Woodard & Curran

Automated Tools for Optimizing Groundwater Monitoring Programs

"Big Data" in Groundwater optimization

Victoria Ward

September 12, 2023

Objective

Reduce the number of wells routinely sampled at long-term monitoring Sites.

Automated Resources

- Data wrangling,
- Mann-Kendall trends,
- List of nearby wells screened at a similar interval,
- Summary Statistics that include comparison to regulatory standards,
- Extent of degradation, and
- Contour optimization.

Automated Data Wrangling with R and Python

- Scripts were developed to:

query site databases,

convert results to consistent units,

select the most representative result across multiple analyses and field duplicates,

calculate temporal averages,

calculate totaled values (e.g., Total VOCs),

convert concentrations to molarity, and

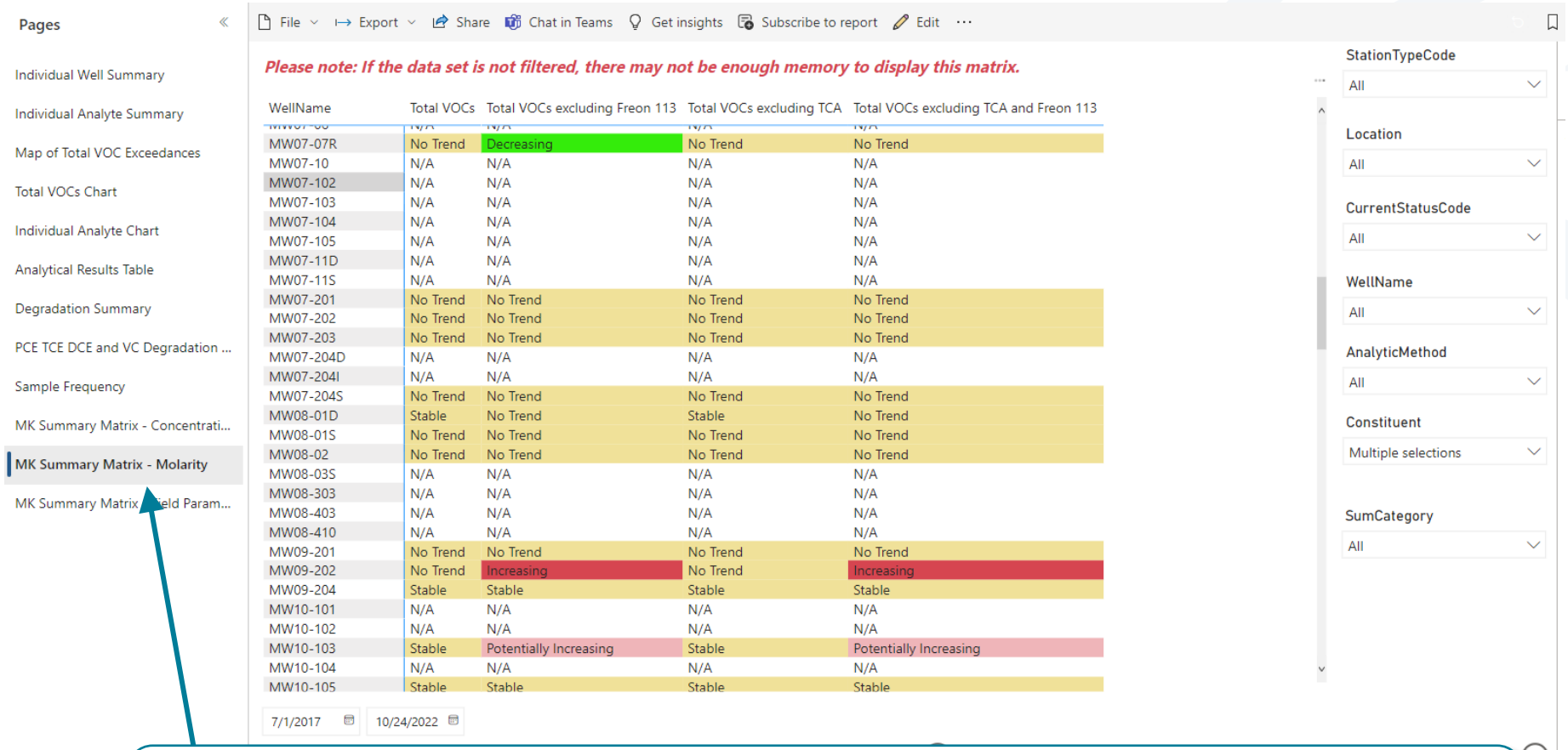
generate an output file that facilitated use of Power BI for calculations and visuals.

Automated Data Wrangling with R and Python

Scripts distributed via Woodard & Curran Github!

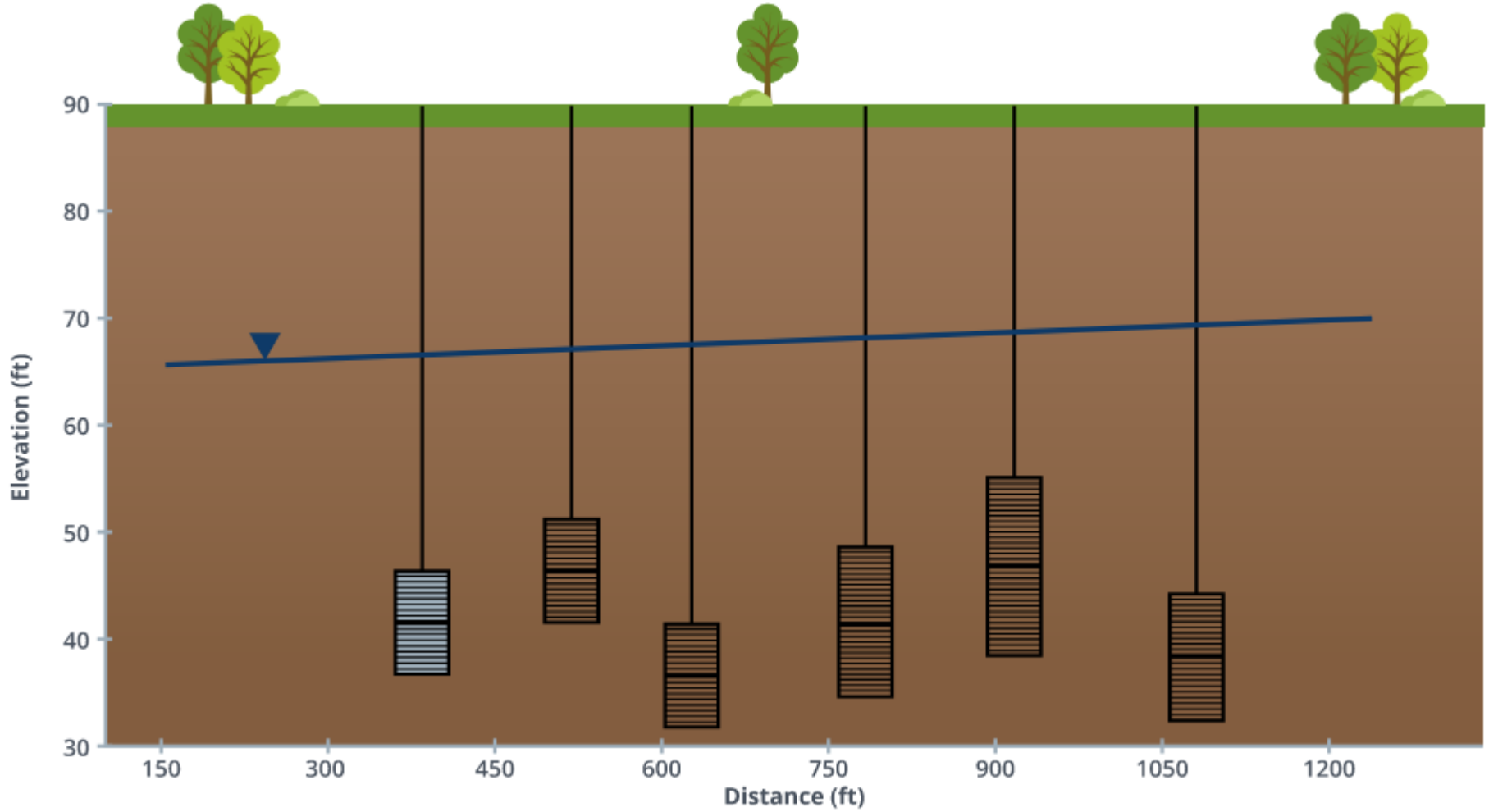
Mann Kendall Trends

(Mann Kendall automation presented at ICEDM 2022)



For total VOCs, the trends were assessed based on the totaled mass of analytes instead of concentrations.

Nearby Wells with Similar Screen Interval



Nearby Wells with Similar Screen Interval

Used an R script to return the following information:

- Nearest Active Well
- The distance to that well
- The screen interval of that well (to easily double check it overlaps)
- The number and names of active wells within 50 ft
- The number and names of all Site wells that have been within 50 ft

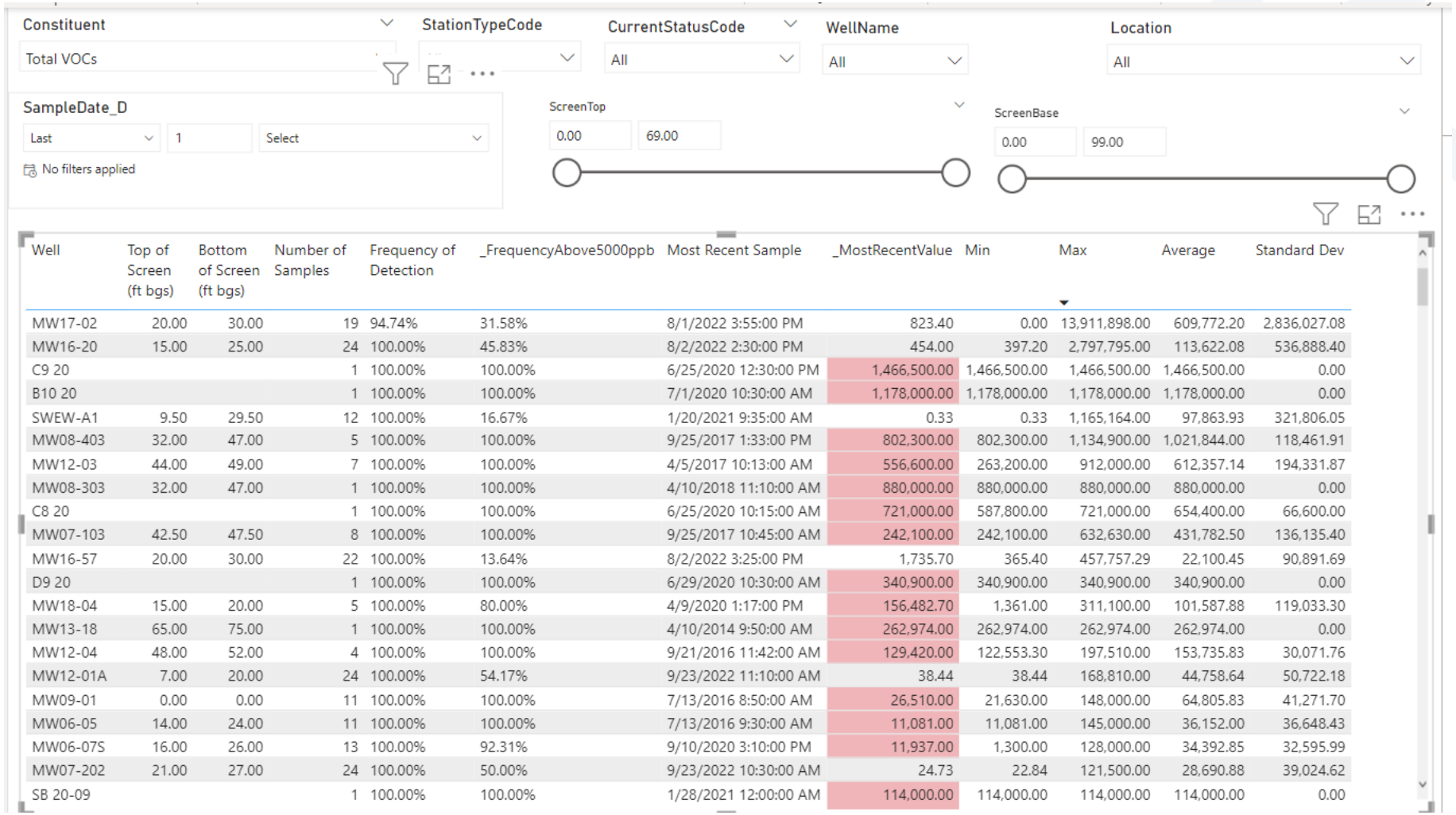
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	OldName	Location_CX	Location_CY	GroundElevation	ScreenedElevation	ScreenTop	ScreenBase	NearestActiveWell	DistanceToNearestActiveWellFt	NearestActiveWellScreenInterval	NumActiveWellsIn50ft	ActiveWellsIn50ft	NumWellsIn50ft	WellsIn50ft
3	GZ-104	712702.75	3047559.32	129.02	(89.02 - 84.02 ft)	40	45	MW14-01	511.0190225	30 - 55 ft (100.51 - 75	0	(ft)	0	(ft)
4	GZ-119R	712772.89	3047629.11	128.17	(83.17 - 78.17 ft)	45	50	MW15-12	744.1689775	45 - 50 ft (74.88 - 69.	0	(ft)	2	GZ-119 (7.66319124124669 ft), GZ-122 (35.4566242047828 ft)
5	MW07-06	712613.51	3047582.51	127.39	(97.39 - 92.39 ft)	30	35	NA	NA	NA	0	(ft)	0	(ft)
6	PP-4D	712757.97	3047589.54	127.46	(97.46 - 92.46 ft)	30	35	NA	NA	NA	0	(ft)	4	PP-2D (30.017438265215 ft), PP-1D (46.3832135584939 ft), PP 41.4322869268026 ft)
7	GZ-116	712828.11	3047629.57	127.32	(102.32 - 92.32 ft)	25	35	MW14-01	529.13517	30 - 55 ft (100.51 - 75	0	(ft)	1	PP-1D (47.3012219714629 ft)
8	GZ-103	712690.78	3047660.42	129.02	(89.02 - 84.02 ft)	40	45	MW14-01	418.2128885	30 - 55 ft (100.51 - 75	0	(ft)	0	(ft)
9	PP-6D	712752.82	3047608.81	127.73	(95.73 - 85.73 ft)	32	42	MW12-08B	786.9459916	37 - 47 ft (67.2 - 57.2	0	(ft)	1	MW02-13 (19.2135629180699 ft)
10	GZ-109	712710.94	3047712.73	129.37	(89.37 - 84.37 ft)	40	45	MW14-01	388.6297331	30 - 55 ft (100.51 - 75	0	(ft)	1	GZ-120 (42.9684372534382 ft)
11	GZ-106	712838.49	3047527.03	124.38	(84.38 - 79.38 ft)	40	45	MW14-01	613.1235276	30 - 55 ft (100.51 - 75	0	(ft)	0	(ft)
12	TGG-6	712796.29	3047717.93	NA	No GSE to calc elevation	10	20	MW92-9R	649.0061521	5 - 15 ft (121.06 - 111	0	(ft)	0	(ft)
13	MW01-02	712930.13	3047633.36	125.95	(90.95 - 80.95 ft)	35	45	MW07-204D	944.7819195	40 - 45 ft (62.95 - 57.	0	(ft)	1	MW01-01 (48.321157107947 ft)
14	GZ-115C	712740.52	3047627.69	128.45	(88.45 - 78.45 ft)	40	50	MW15-12	714.2421449	45 - 50 ft (74.88 - 69.	0	(ft)	4	GZ-119R (32.4011628651353 ft), MW99-4R (24.5151817248246 40.513149137247 ft)
15	MW01-01	712881.89	3047630.55	126.47	(91.47 - 81.47 ft)	35	45	MW07-204D	905.4975425	40 - 45 ft (62.95 - 57.	0	(ft)	2	MW01-02 (48.321157107947 ft), GZI-2 (45.5518600525936 ft)
16	MW02-12A	712746.00	3047589.55	127.87	(109.87 - 104.87 ft)	18	23	NA	NA	NA	0	(ft)	0	(ft)
17	GZ-108	712773.22	3047668.87	128.90	(88.9 - 83.9 ft)	40	45	MW14-01	462.8196017	30 - 55 ft (100.51 - 75	0	(ft)	2	GZ-120 (34.5121572782072 ft), GZI-4 (22.392829209546 ft)
18	GZ-120	712749.65	3047694.08	129.19	(89.19 - 84.19 ft)	40	45	MW14-01	428.3077181	30 - 55 ft (100.51 - 75	0	(ft)	2	GZ-109 (42.9684372534382 ft), GZ-108 (34.5121572782072 ft)
19	MW06-09	712708.50	3047592.57	128.27	(85.27 - 80.27 ft)	43	48	NA	NA	NA	0	(ft)	1	MW06-10 (35.3640636804888 ft)
20	MW07-05	712663.14	3047621.83	127.71	(99.71 - 94.71 ft)	28	33	NA	NA	NA	0	(ft)	0	(ft)
21	MW06-10	712743.21	3047599.34	127.93	(84.93 - 79.93 ft)	43	48	NA	NA	NA	0	(ft)	1	MW06-09 (35.3640636804888 ft)

Automated Summary Statistics

Sitewide Review of Individual Analyte

Power BI DAX Expressions were built to calculate statistics from script-generated input file.

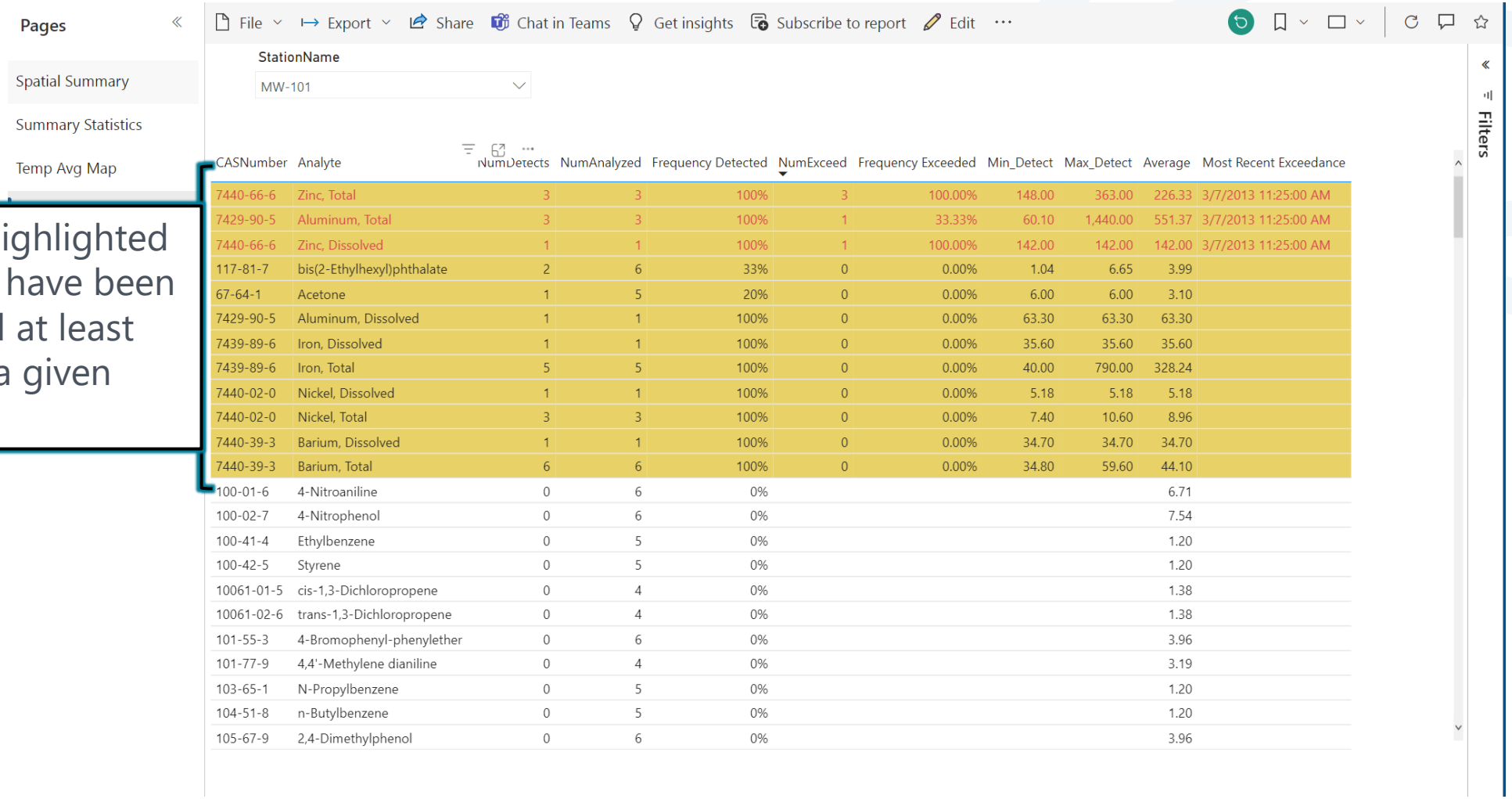
Measures allowed dynamic recalculations



Well	Top of Screen (ft bgs)	Bottom of Screen (ft bgs)	Number of Samples	Frequency of Detection	_FrequencyAbove5000ppb	Most Recent Sample	_MostRecentValue	Min	Max	Average	Standard Dev
MW17-02	20.00	30.00	19	94.74%	31.58%	8/1/2022 3:55:00 PM	823.40	0.00	13,911,898.00	609,772.20	2,836,027.08
MW16-20	15.00	25.00	24	100.00%	45.83%	8/2/2022 2:30:00 PM	454.00	397.20	2,797,795.00	113,622.08	536,888.40
C9 20			1	100.00%	100.00%	6/25/2020 12:30:00 PM	1,466,500.00	1,466,500.00	1,466,500.00	1,466,500.00	0.00
B10 20			1	100.00%	100.00%	7/1/2020 10:30:00 AM	1,178,000.00	1,178,000.00	1,178,000.00	1,178,000.00	0.00
SWEW-A1	9.50	29.50	12	100.00%	16.67%	1/20/2021 9:35:00 AM	0.33	0.33	1,165,164.00	97,863.93	321,806.05
MW08-403	32.00	47.00	5	100.00%	100.00%	9/25/2017 1:33:00 PM	802,300.00	802,300.00	1,134,900.00	1,021,844.00	118,461.91
MW12-03	44.00	49.00	7	100.00%	100.00%	4/5/2017 10:13:00 AM	556,600.00	263,200.00	912,000.00	612,357.14	194,331.87
MW08-303	32.00	47.00	1	100.00%	100.00%	4/10/2018 11:10:00 AM	880,000.00	880,000.00	880,000.00	880,000.00	0.00
C8 20			1	100.00%	100.00%	6/25/2020 10:15:00 AM	721,000.00	587,800.00	721,000.00	654,400.00	66,600.00
MW07-103	42.50	47.50	8	100.00%	100.00%	9/25/2017 10:45:00 AM	242,100.00	242,100.00	632,630.00	431,782.50	136,135.40
MW16-57	20.00	30.00	22	100.00%	13.64%	8/2/2022 3:25:00 PM	1,735.70	365.40	457,757.29	22,100.45	90,891.69
D9 20			1	100.00%	100.00%	6/29/2020 10:30:00 AM	340,900.00	340,900.00	340,900.00	340,900.00	0.00
MW18-04	15.00	20.00	5	100.00%	80.00%	4/9/2020 1:17:00 PM	156,482.70	1,361.00	311,100.00	101,587.88	119,033.30
MW13-18	65.00	75.00	1	100.00%	100.00%	4/10/2014 9:50:00 AM	262,974.00	262,974.00	262,974.00	262,974.00	0.00
MW12-04	48.00	52.00	4	100.00%	100.00%	9/21/2016 11:42:00 AM	129,420.00	122,553.30	197,510.00	153,735.83	30,071.76
MW12-01A	7.00	20.00	24	100.00%	54.17%	9/23/2022 11:10:00 AM	38.44	38.44	168,810.00	44,758.64	50,722.18
MW09-01	0.00	0.00	11	100.00%	100.00%	7/13/2016 8:50:00 AM	26,510.00	21,630.00	148,000.00	64,805.83	41,271.70
MW06-05	14.00	24.00	11	100.00%	100.00%	7/13/2016 9:30:00 AM	11,081.00	11,081.00	145,000.00	36,152.00	36,648.43
MW06-07S	16.00	26.00	13	100.00%	92.31%	9/10/2020 3:10:00 PM	11,937.00	1,300.00	128,000.00	34,392.85	32,595.99
MW07-202	21.00	27.00	24	100.00%	50.00%	9/23/2022 10:30:00 AM	24.73	22.84	121,500.00	28,690.88	39,024.62
SB 20-09			1	100.00%	100.00%	1/28/2021 12:00:00 AM	114,000.00	114,000.00	114,000.00	114,000.00	0.00

Automated Summary Statistics
Review of analyte concentrations at an individual well

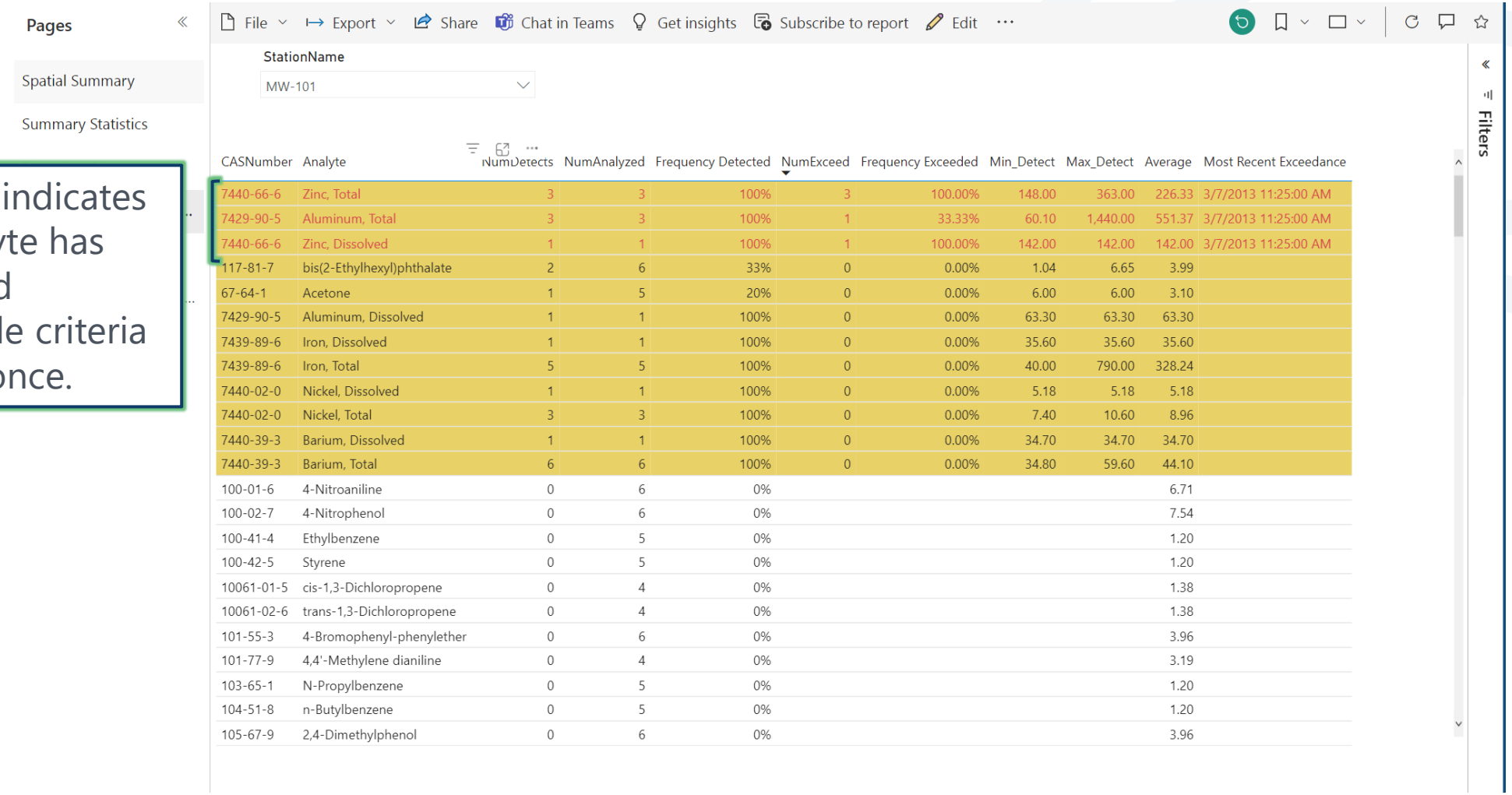
Yellow-highlighted analytes have been detected at least once at a given location.



CASNumber	Analyte	NumDetects	NumAnalyzed	Frequency Detected	NumExceed	Frequency Exceeded	Min_Detect	Max_Detect	Average	Most Recent Exceedance
7440-66-6	Zinc, Total	3	3	100%	3	100.00%	148.00	363.00	226.33	3/7/2013 11:25:00 AM
7429-90-5	Aluminum, Total	3	3	100%	1	33.33%	60.10	1,440.00	551.37	3/7/2013 11:25:00 AM
7440-66-6	Zinc, Dissolved	1	1	100%	1	100.00%	142.00	142.00	142.00	3/7/2013 11:25:00 AM
117-81-7	bis(2-Ethylhexyl)phthalate	2	6	33%	0	0.00%	1.04	6.65	3.99	
67-64-1	Acetone	1	5	20%	0	0.00%	6.00	6.00	3.10	
7429-90-5	Aluminum, Dissolved	1	1	100%	0	0.00%	63.30	63.30	63.30	
7439-89-6	Iron, Dissolved	1	1	100%	0	0.00%	35.60	35.60	35.60	
7439-89-6	Iron, Total	5	5	100%	0	0.00%	40.00	790.00	328.24	
7440-02-0	Nickel, Dissolved	1	1	100%	0	0.00%	5.18	5.18	5.18	
7440-02-0	Nickel, Total	3	3	100%	0	0.00%	7.40	10.60	8.96	
7440-39-3	Barium, Dissolved	1	1	100%	0	0.00%	34.70	34.70	34.70	
7440-39-3	Barium, Total	6	6	100%	0	0.00%	34.80	59.60	44.10	
100-01-6	4-Nitroaniline	0	6	0%					6.71	
100-02-7	4-Nitrophenol	0	6	0%					7.54	
100-41-4	Ethylbenzene	0	5	0%					1.20	
100-42-5	Styrene	0	5	0%					1.20	
10061-01-5	cis-1,3-Dichloropropene	0	4	0%					1.38	
10061-02-6	trans-1,3-Dichloropropene	0	4	0%					1.38	
101-55-3	4-Bromophenyl-phenylether	0	6	0%					3.96	
101-77-9	4,4'-Methylene dianiline	0	4	0%					3.19	
103-65-1	N-Propylbenzene	0	5	0%					1.20	
104-51-8	n-Butylbenzene	0	5	0%					1.20	
105-67-9	2,4-Dimethylphenol	0	6	0%					3.96	

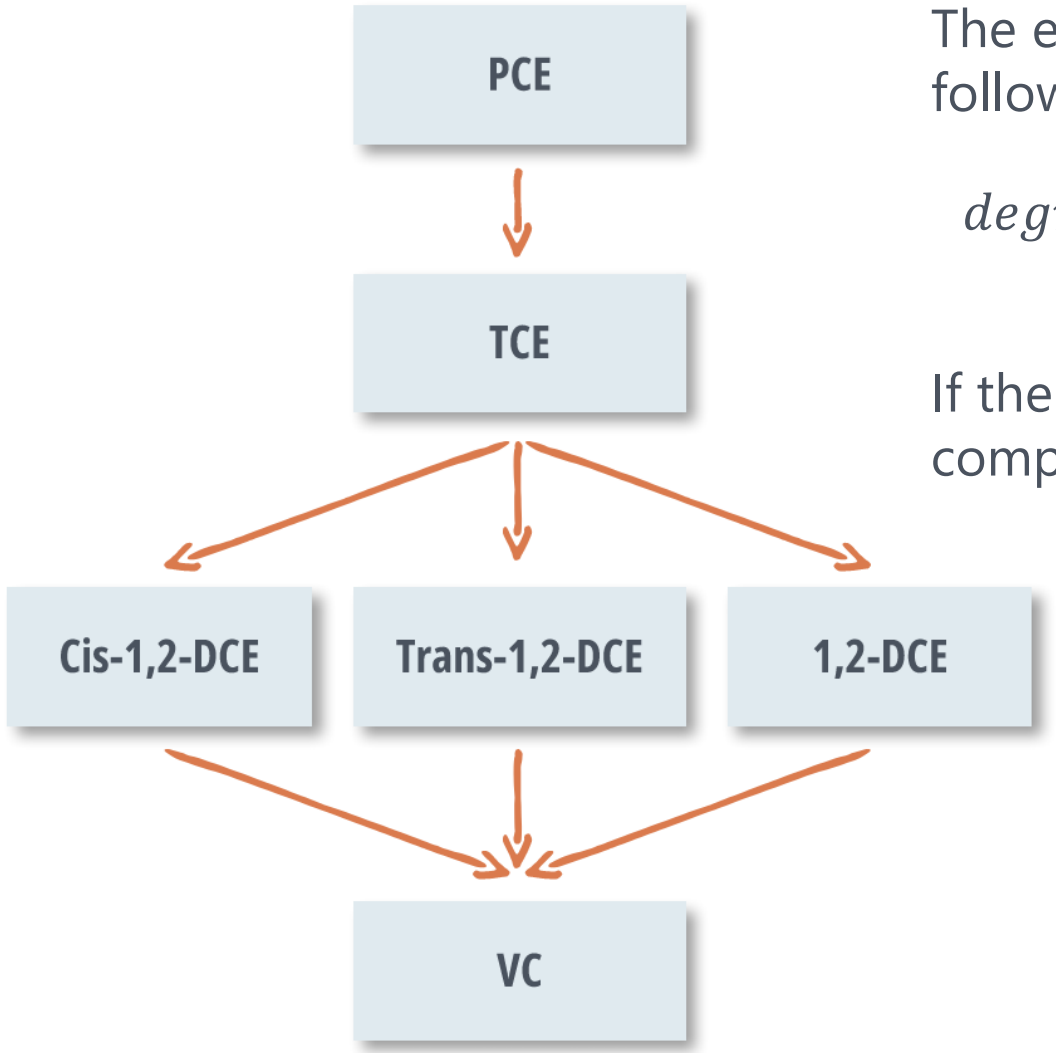
Automated Summary Statistics
Review of analyte concentrations at an individual well

Red text indicates the analyte has exceeded applicable criteria at least once.



CASNumber	Analyte	NumDetects	NumAnalyzed	Frequency Detected	NumExceed	Frequency Exceeded	Min_Detect	Max_Detect	Average	Most Recent Exceedance
7440-66-6	Zinc, Total	3	3	100%	3	100.00%	148.00	363.00	226.33	3/7/2013 11:25:00 AM
7429-90-5	Aluminum, Total	3	3	100%	1	33.33%	60.10	1,440.00	551.37	3/7/2013 11:25:00 AM
7440-66-6	Zinc, Dissolved	1	1	100%	1	100.00%	142.00	142.00	142.00	3/7/2013 11:25:00 AM
117-81-7	bis(2-Ethylhexyl)phthalate	2	6	33%	0	0.00%	1.04	6.65	3.99	
67-64-1	Acetone	1	5	20%	0	0.00%	6.00	6.00	3.10	
7429-90-5	Aluminum, Dissolved	1	1	100%	0	0.00%	63.30	63.30	63.30	
7439-89-6	Iron, Dissolved	1	1	100%	0	0.00%	35.60	35.60	35.60	
7439-89-6	Iron, Total	5	5	100%	0	0.00%	40.00	790.00	328.24	
7440-02-0	Nickel, Dissolved	1	1	100%	0	0.00%	5.18	5.18	5.18	
7440-02-0	Nickel, Total	3	3	100%	0	0.00%	7.40	10.60	8.96	
7440-39-3	Barium, Dissolved	1	1	100%	0	0.00%	34.70	34.70	34.70	
7440-39-3	Barium, Total	6	6	100%	0	0.00%	34.80	59.60	44.10	
100-01-6	4-Nitroaniline	0	6	0%					6.71	
100-02-7	4-Nitrophenol	0	6	0%					7.54	
100-41-4	Ethylbenzene	0	5	0%					1.20	
100-42-5	Styrene	0	5	0%					1.20	
10061-01-5	cis-1,3-Dichloropropene	0	4	0%					1.38	
10061-02-6	trans-1,3-Dichloropropene	0	4	0%					1.38	
101-55-3	4-Bromophenyl-phenylether	0	6	0%					3.96	
101-77-9	4,4'-Methylene dianiline	0	4	0%					3.19	
103-65-1	N-Propylbenzene	0	5	0%					1.20	
104-51-8	n-Butylbenzene	0	5	0%					1.20	
105-67-9	2,4-Dimethylphenol	0	6	0%					3.96	

Extent of Degradation

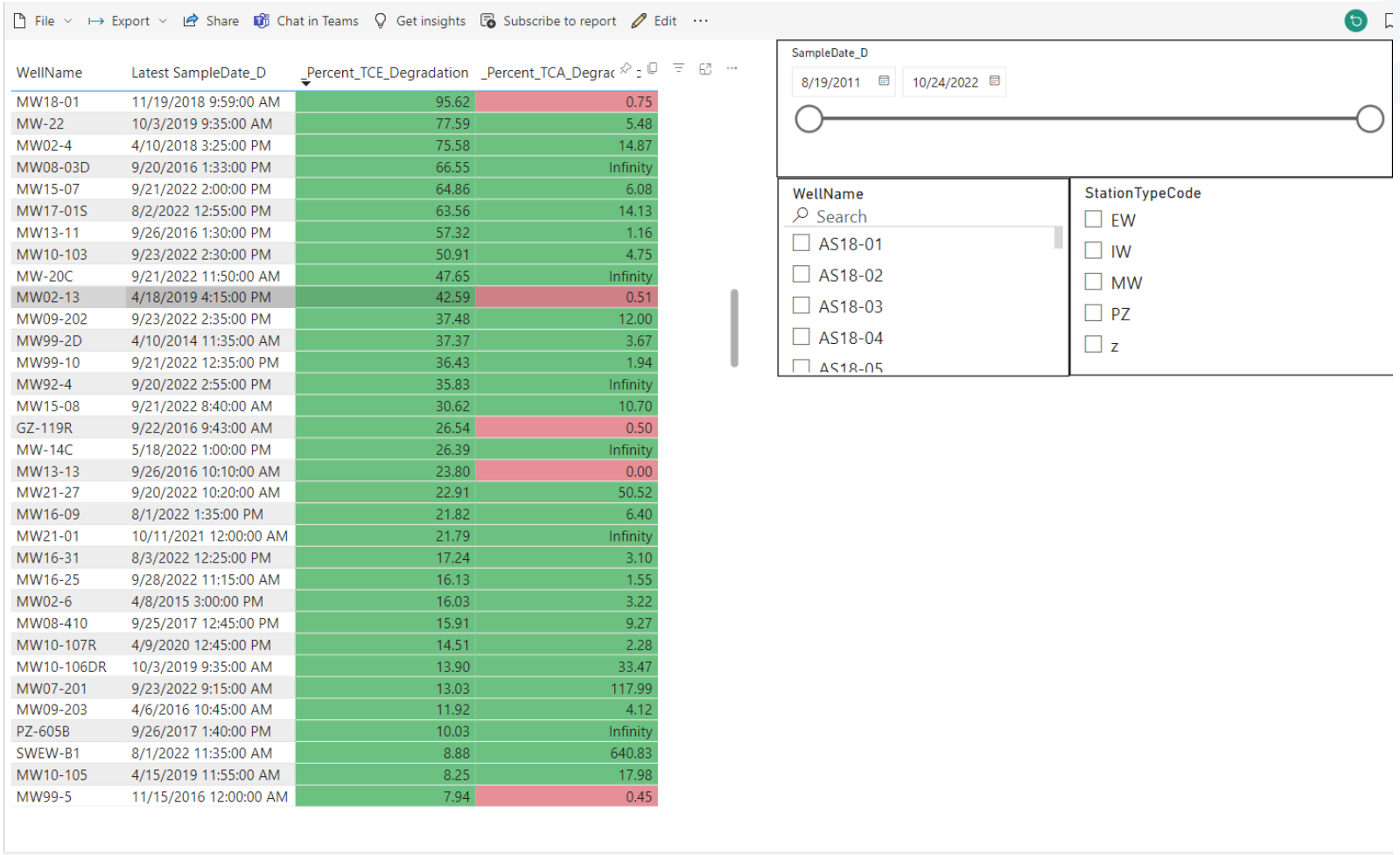


The extent of degradation was calculated using the following equation:

$$degradation = \frac{molarity\ of\ degradation\ by-products}{molarity\ of\ original\ compound}$$

If the degradation ratio is **greater than one**, the compound is considered to be degrading at that well.

Extent of Degradation – Power BI Display



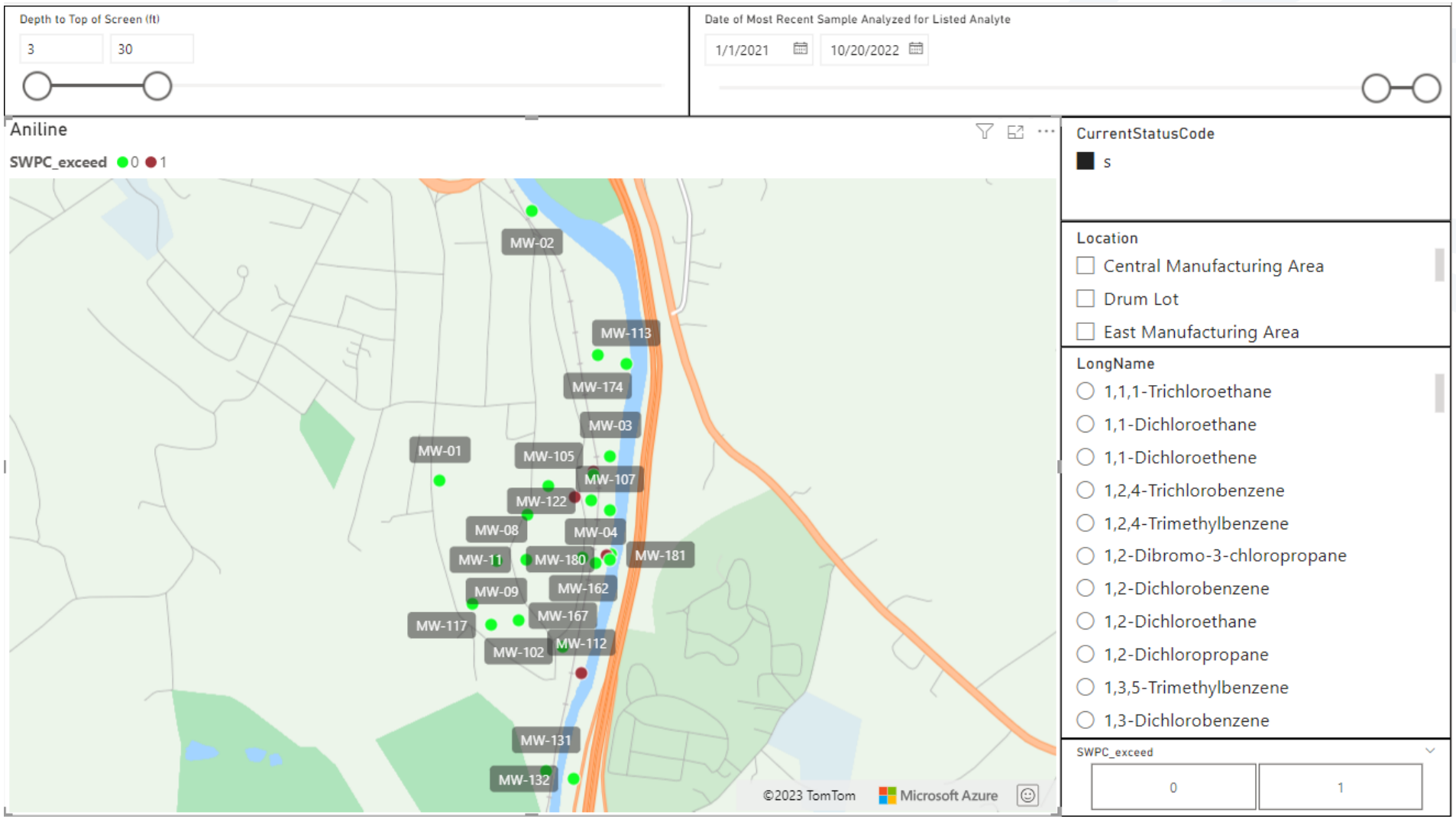
WellName	Latest SampleDate_D	_Percent_TCE_Degradation	_Percent_TCA_Degrac
MW18-01	11/19/2018 9:59:00 AM	95.62	0.75
MW-22	10/3/2019 9:35:00 AM	77.59	5.48
MW02-4	4/10/2018 3:25:00 PM	75.58	14.87
MW08-03D	9/20/2016 1:33:00 PM	66.55	Infinity
MW15-07	9/21/2022 2:00:00 PM	64.86	6.08
MW17-01S	8/2/2022 12:55:00 PM	63.56	14.13
MW13-11	9/26/2016 1:30:00 PM	57.32	1.16
MW10-103	9/23/2022 2:30:00 PM	50.91	4.75
MW-20C	9/21/2022 11:50:00 AM	47.65	Infinity
MW02-13	4/18/2019 4:15:00 PM	42.59	0.51
MW09-202	9/23/2022 2:35:00 PM	37.48	12.00
MW99-2D	4/10/2014 11:35:00 AM	37.37	3.67
MW99-10	9/21/2022 12:35:00 PM	36.43	1.94
MW92-4	9/20/2022 2:55:00 PM	35.83	Infinity
MW15-08	9/21/2022 8:40:00 AM	30.62	10.70
GZ-119R	9/22/2016 9:43:00 AM	26.54	0.50
MW-14C	5/18/2022 1:00:00 PM	26.39	Infinity
MW13-13	9/26/2016 10:10:00 AM	23.80	0.00
MW21-27	9/20/2022 10:20:00 AM	22.91	50.52
MW16-09	8/1/2022 1:35:00 PM	21.82	6.40
MW21-01	10/11/2021 12:00:00 AM	21.79	Infinity
MW16-31	8/3/2022 12:25:00 PM	17.24	3.10
MW16-25	9/28/2022 11:15:00 AM	16.13	1.55
MW02-6	4/8/2015 3:00:00 PM	16.03	3.22
MW08-410	9/25/2017 12:45:00 PM	15.91	9.27
MW10-107R	4/9/2020 12:45:00 PM	14.51	2.28
MW10-106DR	10/3/2019 9:35:00 AM	13.90	33.47
MW07-201	9/23/2022 9:15:00 AM	13.03	117.99
MW09-203	4/6/2016 10:45:00 AM	11.92	4.12
PZ-605B	9/26/2017 1:40:00 PM	10.03	Infinity
SWEW-B1	8/1/2022 11:35:00 AM	8.88	640.83
MW10-105	4/15/2019 11:55:00 AM	8.25	17.98
MW99-5	11/15/2016 12:00:00 AM	7.94	0.45

Power BI DAX Expressions were built to calculate ratios from script-generated input file.

The input file stored concentration and molarity.

Regulatory Exceedance Map

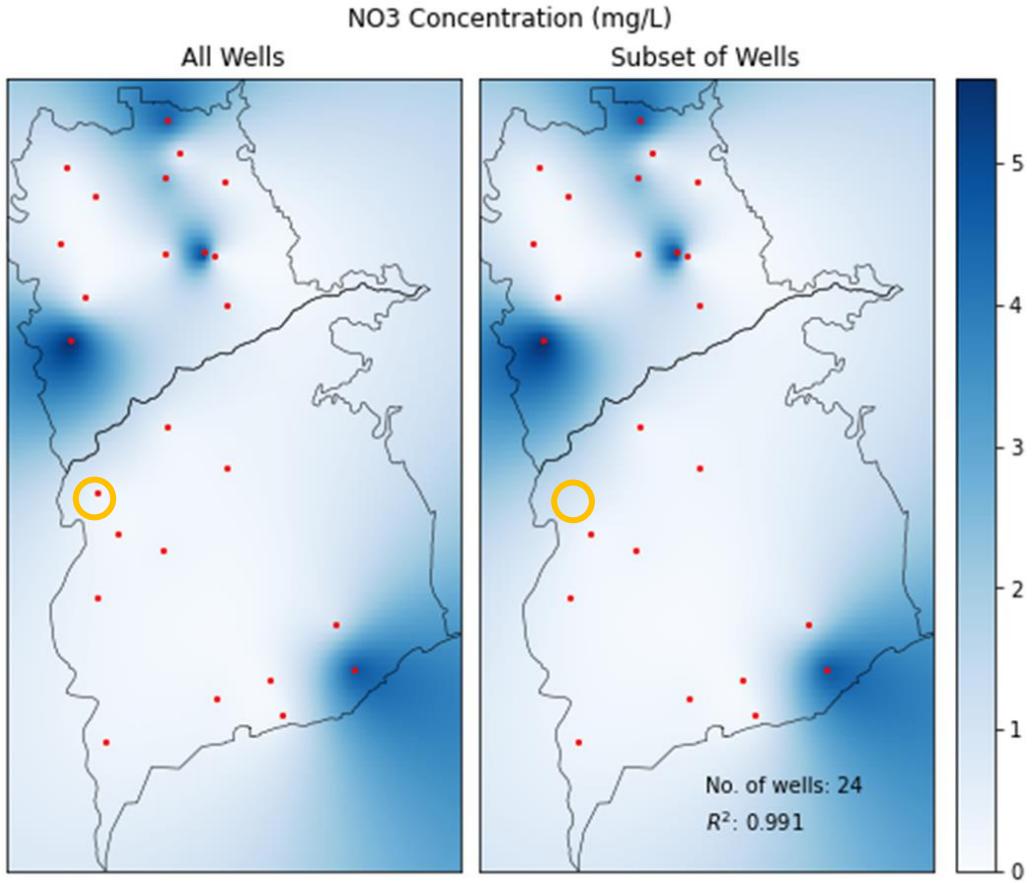
Input data provided by Python script to evaluate last 4 samples collected from each well.



Contour Optimization

- Identify representative wells for long-term, basin-wide groundwater quality monitoring using spatial distribution

- Methodology:
  1. Create concentration contours based on the constituents' concentrations on each well
  2. Remove the well that provides the **least** amount of information to the contour for **all** constituents
  3. Repeat Step #2 and stop when a threshold is met



Yuba Subbasin – California

Contour Optimization

- Yuba Subbasin results:
  - From 55 wells, 26 wells were selected for long-term groundwater quality monitoring
  - Maintaining the spatial distribution of the constituents' concentration
- Tool provides flexibility
  - Can be applied to different subbasins
  - A subset of wells can be set as fixed
    - Wells that exceed Primary MCLs
- Provides a scientific base for establishing a high-quality, cost-effective regional groundwater quality monitoring network

Project Conclusions:

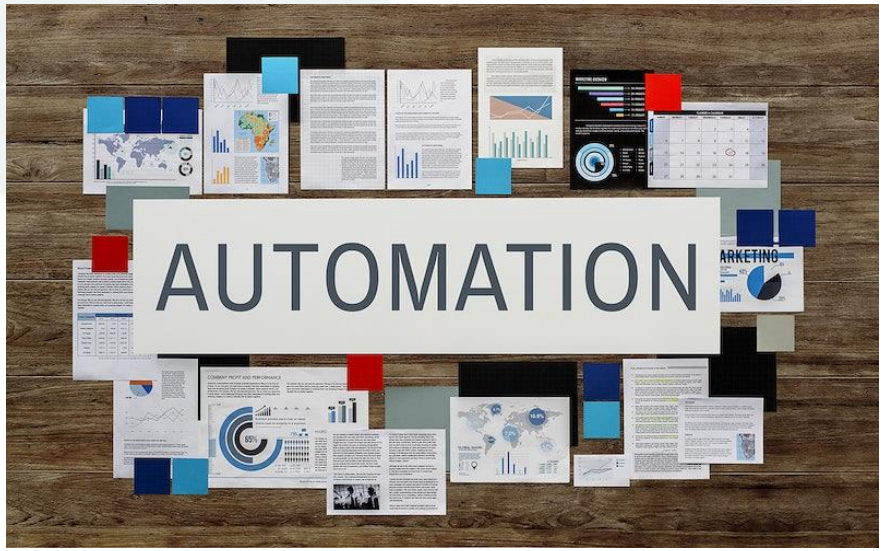
Site	% reduction in routine wells monitored	% of remaining wells with reduced sampling frequency	Hours of fieldwork saved per sampling event
Example Site #1	30	40	19
Example Site #2	40	0*	50–60

Notable cost savings

Increased project sustainability

Return on Investment from Scalable Tools

Tool	Hours Saved (range from small to large site)
Mann Kendall	10–100
Spatial Representation	2–200
Summary Statistics	5–20
Degradation Evaluation	10–100



GitHub

Next Steps

- Incorporate monitoring optimization tools into Power BI interface connected to multi-project Azure SQL Database

Woodard & Curran

Questions?

September 12, 2023