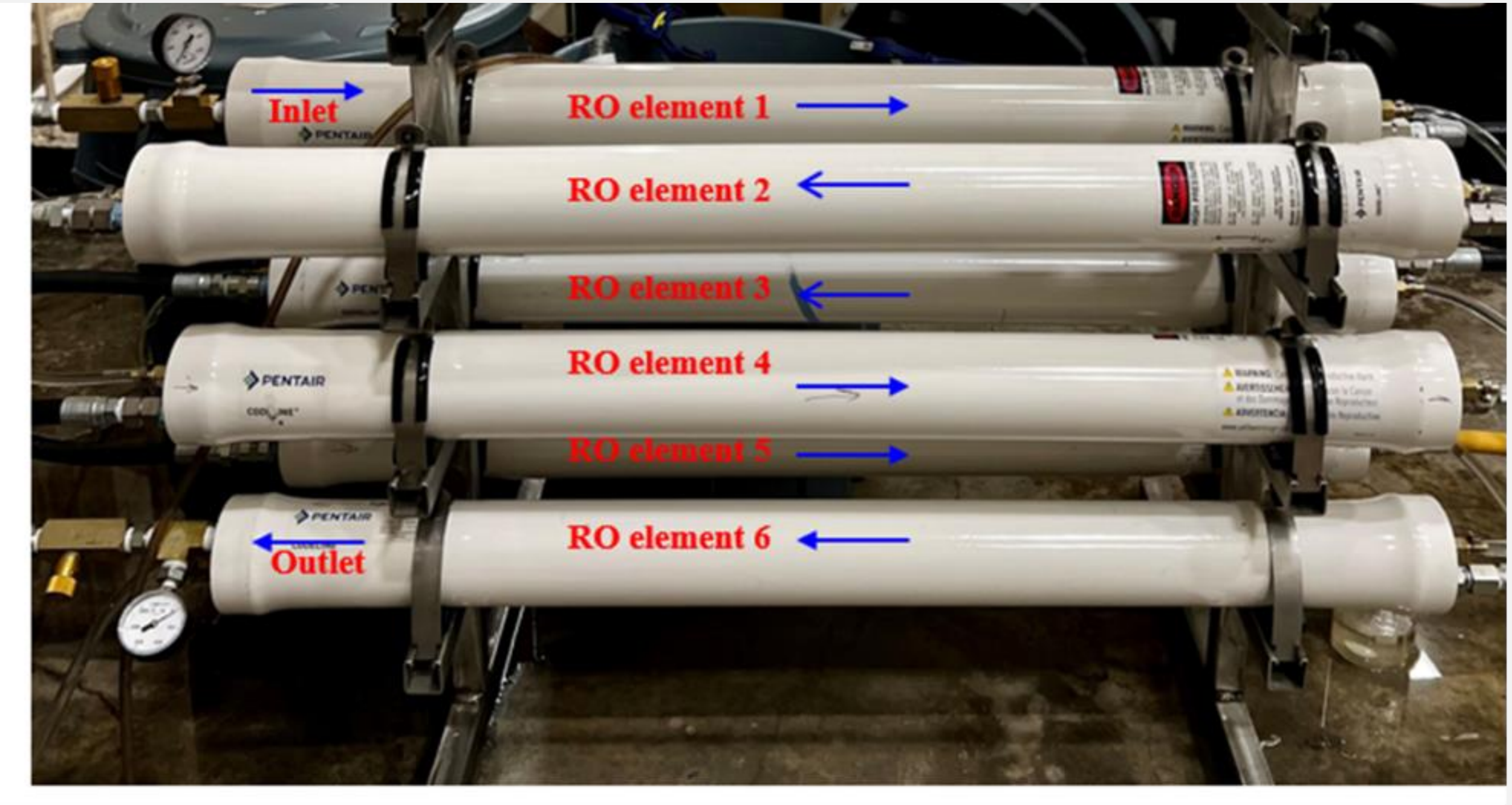
Experimental setup at WVU

Nanofiltration System

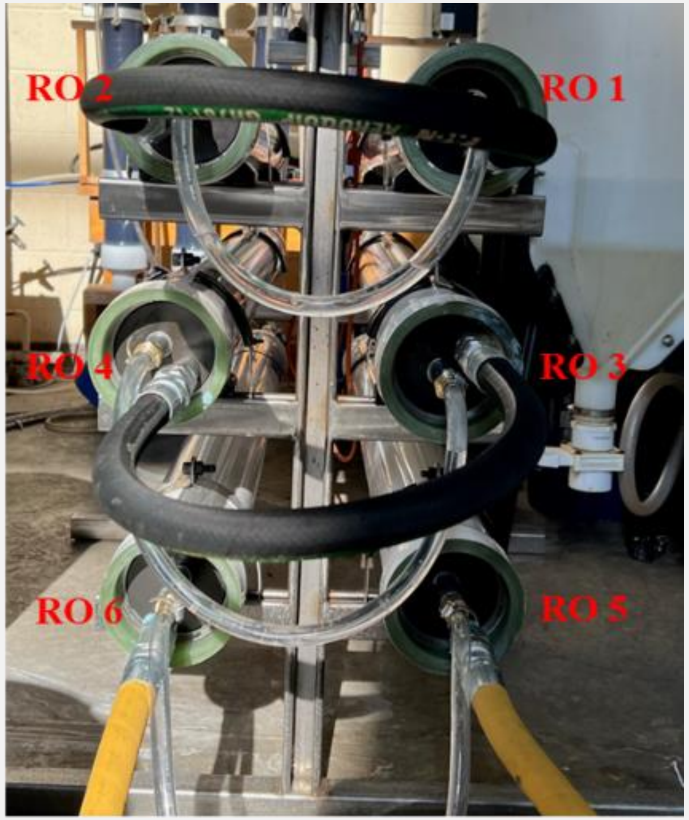


Four NF 270-4040 elements connected in parallel

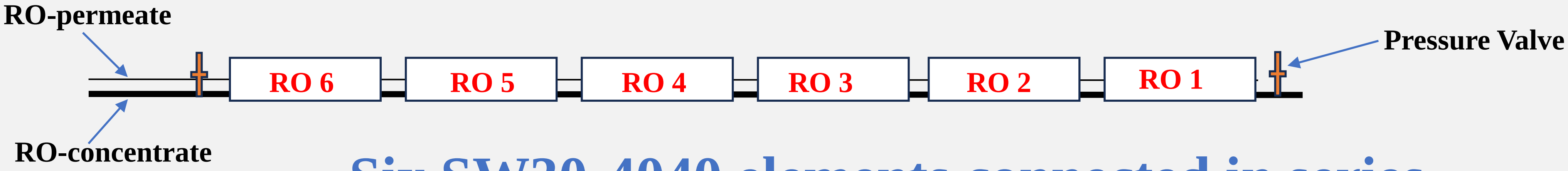
Reverse Osmosis (RO) System



(Front view)

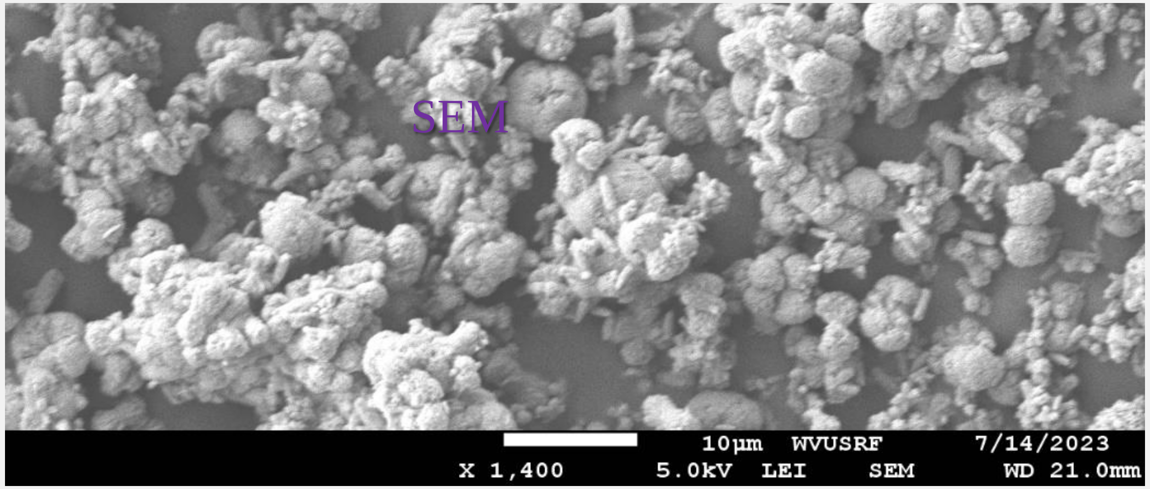


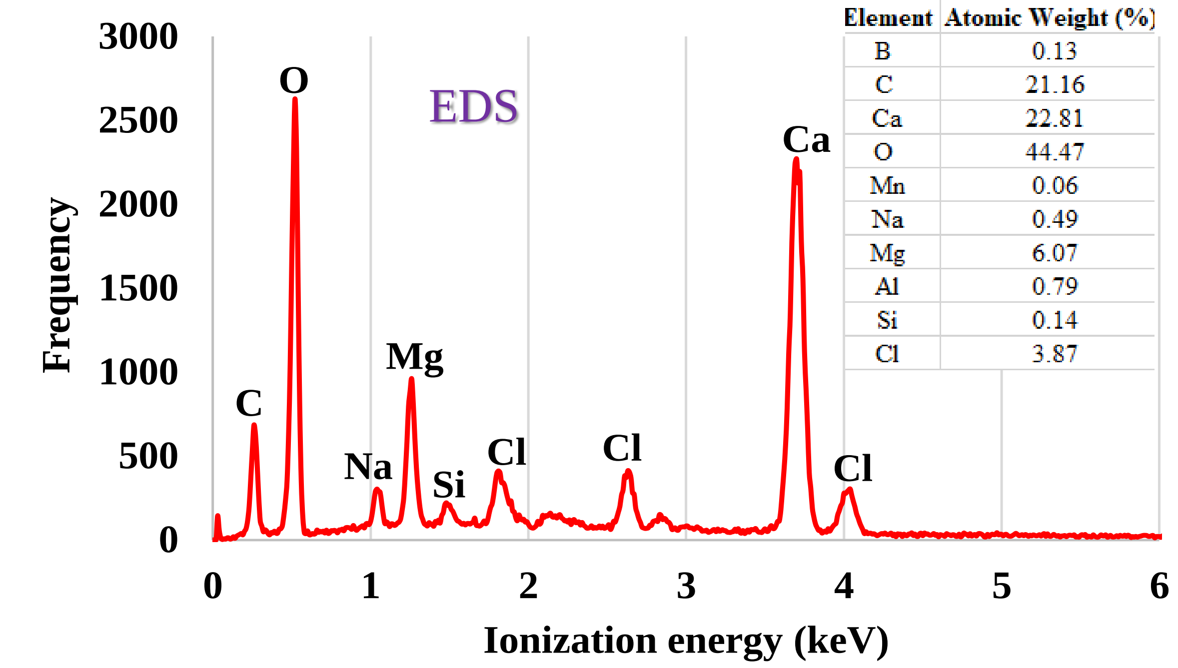
(Side view)



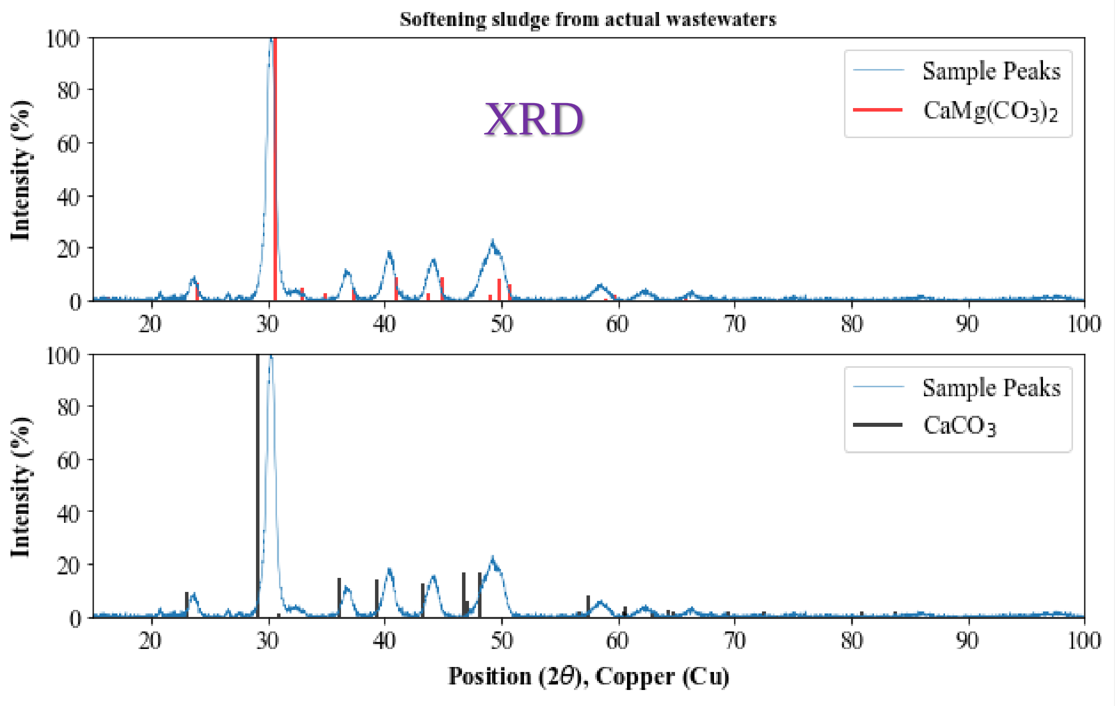
Six SW30-4040 elements connected in series

Calcite ($CaCO_3$) Production from Softening



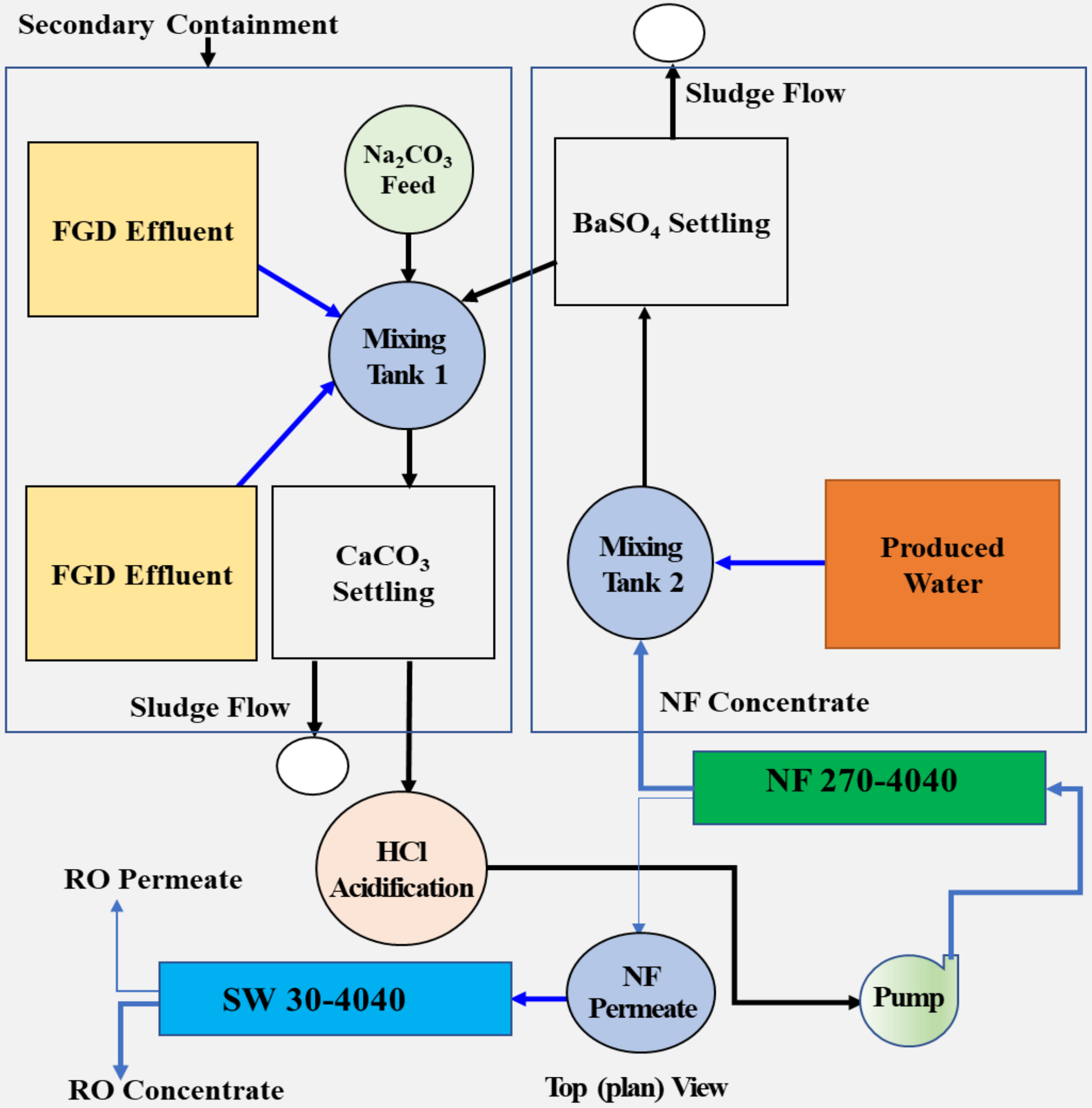


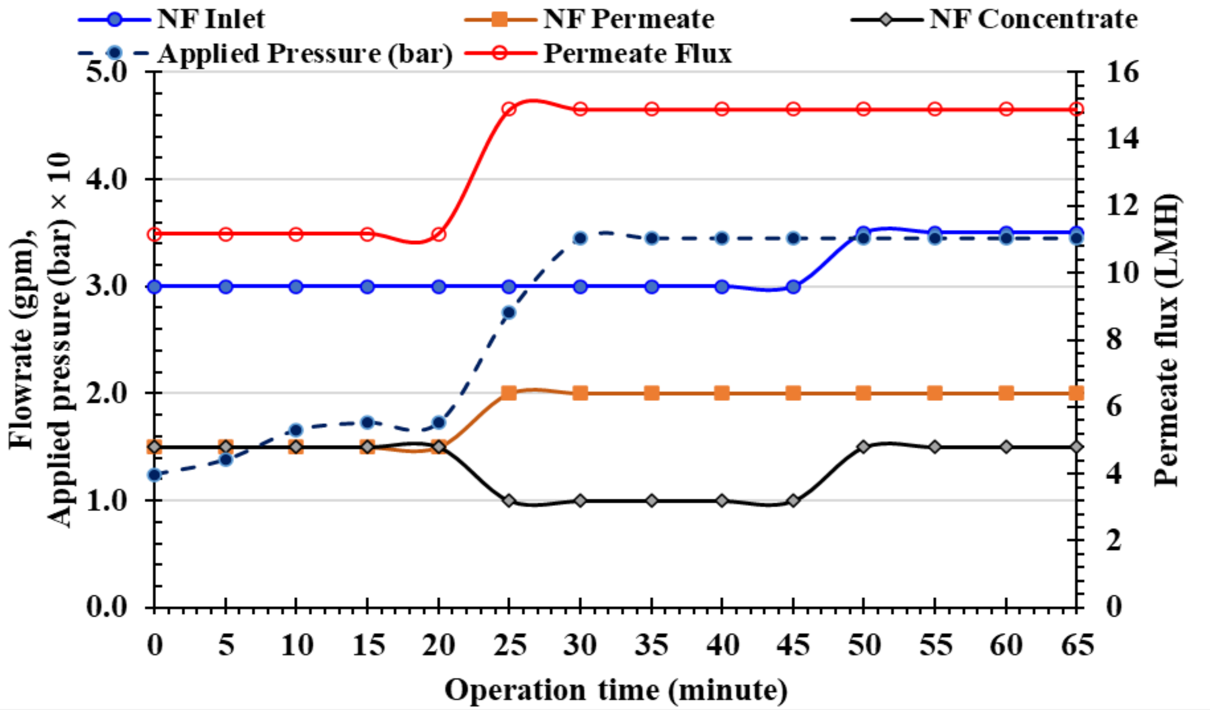
Element	Atomic Weight (%)
B	0.13
C	21.16
Ca	22.81
O	44.47
Mn	0.06
Na	0.49
Mg	6.07
Al	0.79
Si	0.14
Cl	3.87



- Na_2CO_3 requirement: ~35 kg /m³ mixture
- Production yield: ~30 kg/m³ mixture (high-yield)
- SEM-EDS & XRD: calcite ($CaCO_3$)

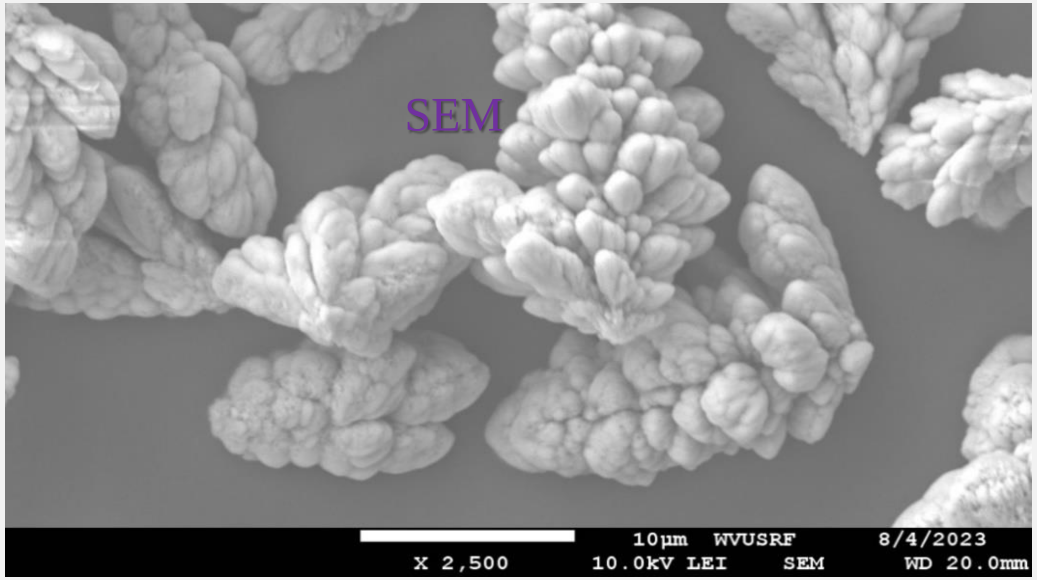
NF Operational Results

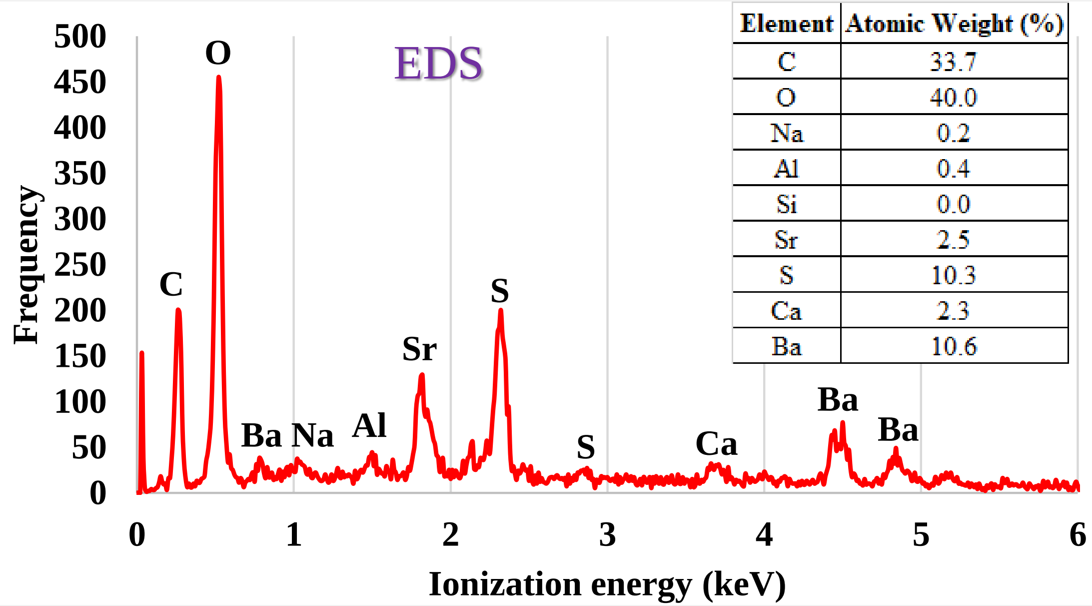




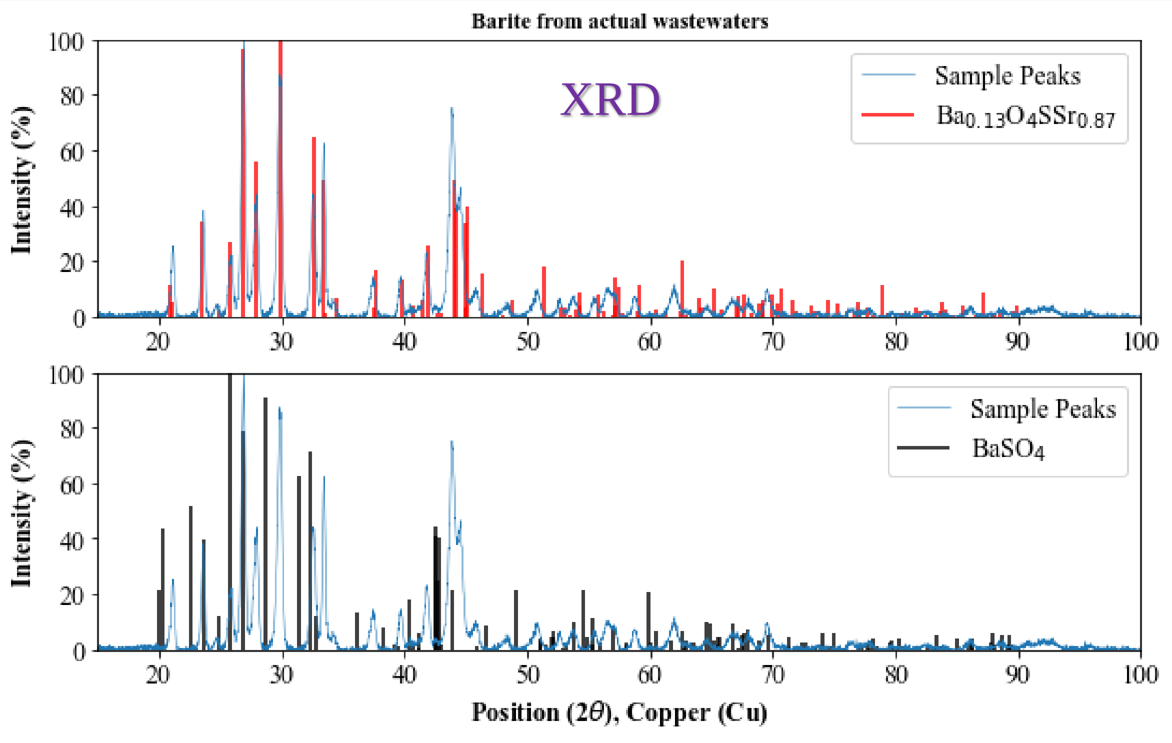
Parameter	0-45 min	(45-65 min)*
FGD flow (gpm)	3.0	1.25
NF inlet flow (gpm)	**3.0**	**3.5**
Feed pressure (bar)	24.3	34.5
NF-permeate (gpm)	**1.8**	**2.0**
NF-concentrate (gpm)	1.2	1.5
PW flow (gpm)	1.3	1.5
Permeate flux (LMH)	13.0	14.9
NF-permeate recovery (%)	**60**	**67**

NF-conc: PW Mixing - Barite ($BaSO_4$) Production



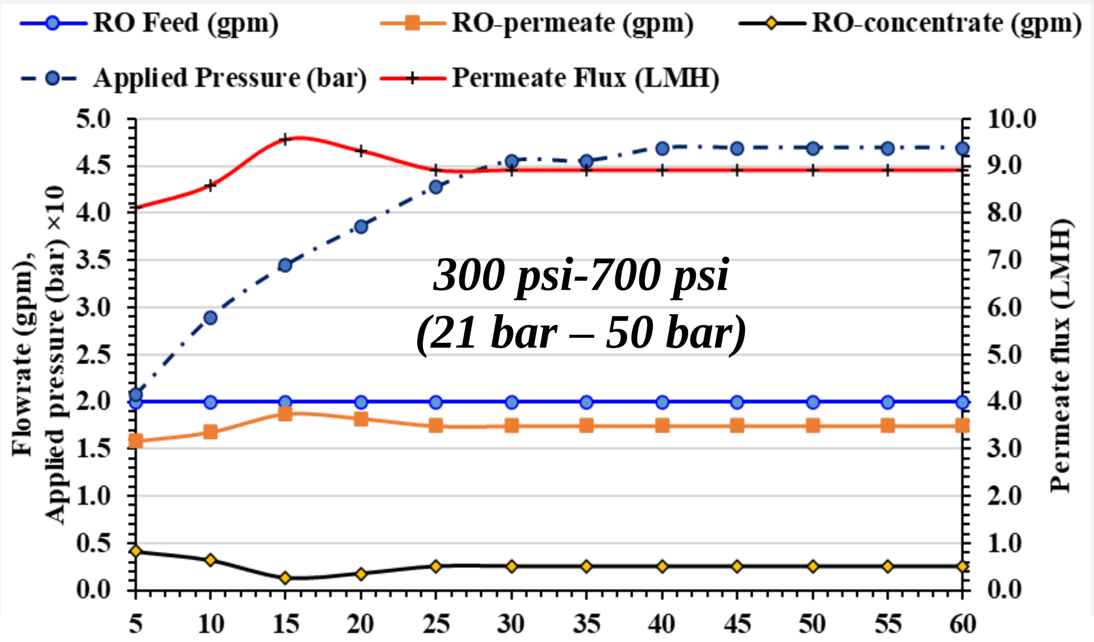


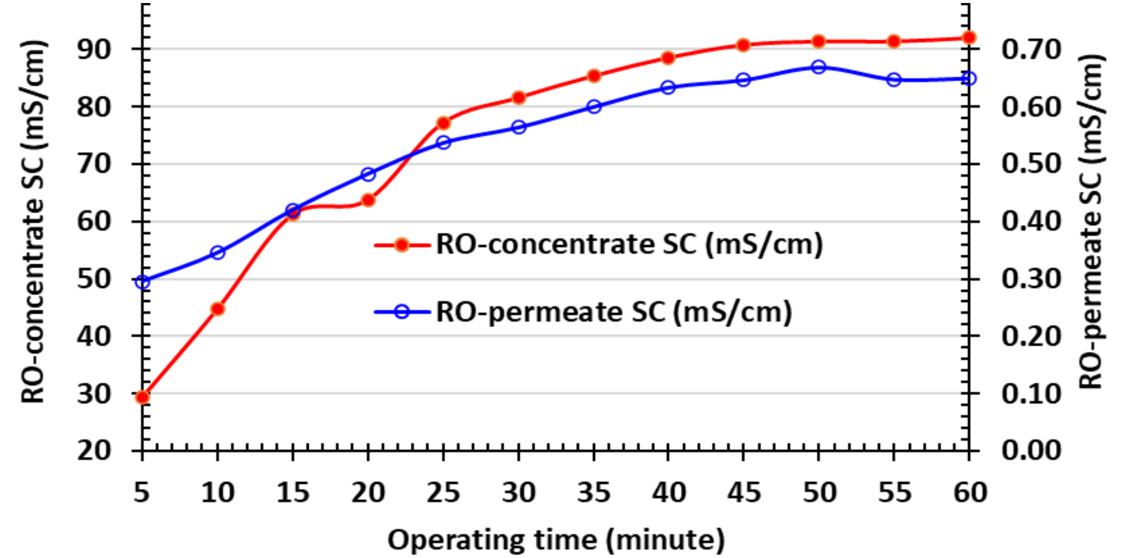
Element	Atomic Weight (%)
C	33.7
O	40.0
Na	0.2
Al	0.4
Si	0.0
Sr	2.5
S	10.3
Ca	2.3
Ba	10.6



- Dry density: ~4.1 g /cm³ **Meets API Specs**
- Production yield: ~7.5 kg/m³ mixture
- SEM-EDS & XRD: Barite ($BaSO_4$)

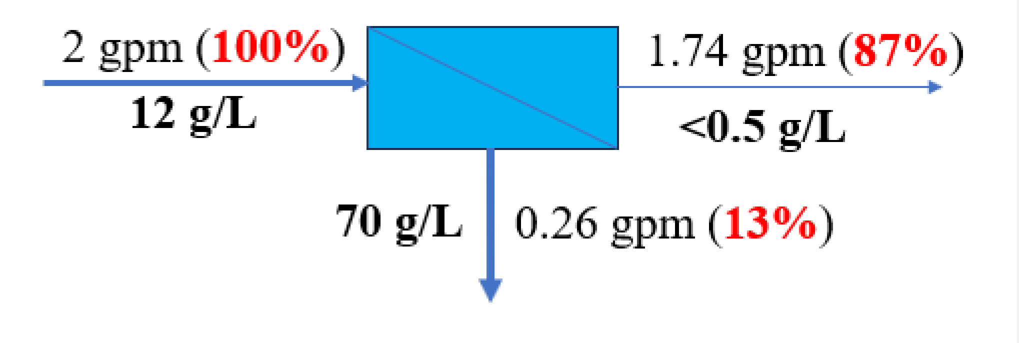
Low Salinity Water Recovery by Reverse Osmosis





Analyte	RO Inlet	RO-concentrate	RO-permeate
		mg/L	
B	189	498	117
Ba^{2+}	0.07	0.43	0.006
Ca^{2+}	**453**	**2,520**	0.6
Mg^{2+}	**1,270**	**7,321**	1.6
Mn^{2+}	17	96	0.024
Na^{+}	**1,790**	**9,353**	130
Sr^{2+}	7	44	0.01
Cl^{-}	**6,928**	**39,076**	182
SO_4^{2-}	207	2,045	-
TDS	**12,000**	**70,000**	**<500**

Low-salinity



Results Summary - FGD-PW Co-treatment

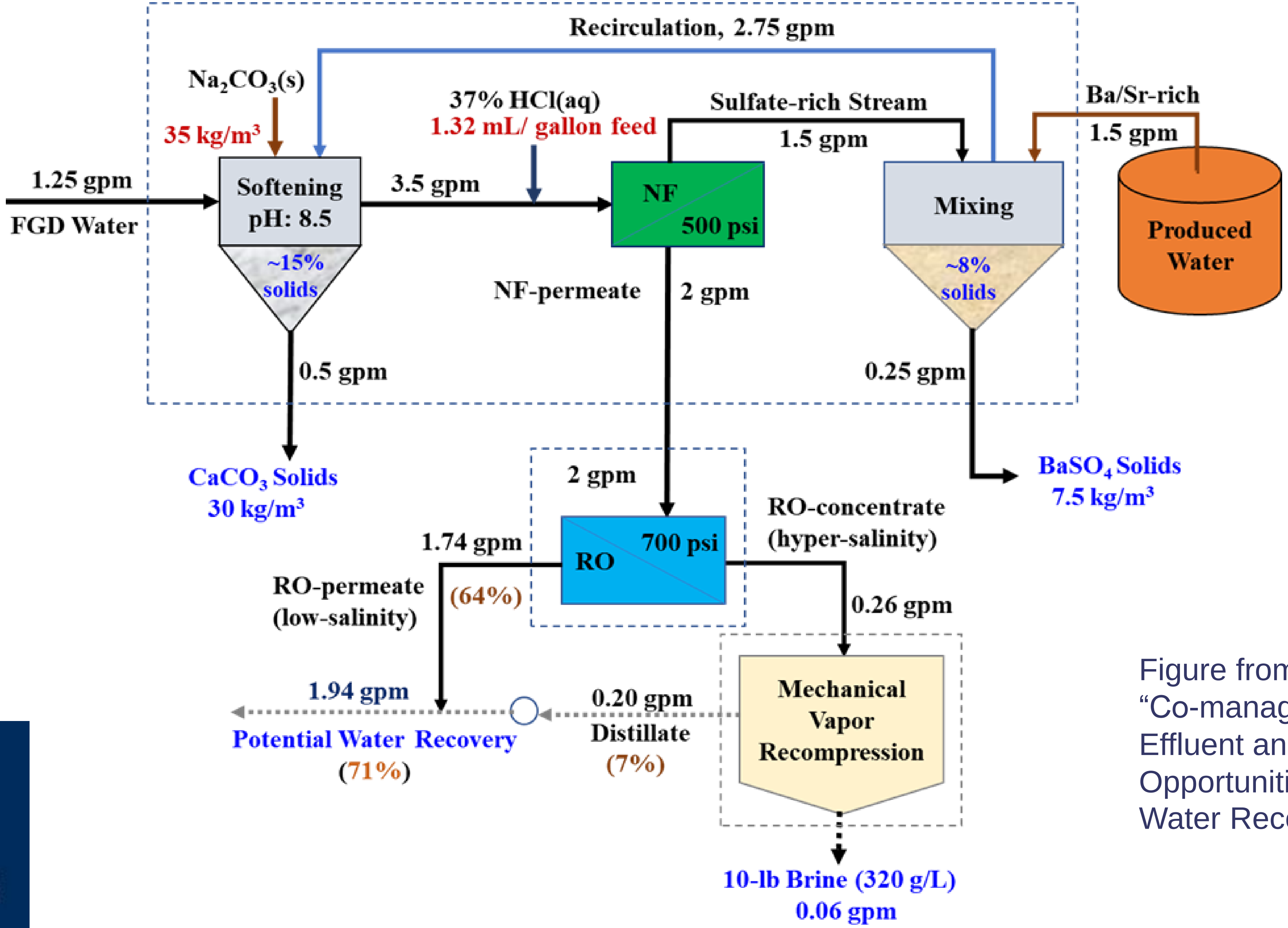


Figure from: Ahmed *et al*., 2024, "Co-managing Flue Gas Desulfurized Effluent and Produced Water Offers Opportunities of Critical Minerals and Water Recovery, *under review*.

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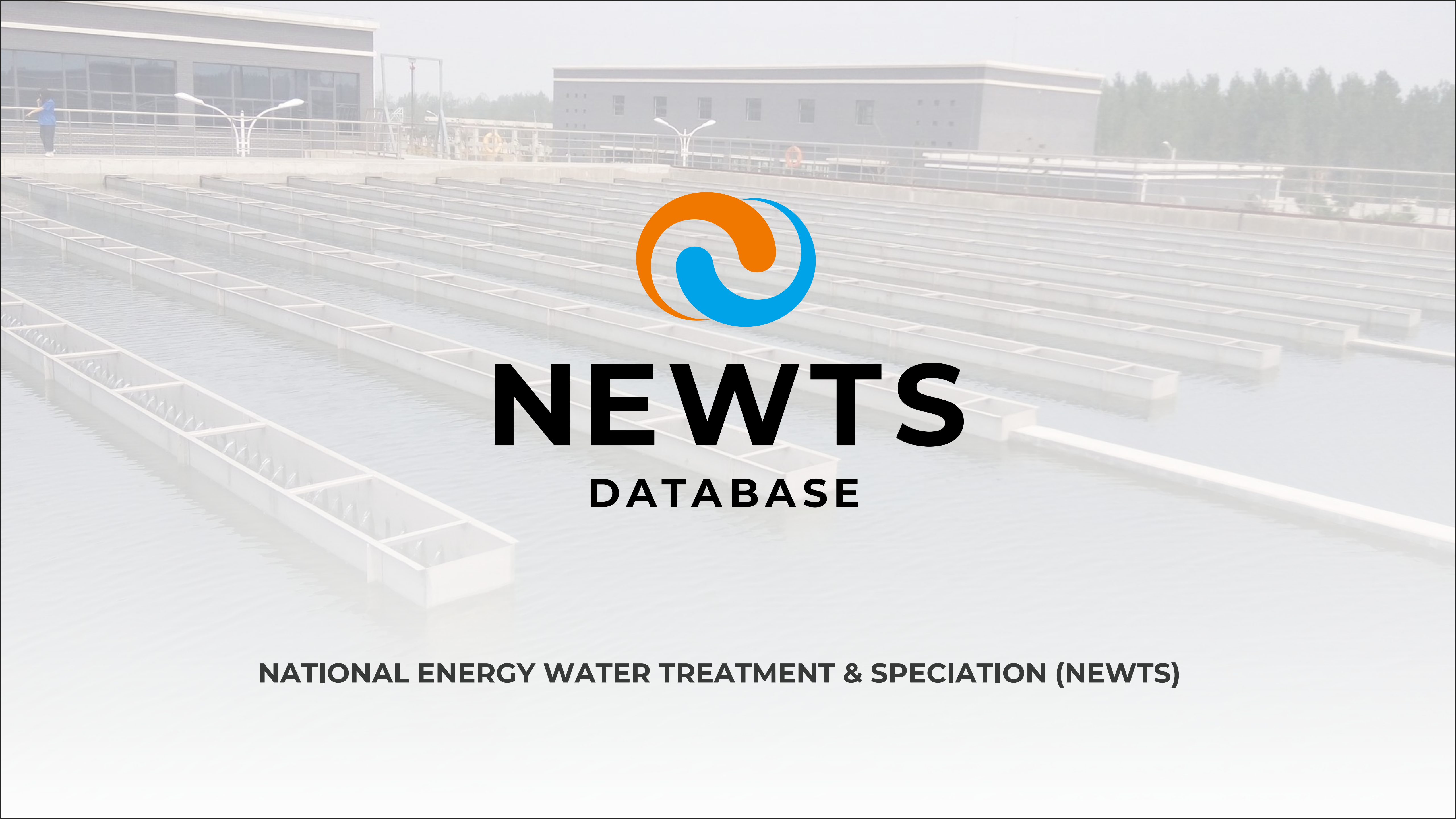
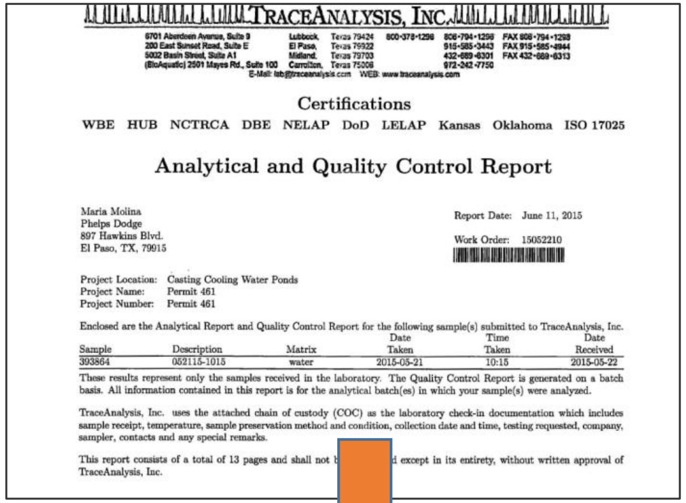

NEWTS
DATABASE
NATIONAL ENERGY WATER TREATMENT & SPECIATION (NEWTS)

Motivation for NEWTS Database

Prior state of energy-water data

- Energy process wastewater dataset were **incomplete**, **non-standardized**, and/or **difficult to access**
- Regulated by different **federal and state agencies**
  - Many datasets were not easily downloadable
- Many datasets list elements, not the species or redox state, e.g. Fe(II) vs. Fe(III)
- Existing datasets are initially **not formatted** for input into modeling and water treatment software

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



TRACEANALYSIS, INC.

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(BioAquatic) 2501 Mayes Rd., Suite 100	Carrollton,	Texas 75006		972•242•7750	

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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

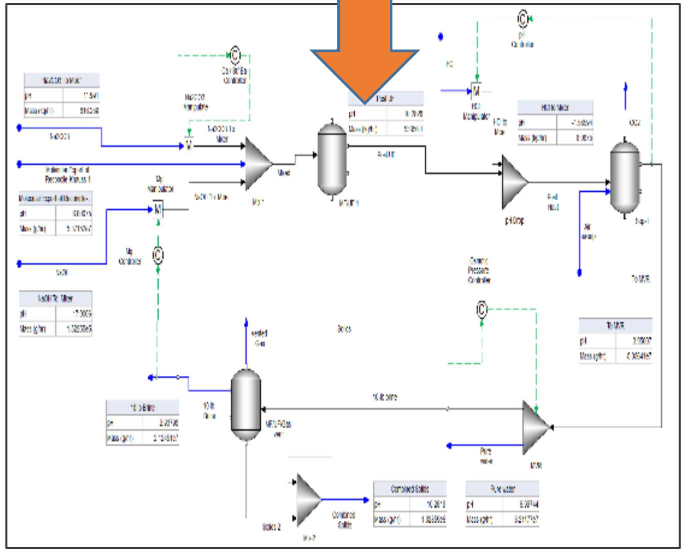
Enclosed are the Analytical Report and Quality Control Report for the following sample(s) submitted to TraceAnalysis, Inc.

Sample	Description	Matrix	Date Taken	Time Taken	Date Received
393864	052115-1015	water	2015-05-21	10:15	2015-05-22

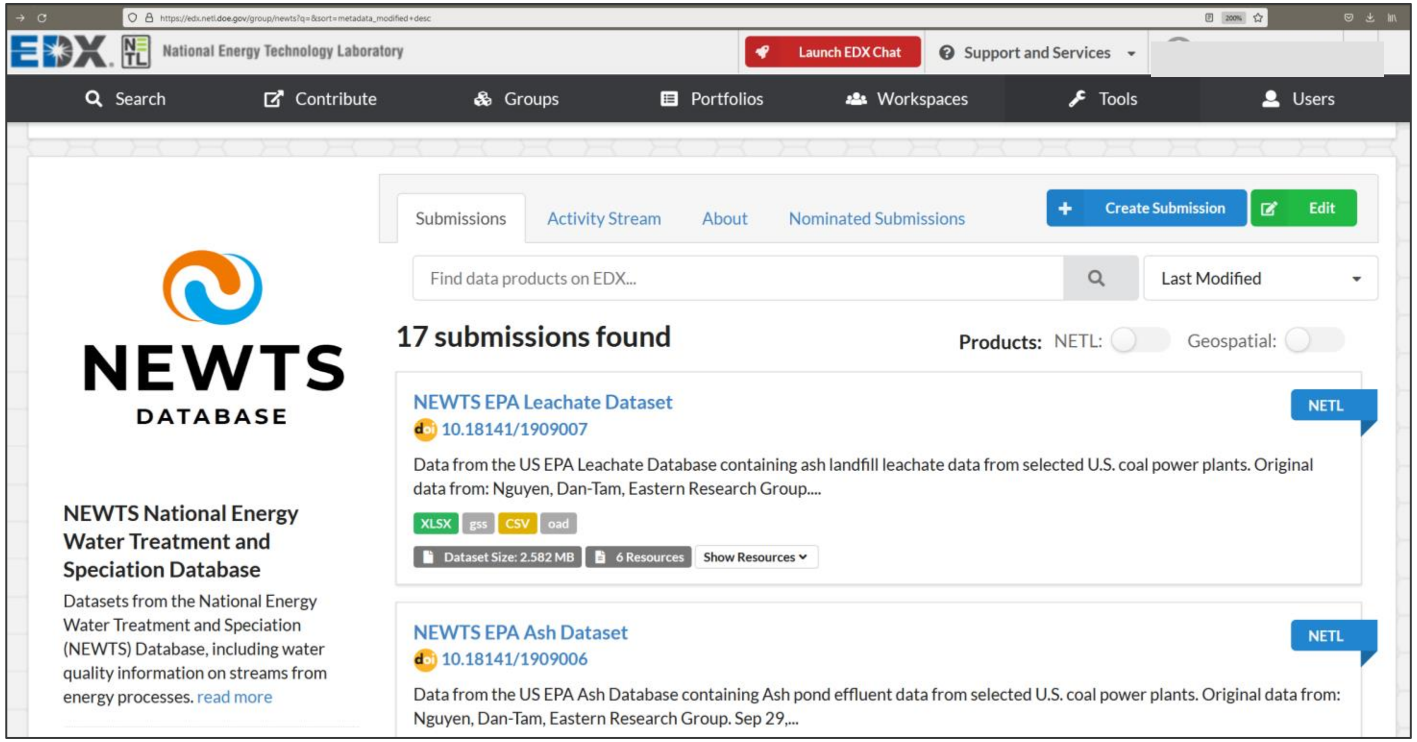
These results represent only the samples received in the laboratory. The Quality Control Report is generated on a batch basis. All information contained in this report is for the analytical batch(es) in which your sample(s) were analyzed.

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 b[illegible]d except in its entirety, without written approval of TraceAnalysis, Inc.



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

National Energy Water Treatment & Speciation Database

Leveraging NETL R&D Core Capabilities

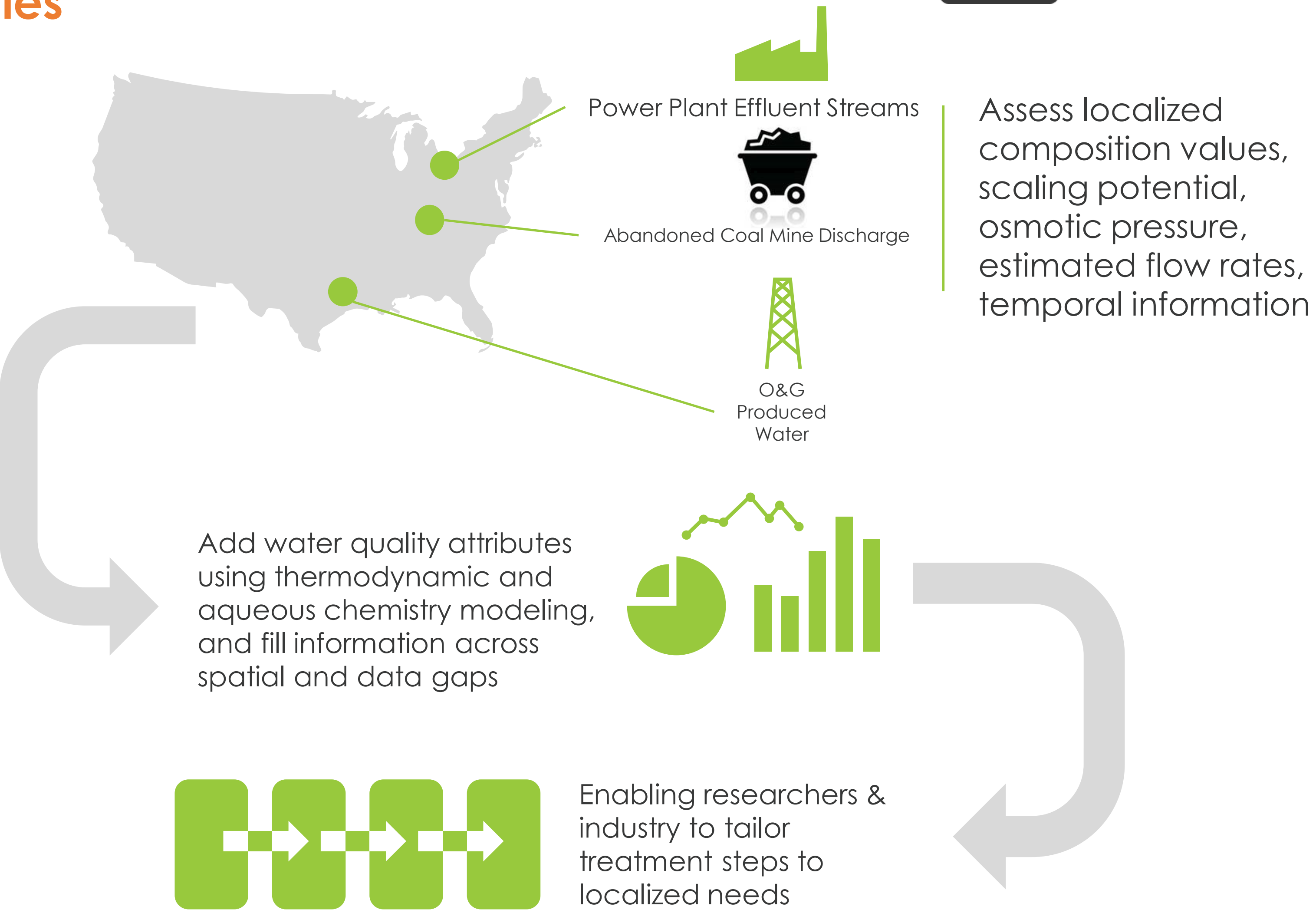
Solution: Develop a Nationwide Energy Wastewater Data System

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

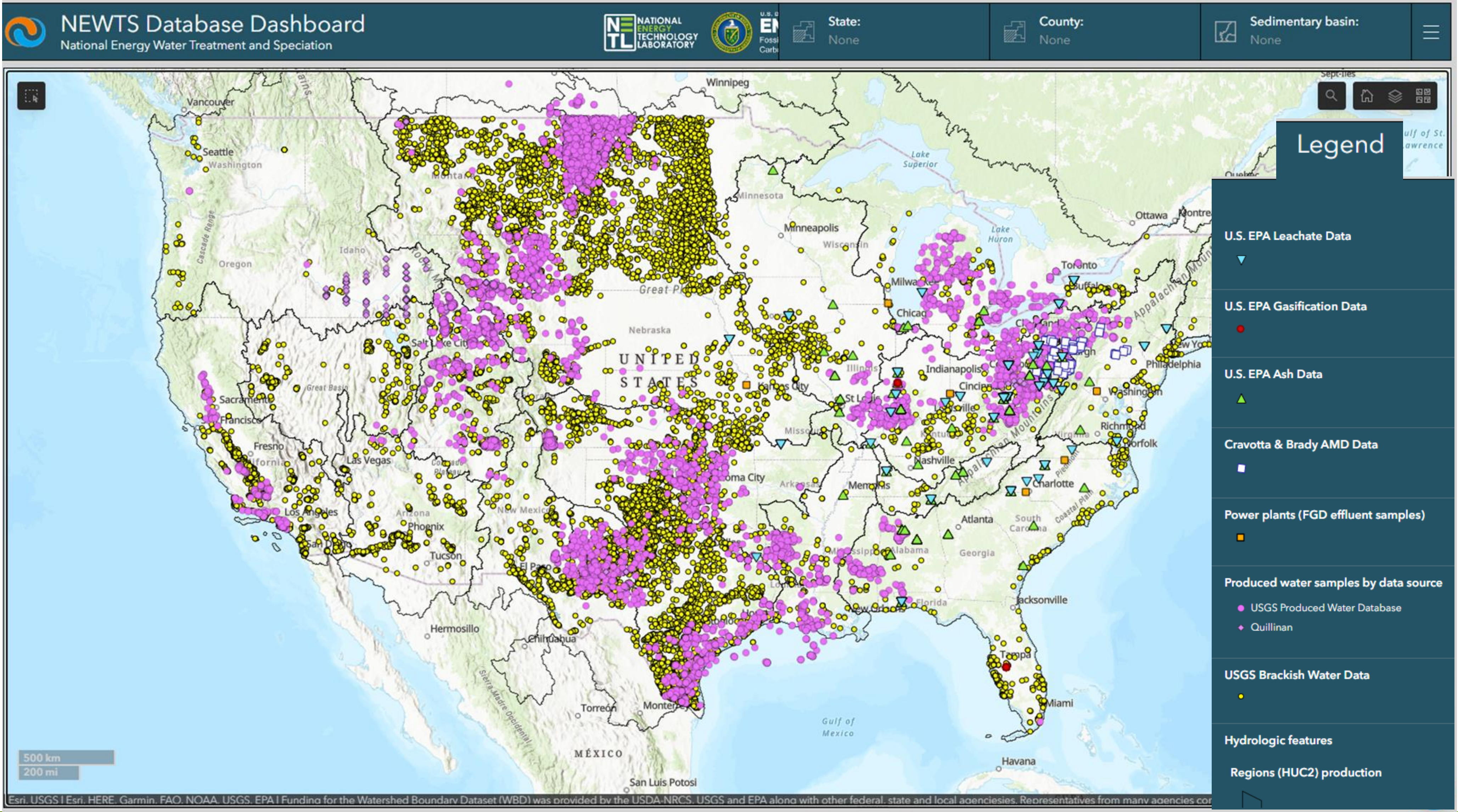
➢ Enables **<u>design of localized treatment</u>**

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

Energy Data exchange



NEWTS Federal Level Dashboard



Enables data visualization, exploration, and download

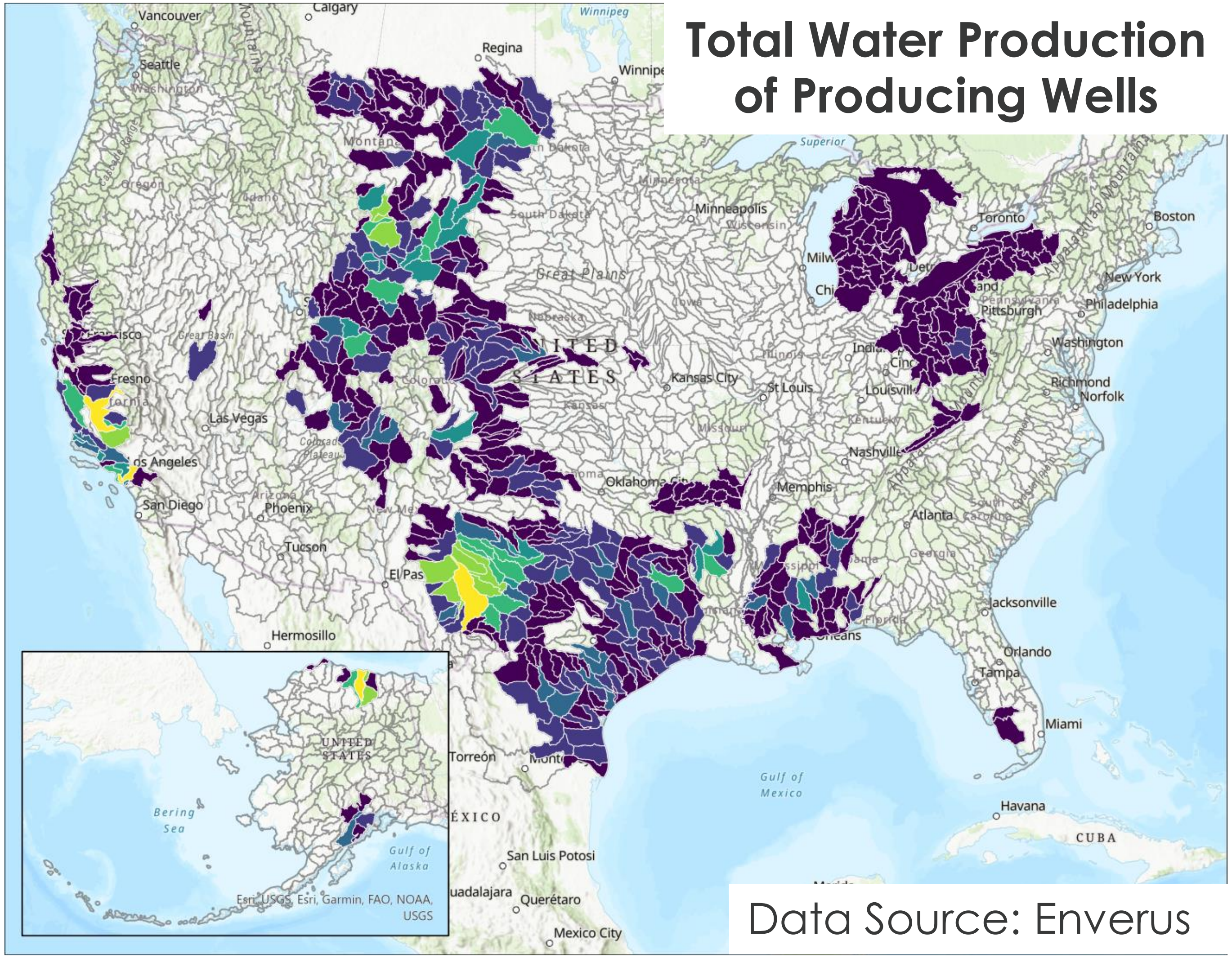
Integrating Water Volume Data

- 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

Total Water Production of Producing Wells

Millions of Barrels of Water

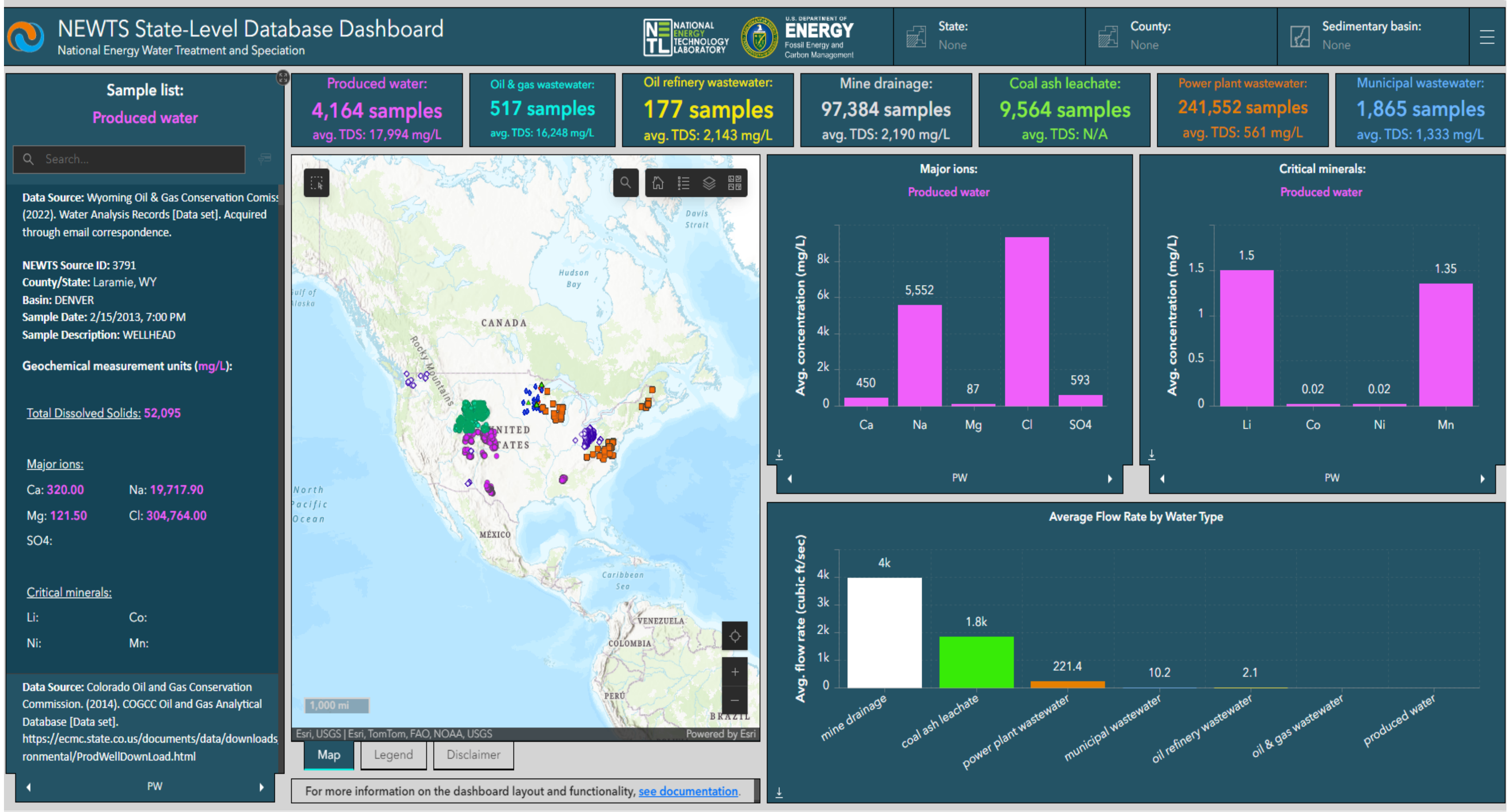
Dark purple	< 100
Purple	100 – 500
Blue	500 – 1,000
Teal	1,000 – 2,000
Green	2,000 – 5,000
Light green	5,000 – 10,000
Yellow	10,000 – 21,370



Data Source: Enverus

New! NEWTS State-Level Dashboard

Visualization tool for energy-related waste streams

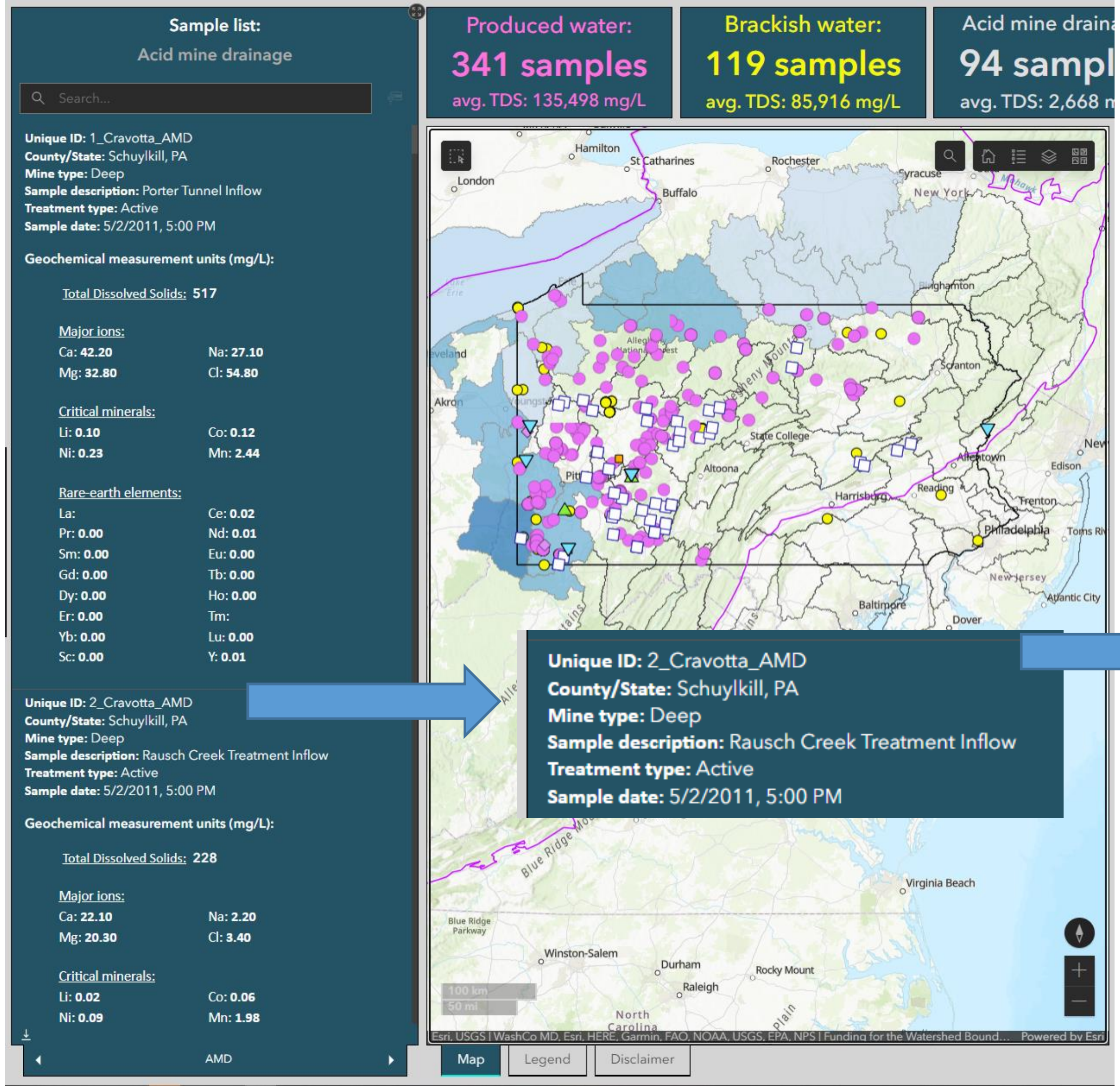


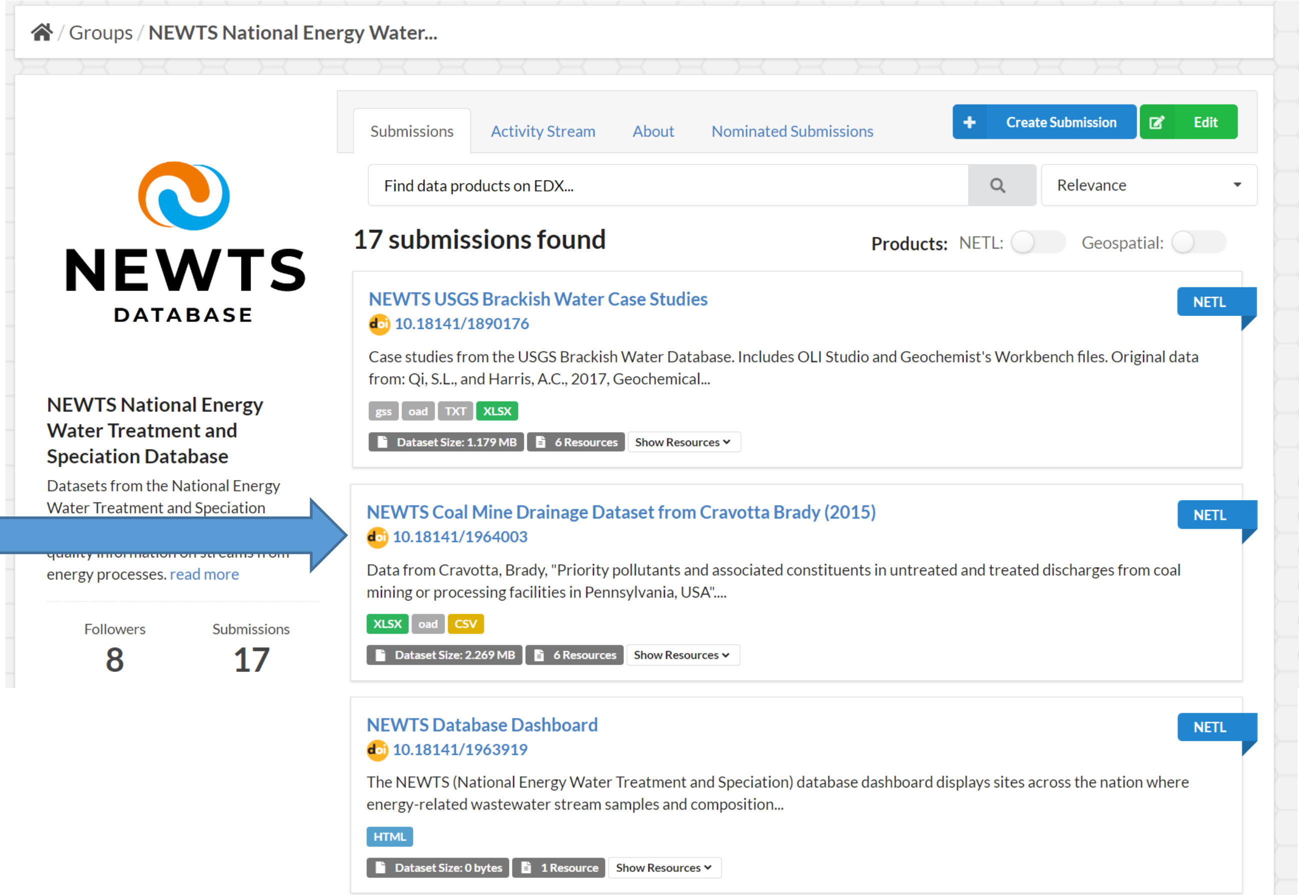
- 360,000+ samples
- Data from state agencies, industry, & localized research projects
- Aggregated using python & attribute mapping schema
- Water types:
  - produced water
  - oil & gas
  - mine drainage
  - power plants

NEWTS State-Level Dashboard NEWTS Dashboard Storymap

Connecting NEWTS Dashboard to the Database

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





Connecting NEWTS Dashboard to the Database

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

NEWTS Coal Mine Drainage Dataset from Cravotta Brady (2015)

doi 10.18141/1964003

License(s):
License Not Specified

Data from Cravotta, Brady, "Priority pollutants and associated constituents in untreated and treated discharges from coal mining or processing facilities in Pennsylvania, USA". Applied Geochemistry, 2015. https://doi.org/10.1016/j.apgeochem.2015.03.001

Dataset includes information on water quality composition including inorganic compounds from untreated and treated streams of coal-mine discharge from coal mining and coal processing locations. Data is provided in the original version as well as in a summarized version for easy input into aqueous chemistry modeling software.

Followers: 0

+ Follow

- 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		[illegible]flow	Rausch Creek Trea	Si
MINE_NUM		Some Mines have multiple Streams			1	2	
STAID		Station identifier used by US[illegible]			4.03619E+14	4.03748E+14	
Lon_dd					40.60056	40.62994	
Lat_dd					-76.50583	-76.55399	-
Mine_Type					Deep	Deep	D
Pas[illegible]					Active	Active	P
[illegible]					CaO	CaO	W
[illegible]flow_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

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

	D	E	F	G	H	I	J	K	L	
4	State			Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar	Pennsylvar	Penr
5	State Code			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 Diss	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	48.76859	38.07548	11.4926	26.0832	40.
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

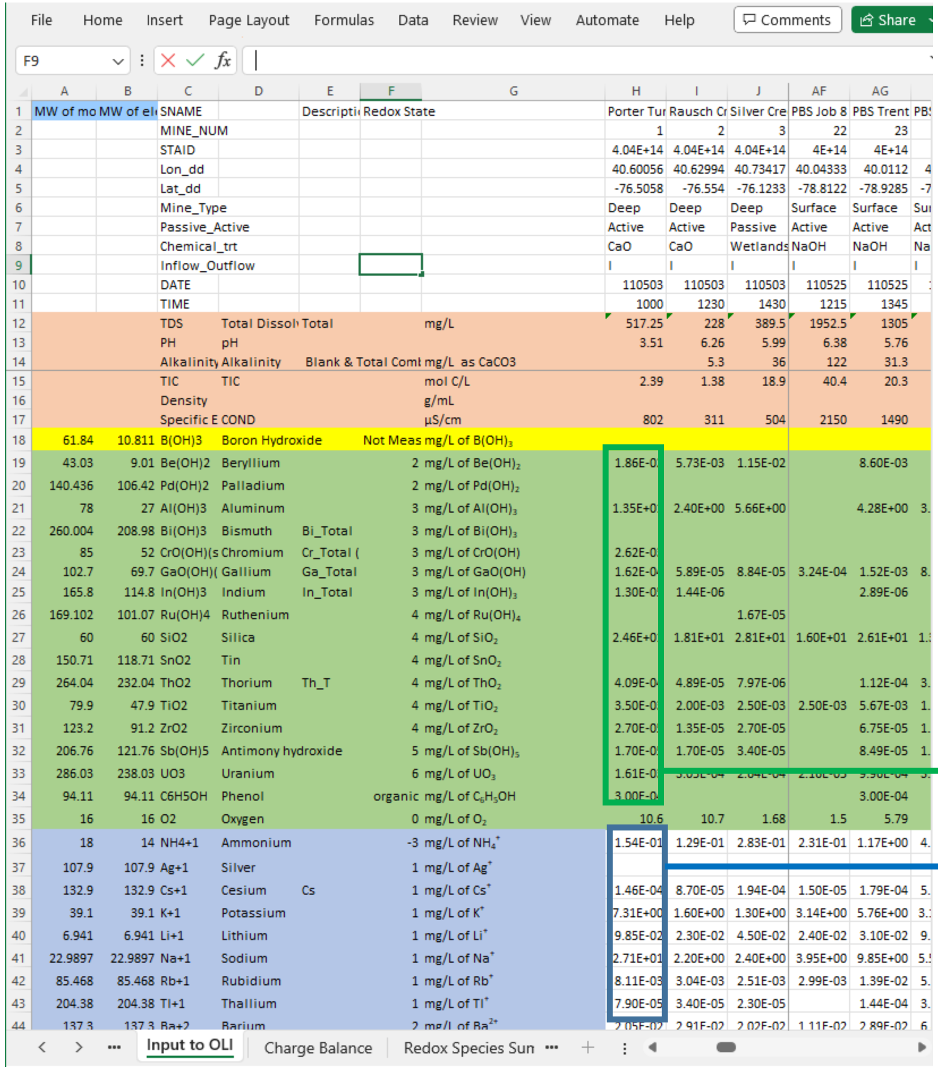
Templates to easily input into GWB Geochemist's Spreadsheet (GSS)

		1
Sample ID		
pH		
Carbonate alkality	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	

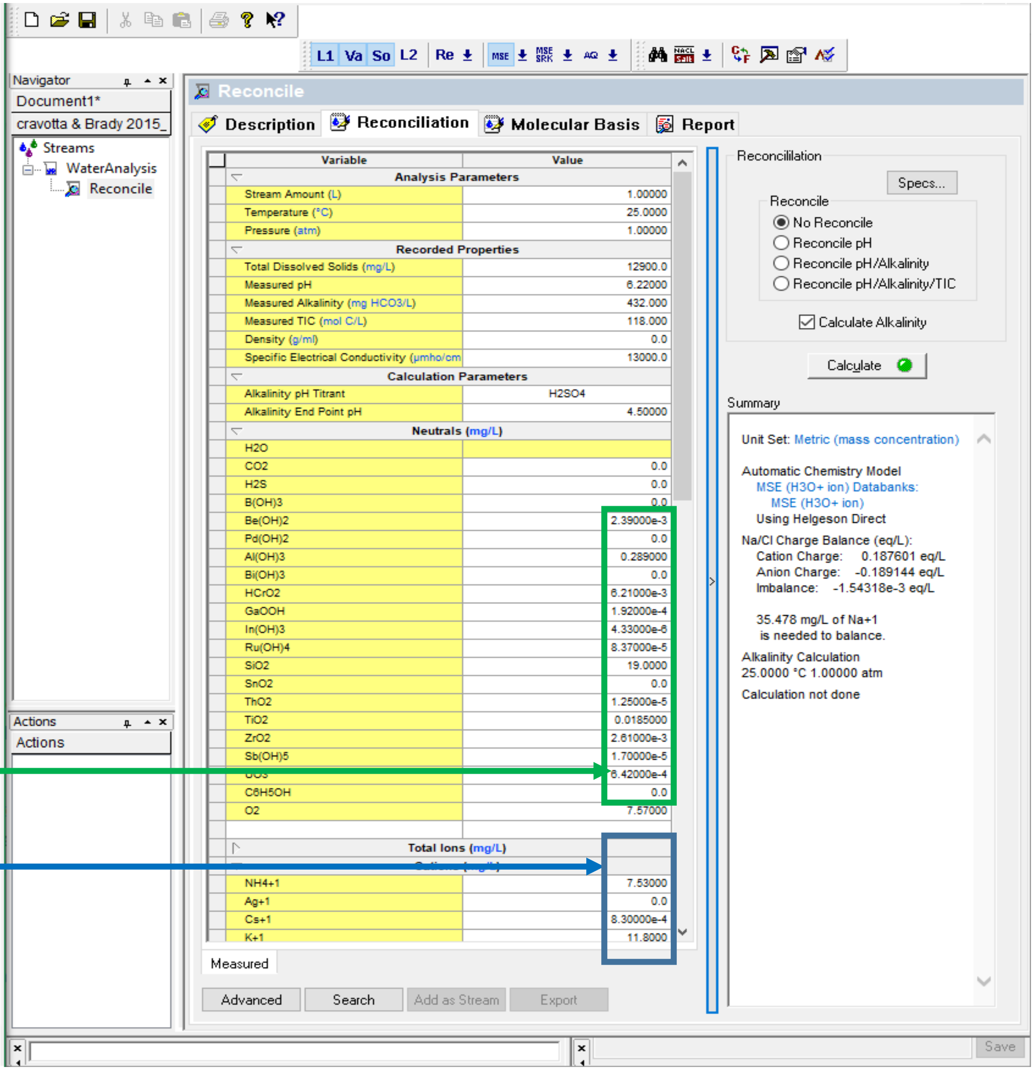
+ sample

Ease of Input into Aqueous Chemistry Software

NATIONAL ENERGY TECHNOLOGY LABORATORY

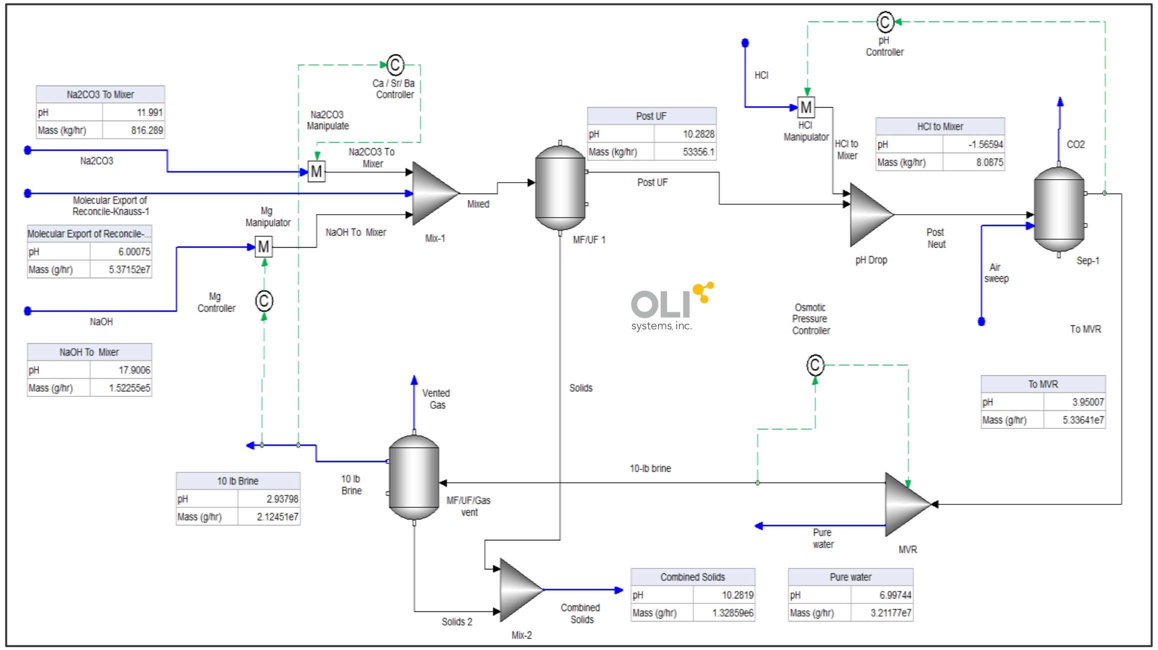


Templates to easily input into OLI Studio

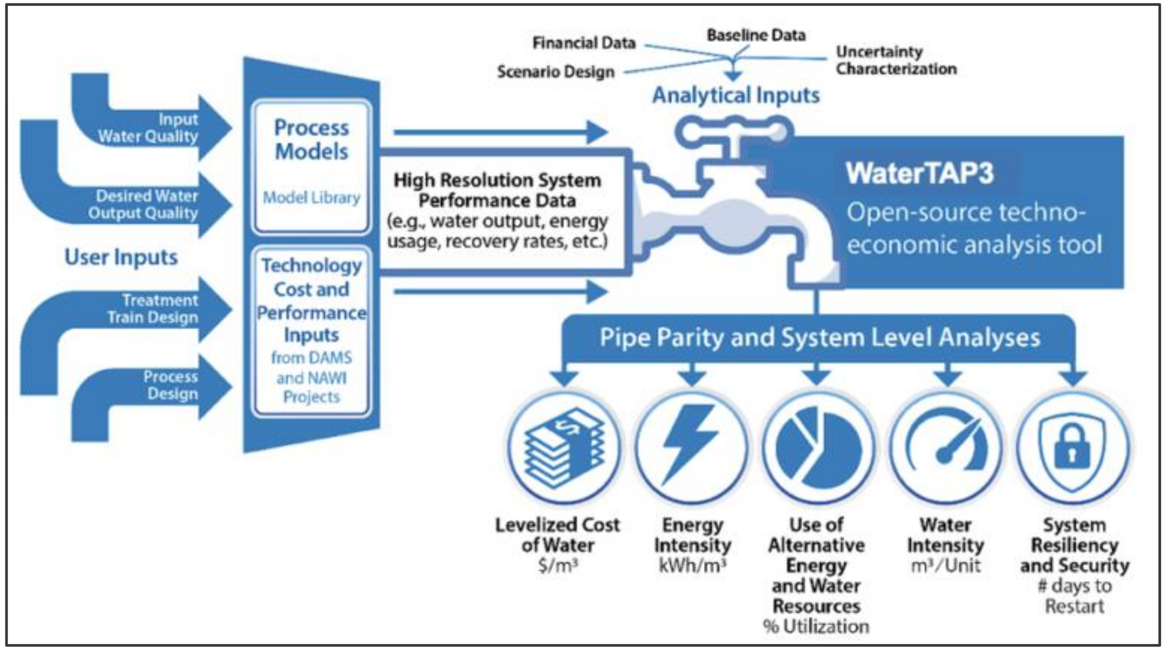


Integration with Modeling Software

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

Data Catalog and Citing Datasets with DOI#'s

NATIONAL ENERGY TECHNOLOGY LABORATORY

	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/d OW-2009-0819-5640

- 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

Followers: 0

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Authors

Nicholas Siefert | Zineb BELARBI | Alison Fritz | Madison Wenzlick

Citation (Click to Copy)

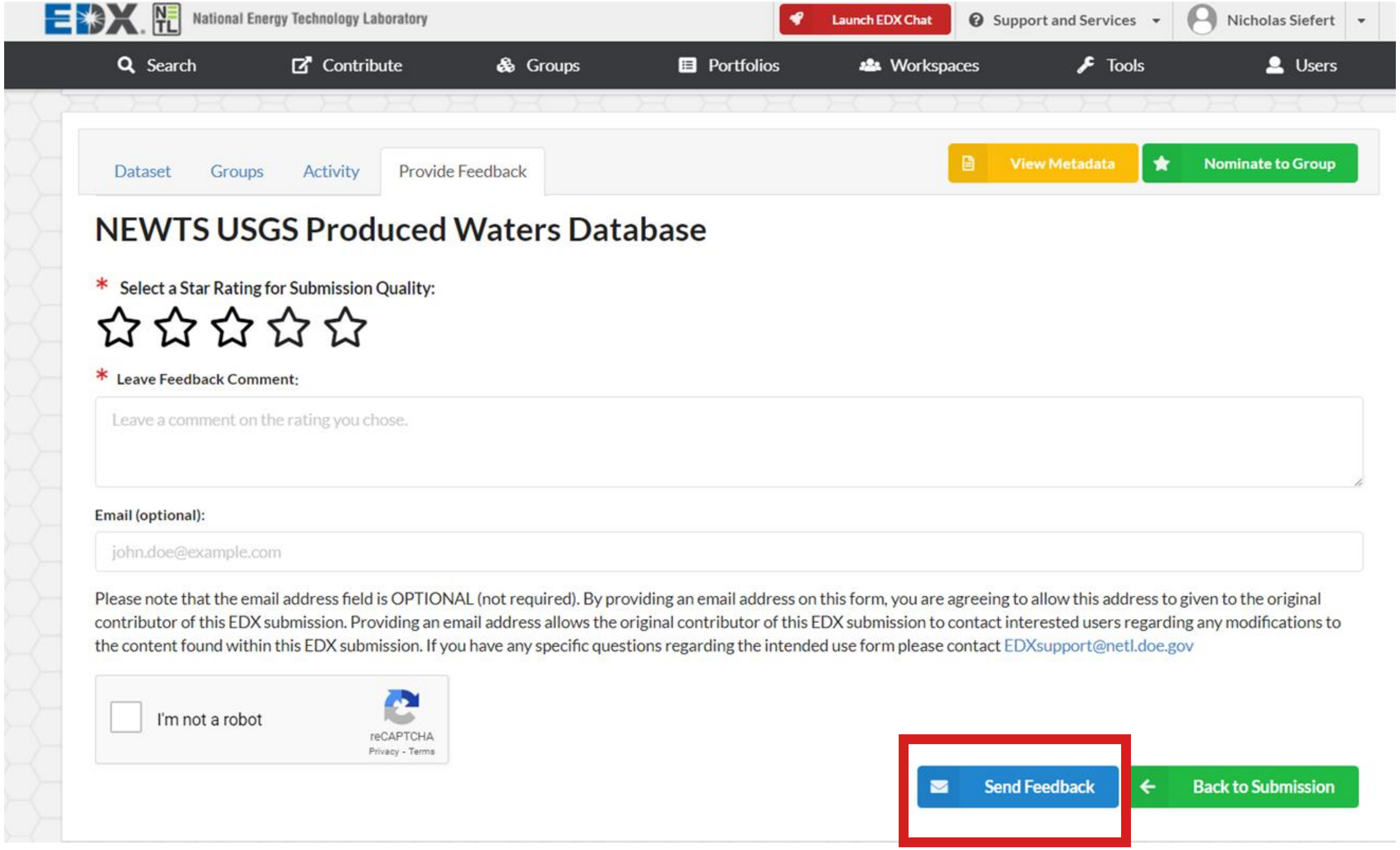
Nicholas Siefert, Zineb Belarbi, Alison Fritz, Madison Wenzlick, NEWTS EPA Leachate Case Studies, 1/13/2023, https://edx.netl.doe.gov/dataset/newts-epa-leachate-case-studies, DOI: 10.18141/1909011

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



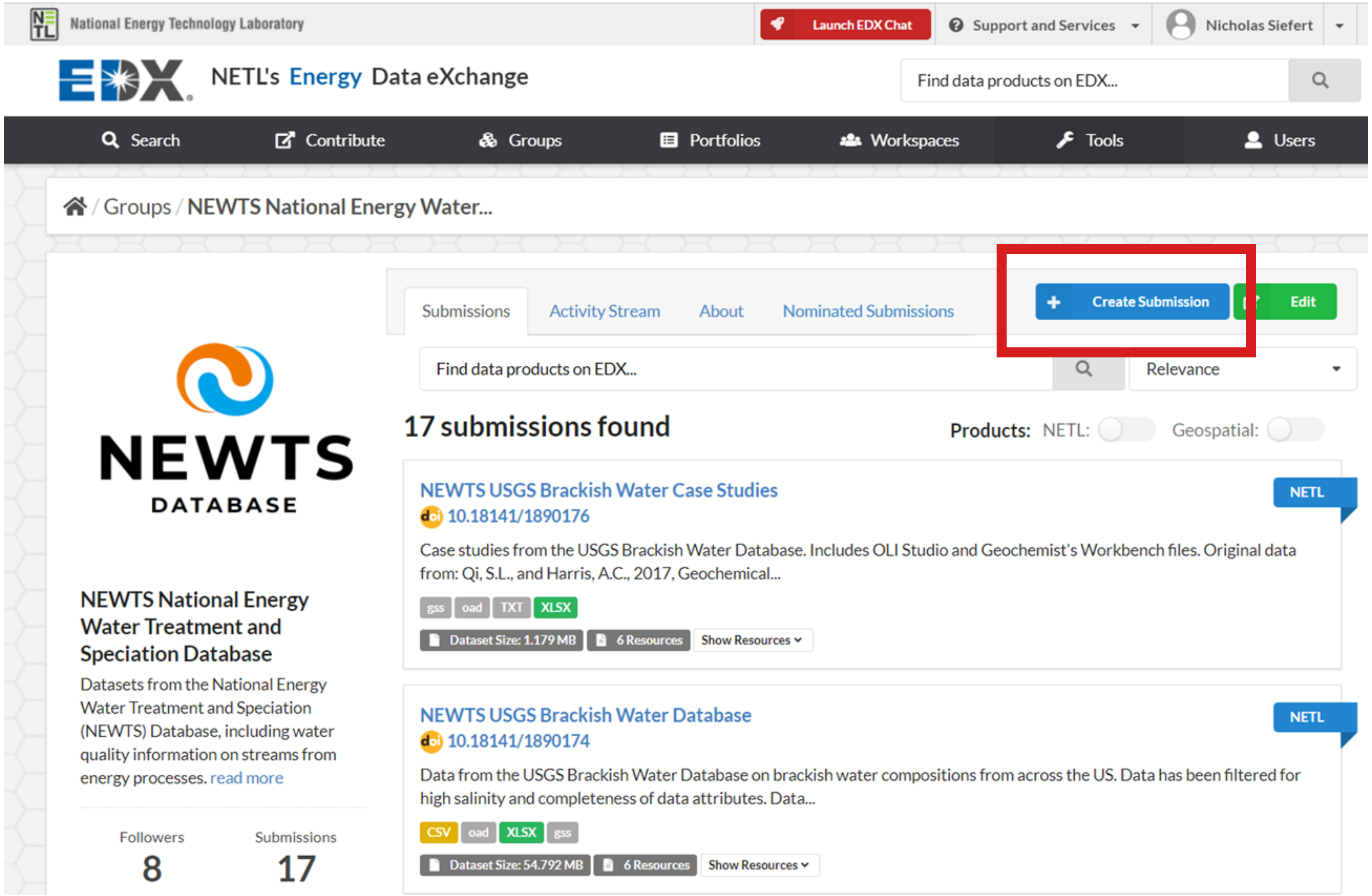
Creating Your Own Data Submission

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



NETL RESOURCES

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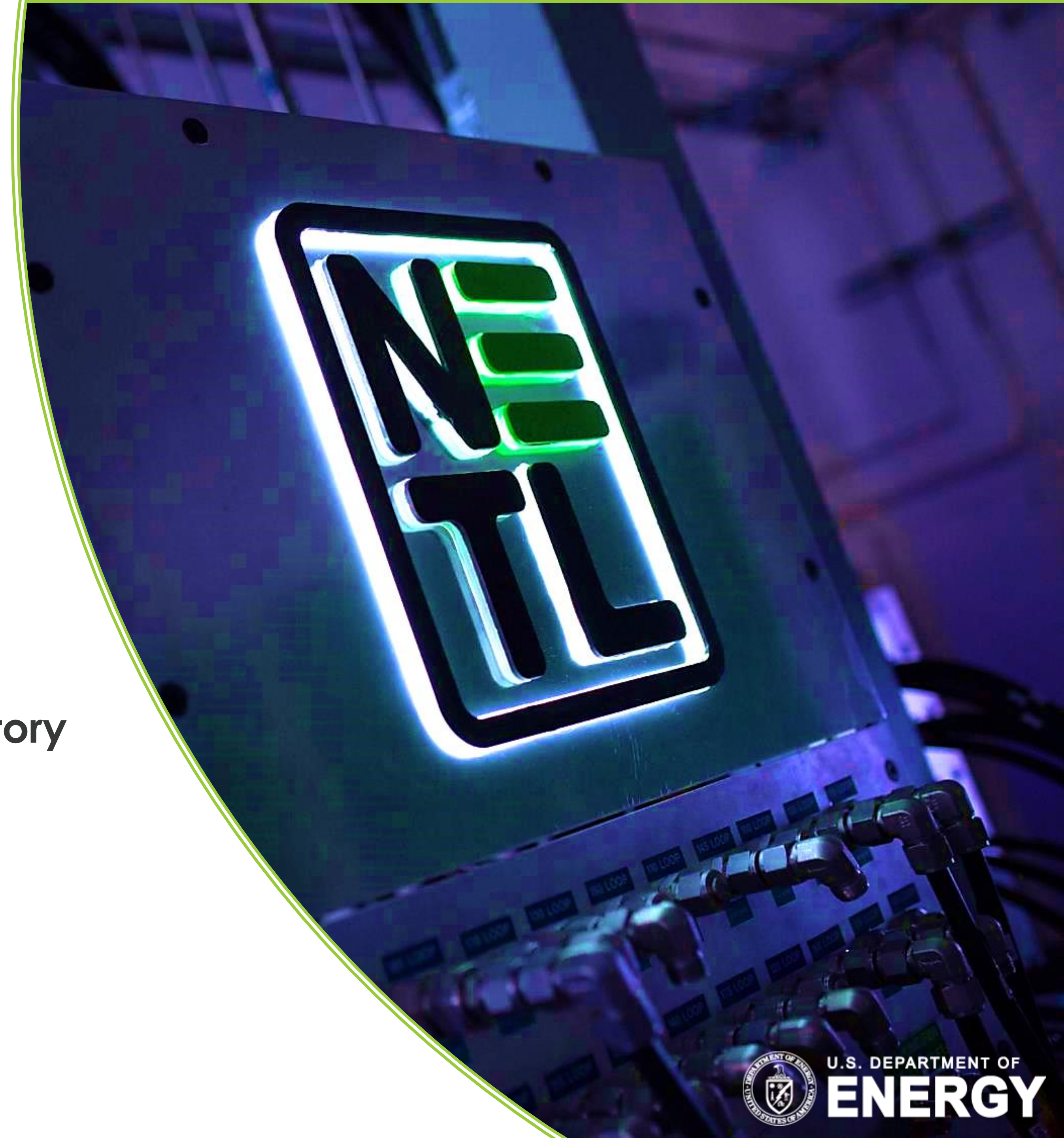
NEWTS
DATABASE

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



NEWTS Team & Contact Information

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[6]Carbon Capture Scientific, 2940 Industrial Blvd, Bethel Park, PA, 15102, USA

Task#5: Metrics Development

Developed Mission Metrics

Developing meaningful water program metrics that will resonate with stakeholders

Emissions-Reduction
- Tons CO_2 abated
- Energy Savings/ CO_2 per kWh
- CO_2 per kg of hydrogen
- Water Consumption/Usage Savings

Economic Impact
- Exports
- Impact to GDP
- Reduction in cost of water / $$ savings from efficiency gains
- Reduced Downtime

Environmental Justice & DEIA
- Social & environmental impact to disadvantaged communities
- Workforce development
- Access to clean and safe water / clean water production
- Collabs with underserved communities
- Increased energy resiliency and democracy

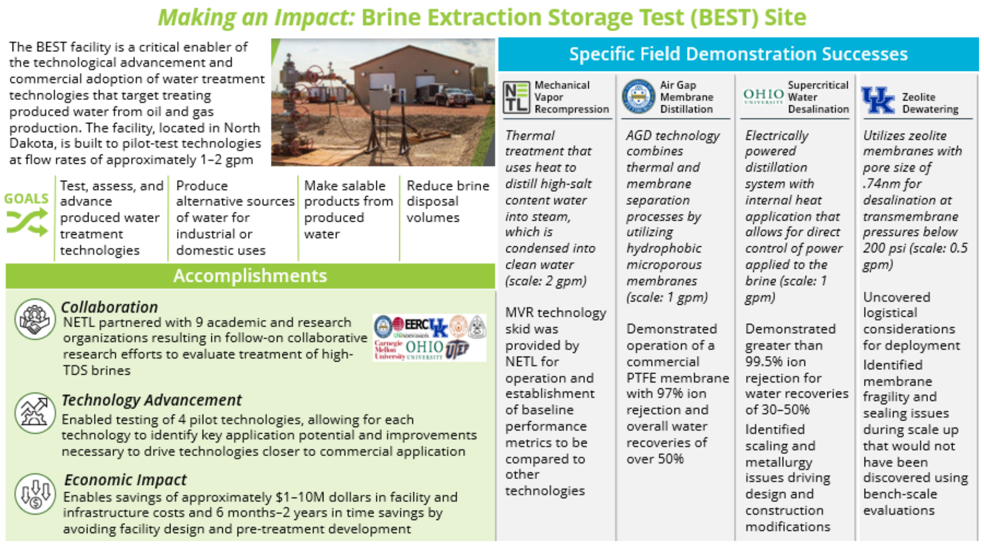
American Jobs
- Developing STEM Workforce
- Jobs supported
- Upskilling workforce

Collaboration and Program Interoperability
- Trainings given
- University partnerships
- Industry partnerships
- Knowledge transfer via patents, publications and conferences
- Deployment/use of demonstration test-beds

Water Infrastructure
- Modernization of water infrastructure
- Power Plant system improvements
- Improving availability

Applied to Projects

Applied metrics to RIC project to communicate accomplishments and utilize as template for communicating successes of projects across the program



***Making an Impact:* Brine Extraction Storage Test (BEST) Site**

The BEST facility is a critical enabler of the technological advancement and commercial adoption of water treatment technologies that target treating produced water from oil and gas production. The facility, located in North Dakota, is built to pilot-test technologies at flow rates of approximately 1–2 gpm

GOALS
- Test, assess, and advance produced water treatment technologies
- Produce alternative sources of water for industrial or domestic uses
- Make salable products from produced water
- Reduce brine disposal volumes

Accomplishments

Collaboration
NETL partnered with 9 academic and research organizations resulting in follow-on collaborative research efforts to evaluate treatment of high-TDS brines

Technology Advancement
Enabled testing of 4 pilot technologies, allowing for each technology to identify key application potential and improvements necessary to drive technologies closer to commercial application

Economic Impact
Enables savings of approximately $1–10M dollars in facility and infrastructure costs and 6 months–2 years in time savings by avoiding facility design and pre-treatment development

Specific Field Demonstration Successes

Mechanical Vapor Recompression	Air Gap Membrane Distillation	Supercritical Water Desalination	Zeolite Dewatering
Thermal treatment that uses heat to distill high-salt content water into steam, which is condensed into clean water (scale: 2 gpm)	*AGD technology combines thermal and membrane separation processes by utilizing hydrophobic microporous membranes (scale: 1 gpm)*	*Electrically powered distillation system with internal heat application that allows for direct control of power applied to the brine (scale: 1 gpm)*	*Utilizes zeolite membranes with pore size of .74nm for desalination at transmembrane pressures below 200 psi (scale: 0.5 gpm)*
MVR technology skid was provided by NETL for operation and establishment of baseline performance metrics to be compared to other technologies	Demonstrated operation of a commercial PTFE membrane with 97% ion rejection and overall water recoveries of over 50%	Demonstrated greater than 99.5% ion rejection for water recoveries of 30–50% Identified scaling and metallurgy issues driving design and construction modifications	Uncovered logistical considerations for deployment Identified membrane fragility and sealing issues during scale up that would not have been discovered using bench-scale evaluations

**1 of 2 infographics developed to communicate accomplishments of Water Management Program*

Task#5: DOE HQ Annual Accomplishments Report

Applied metrics across the entire program to communicate successes in the DOE Annual Accomplishments Report

Demonstrated
7 technologies

Launched
3 First-of-its kind digital tools

8,500 Downloads of digital tools utilized by

30 organizations 30 state agencies

Water Management Technology voted
Top 100
Private companies to make significant market impact

Technology enables single powerplant to capture
150M
gallons of water a year

Enough to provide water to
1,369
Average American households for a year

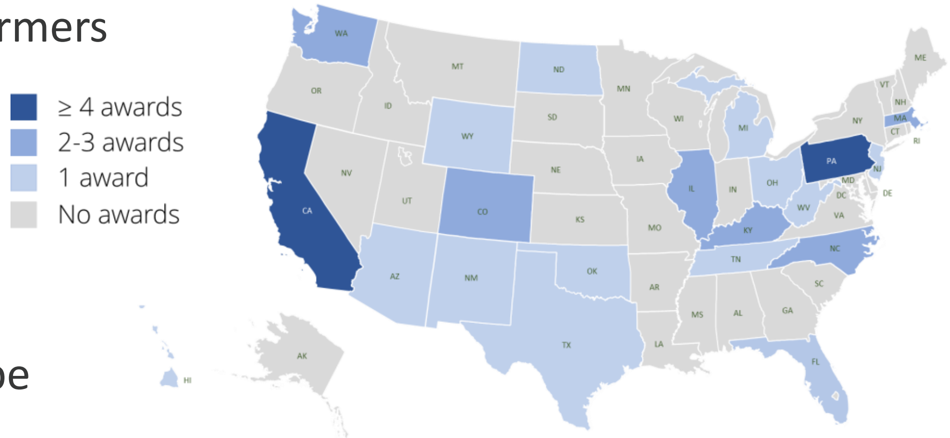
Upskilled and trained
115
Students, university faculty, and state and regulatory employees

NETL PI: Erik Shuster, Systems Analysis PI: Haleigh Heil

Task#5: Portfolio Analysis

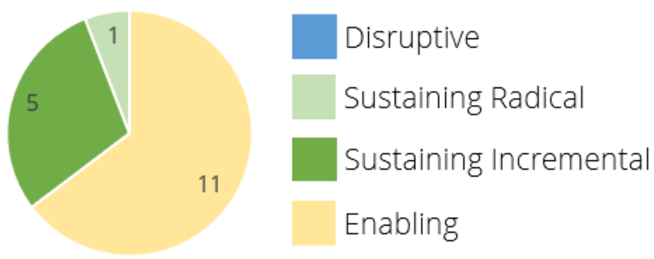
Conducted historical portfolio analysis of the Water Management Portfolio since 2018

Geographical Distribution of Performers

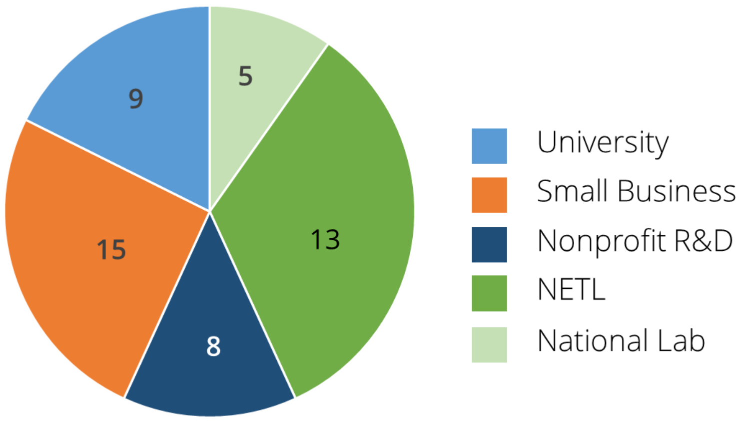


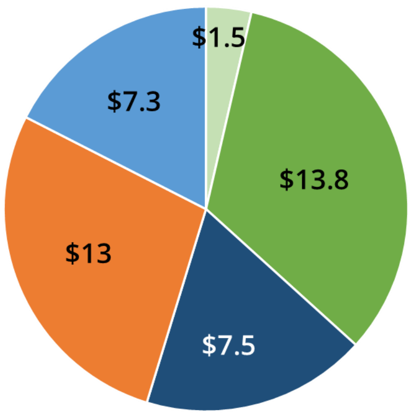
Development Horizons and Technology Types

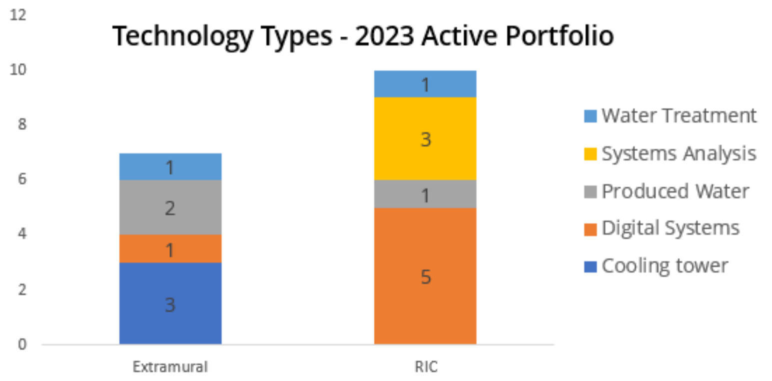
Current Portfolio (As of 8/21/23)



DOE Investment by Performer Type







Back-up Slides for Conference Proceedings

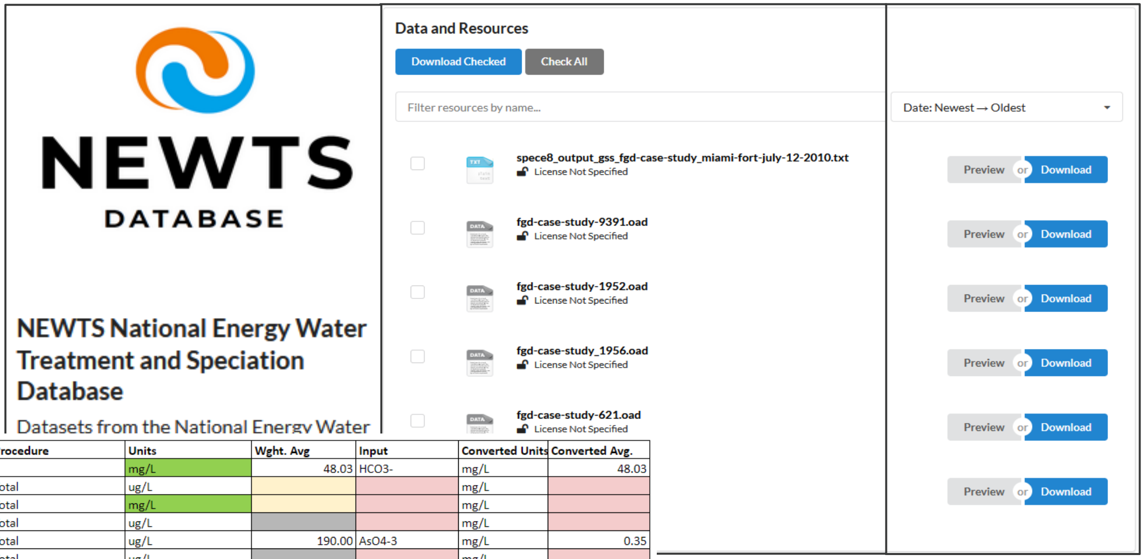
Integration with Modeling Software

Leveraging tools for filling data gaps & modeling treatment

NATIONAL ENERGY TECHNOLOGY LABORATORY

<u>Integrating data streams</u> 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

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-}	

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

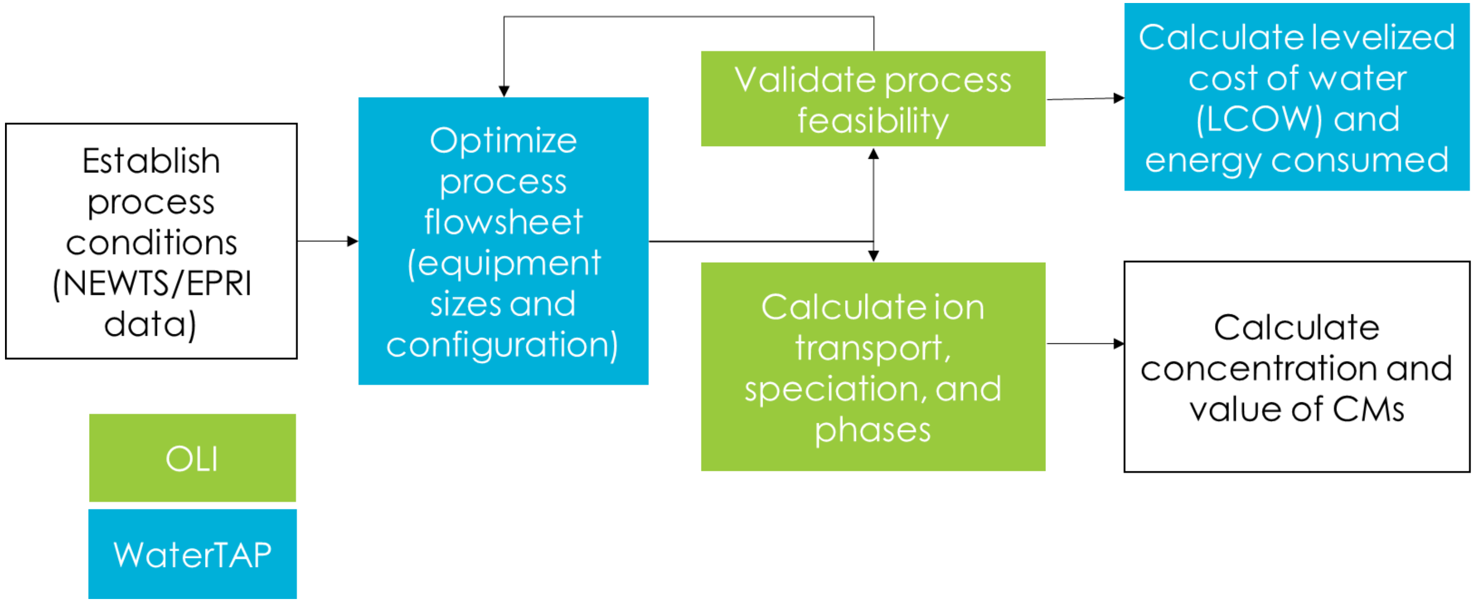
Kinetic induction time for scaling can be estimated for Barite, Gypsum, Calcite, and Celestine with others (silica) likely in the future

Task 2: Treatment and Byproduct Recovery Baseline for Leachate and Produced Waters

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

To understand the performance improvements of new technologies, it is important to develop a baseline.

- Calculated median composition data for leachate and produced water
- Developed performance and cost estimates for landfill and impoundment leachate and produced water



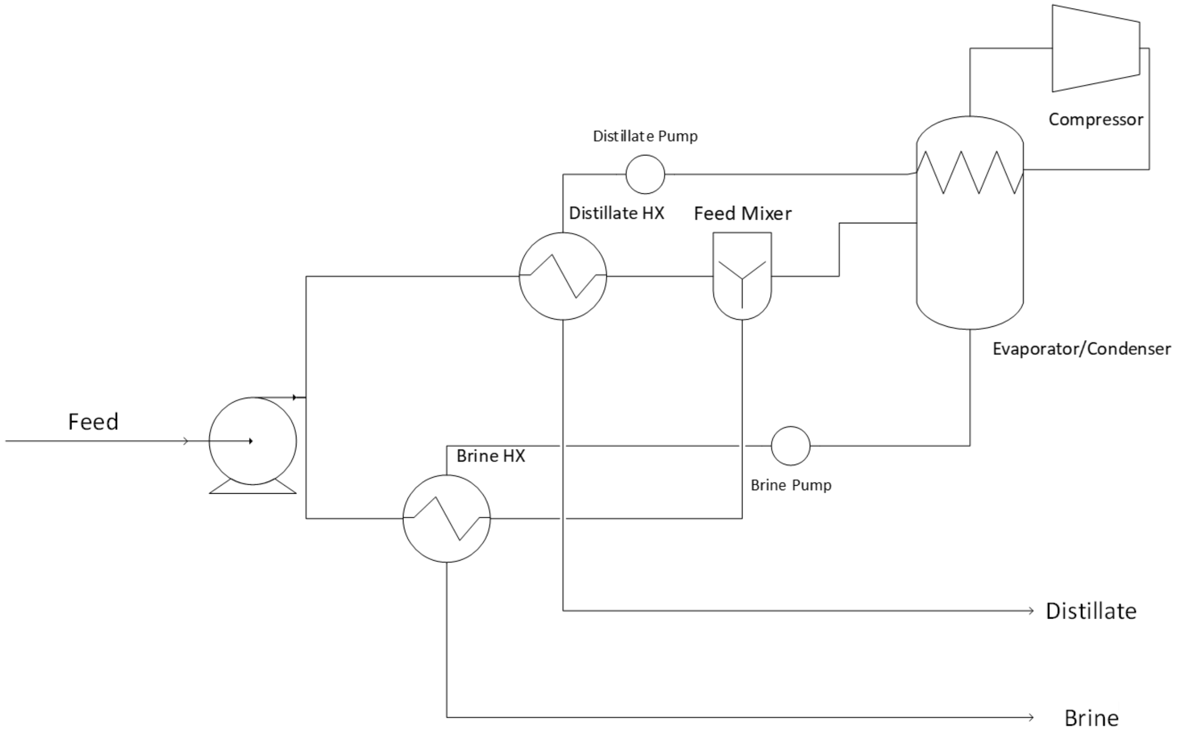
NEWTS USGS Produced Water Database Compositions, key parameters adjusted using CoDaRT

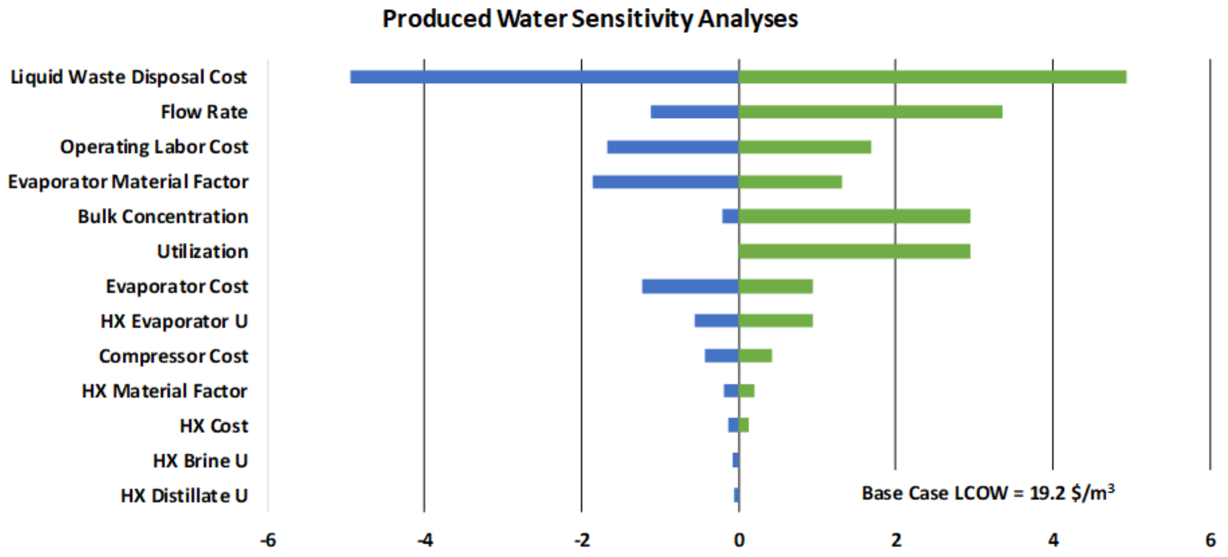
Parameter Name	Median Value	ML-Adjusted Value
TDS, mg/L	101,336	
Ammonia, mg/L	96	
Barium, mg/L	2.355	
Boron, mg/L	19.51	
Bicarbonate, mg/L	231.005	
Bromine, mg/L	224	
Calcium, mg/L	3,127.5	
Carbonate, mg/L	48.885	
Chlorides, mg/L	59,200	59,200
Iodine, mg/L	10	
Iron, mg/L	21	
Lithium, mg/L	10.75	9.22
Magnesium, mg/L	889.115	895.13
Manganese, mg/L	0.885	
Potassium, mg/L	402.87	
Silicon, mg/L	12	
Sodium, mg/L	31,275	31,055
Strontium, mg/L	123.755	
Sulfate, mg/L	1,438.375	

Task 2: Treatment and Byproduct Recovery Baseline for Leachate and Produced Waters

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

Mechanical vapor compression was selected for produced water treatment based on a literature review.





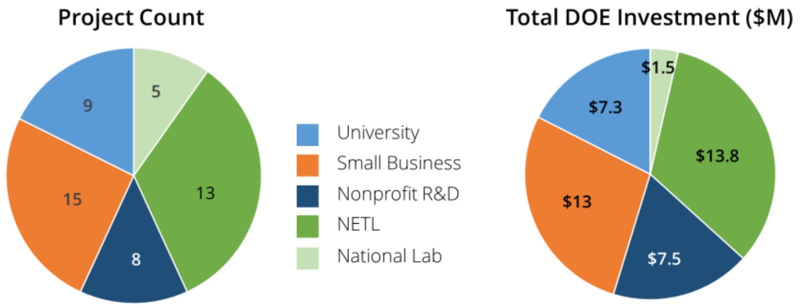
Preliminary Results

The levelized cost of water (LCOW)was calculated for this system. A sensitivity analysis shows the LCOW is heavily dependent on liquid waste disposal.

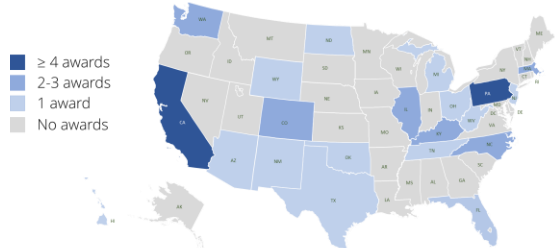
Task#5: Portfolio Analysis

Conducted historical portfolio analysis of the Water Management Portfolio since 2018

DOE Investment by Performer Type

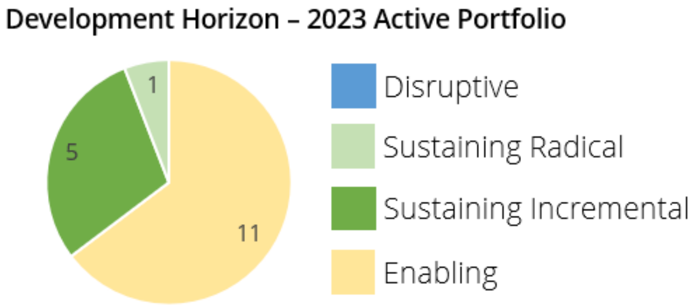


Geographical Distribution of Performers

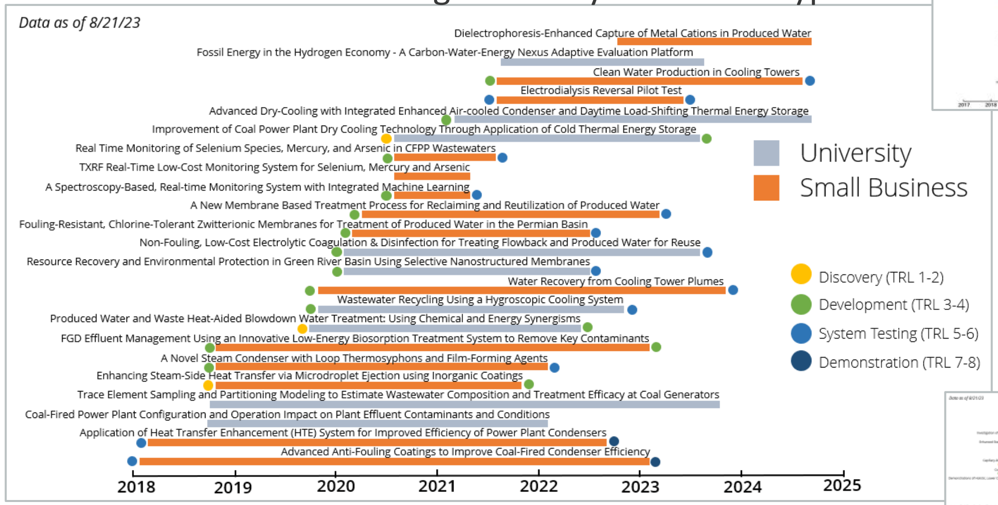


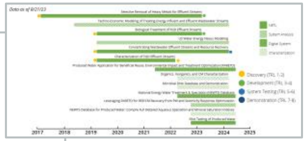
Development Horizons and Technology Types

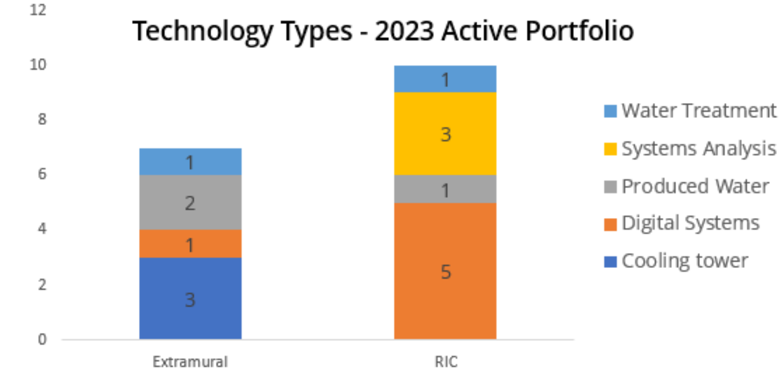
Current Portfolio (As of 8/21/23)



TRL Progression by Performer Type







NETL PI: Erik Shuster, Systems Analysis PI: Haleigh Heil

Task#5: R&D Portfolio Strategy

NATIONAL ENERGY TECHNOLOGY LABORATORY

Developed paper of R&D Portfolio Strategy best practices

1 Introduction

Many research and development (R&D) programs, particularly those focused on foundational technology advancement in complex, dynamic sectors, must navigate through a lot uncertainty and a market fog of war [1]. Various converging variables, including market, societal, political, technological, and organizational factors contribute to this complexity. Many innovations encounter adoption inertia that stem from slow policy and regulation development, expensive retrofitting of legacy infrastructure, and a high degree of technology integration and can result in a technology succumbing to the "Valley of Death". Not only do R&D organizations have to react and interact with these evolving external factors, but they must also manage complex internal dynamics. Given these challenges, there is a need for organizations to develop and nurture internal innovation ecosystems to support navigating these complexities.

An innovation ecosystem, as defined by Grandstrand and Holgersson in their 20-year review of the term, is the "evolving set of actors, activities, and artifacts, and the institutions and relations, including complementary and substitute relations, that are important for the innovative performance of an actor or a population of actors" [2]. In other words, dynamic networks of individuals, resources, entities, and the complementary or substitute interactions between them that catalyze new products, processes, systems, or markets altogether. There can be multiple innovation ecosystems in an industry or dynamic market, and an organization can find itself to be one innovation ecosystem among many.

Recognizing this concept and acknowledging that technology development in dynamic industries requires a convergence of both internal and external ecosystems can guide R&D managers in crafting program and portfolio strategies that not only align with organizational priorities, but also effectively leverage expansive networks. In order to effectively leverage these networks, R&D programs must deeply understand their own operational dynamics and capabilities to nurture their internal innovation ecosystems. One way this can be achieved is through undertaking regular, comprehensive portfolio analyses. This is also critical for benchmarking, allowing a program to measure performance against key metrics, understand and address capabilities gaps, leverage synergies across the organization, and avoid redundancies. The following paper outlines several key elements for conducting an analysis of an organization's portfolio and shaping a portfolio strategy. These elements, while not prescriptive, offer a set of suggestions intended to guide strategic thinking.

1. Setting Program Goals (see Section 2)
2. Defining Portfolio Ambitions (see Section 3)
3. Optimizing Internal Innovation and External Collaborations (see Section 4)
4. Tracking and Strategizing Investments Across Technology Readiness Levels (see Section 5)

The following sections will delve into these concepts, offering high level insight on facilitating these activities.

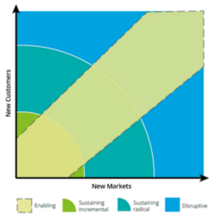
3 Defining Portfolio Ambitions

Developing a portfolio to be a collective group of investments that are complementary and represent the right balance of risk and reward is necessary to ensure technology progression is taking place. This supports an organization in achieving goals through thoughtful diversification of short-/long-term initiatives, high/lower risk initiatives, and high/lower spend initiatives.

Various takes on the definitions and scales for innovation, such as Tushman and Anderson's "incremental" versus "breakthrough" technology [3], Clayton Christenson's "sustaining" versus "disruptive" theory [4], and Nagji and Tuff's "core," "adjacent," and "transformational" ambition definition [5], help describe the range of development horizons a long-term R&D program will typically spread initiatives against (see Exhibit 3-1):

- *Sustaining incremental*: initiatives close to core capabilities that make small, incremental changes to current capabilities, processes, or technologies
- *Sustaining radical*: initiatives that build on current capabilities and technology, but address adjacent markets or opportunities and have increased impact relative to *sustaining incremental*
- *Disruptive*: high-risk projects that, if successful, have the potential to transform the market

Exhibit 3-1. Range of development horizons



Adapted from Nagji and Tuff [5]

R&D programs may also possess a range of technologies or initiatives that do not fit within the conventional categorization of the technology readiness level (TRL) scale (see Exhibit 5-2). Enabling technologies or initiatives support further technological, procedural, or system innovation. Examples include digital tools, software, database development, and applied or

4 Optimizing Internal Innovation and External Collaborations

To maximize technological advancements and financial resources, it is necessary to find the right balance of engaging in internal, proprietary innovation versus investing in external capabilities and partnerships. Research suggests organizations outsource at least 30 percent of R&D activities to ensure R&D is not happening in a vacuum and the organization is gathering insights from other perspectives and specialized knowledge from external sources [8]. If an organization is conducting most R&D activities in-house, they risk neglecting diverse perspectives and specialized knowledge. However, if they outsource the majority of their R&D to external entities, a large portion of their subject matter expertise, knowledge, or technology development no longer lives within the organization. The division of the innovation ecosystem—universities and labs specializing in research while corporations and businesses specialize in demonstration and scaling—has made it harder to bridge the gap from innovative research in the lab to successful, applicable technologies and products on the market [8]. Crafting a thoughtful strategy on how to engage the broader ecosystem is critical for leveraging external synergies, obtaining specialized skills and expertise, and orchestrating collaboration across innovation ecosystems.

How to Balance Internal Versus External Investment

Before determining what the ideal spread of internal versus external investment will look like, an organization needs to understand their current state. Compiling a robust inventory of current initiatives and having a strong understanding of organizational goals, core competencies, and how projects align to goals can support the identification of gaps or opportunities to meet the desired future state of the organization. Again, this will require individual assessment of the projects within the portfolio. The questions listed in Exhibit 4-1 can serve as a starting point in identifying organizational vision and objectives, core competencies, and future capability development/procurement.

Exhibit 4-1. Assessment questions

Organizational Vision and Objectives	• What is the primary mission and goal of the organization? • How do organizational R&D activities align with and support overarching organizational goals? • How do organizational goals and the corresponding R&D portfolio address broader societal needs and challenges?
Core Competencies	• What are the core competencies that define the organization and its activities? • What expertise and specialized skills do personnel possess that are critical to success? • What unique facilities, equipment, and knowledge does the organization possess that supports strategic goals?
Future Capability Development/ Procurement	• What complementary capabilities are required to achieve goals that do not currently exist within the organization? • What gaps exist in the technology areas/initiatives/programs of the organization?