

DQM UTILIZATION IN A PFAS WORLD

PRESENTED BY SCOTT WILSON

WHAT ARE PFAS?

- Per- and polyfluoroalkyl substances
 - Essentially, carbon chains with many C-F bonds
 - C-F bonds are strong and stable *for better and for worse*
- Numerous industrial, commercial, and household uses
 - Ubiquitous in everyday life
- Ever so persistent in the environment
- Seems PFAS are rather toxic to us
 - Average blood levels in U.S. General Population:
 - PFOA, 1.4 ug/L
 - PFOS, 4.3 ug/L



Perfluorooctanoic acid
(PFOA)



Perfluorooctanesulfonic acid
(PFOS)

Plus many, many more

We are going to start seeing a lot more PFAS data in our databases

- PFAS are currently a focus of intense regulatory investigation
 - Between 2016 and 2020 alone, Navy began PFAS investigations at 108 unique sites
 - In August, EPA proposed addition of PFOA and PFOS to CERCLA (Superfund)
- EPA Draft Method 1633 (*“The Dream Team Method”*)
 - Rapidly coming online for DoD projects
 - Several large labs have received DoD accreditation within last few months
 - Validation guidance incoming
- Important 1633 guidance documents expected to drop soon
 - One of the last remaining puzzle pieces
 - Little birdies tell me . . .

WHAT IS DATA VALIDATION (IN ESSENCE)?

- Analyte- and sample-specific assessment of data relative to project criteria
- Does my data meet project needs and goals?
- Is my data legally defensible?
- Data validation *informs* end-user of limitations and usability
 - NOT the exclusive be-all and end-all



Depth of review indicated by a LEVEL or STAGE

STAGE 1

- Sample results + Field QC

STAGE 2A

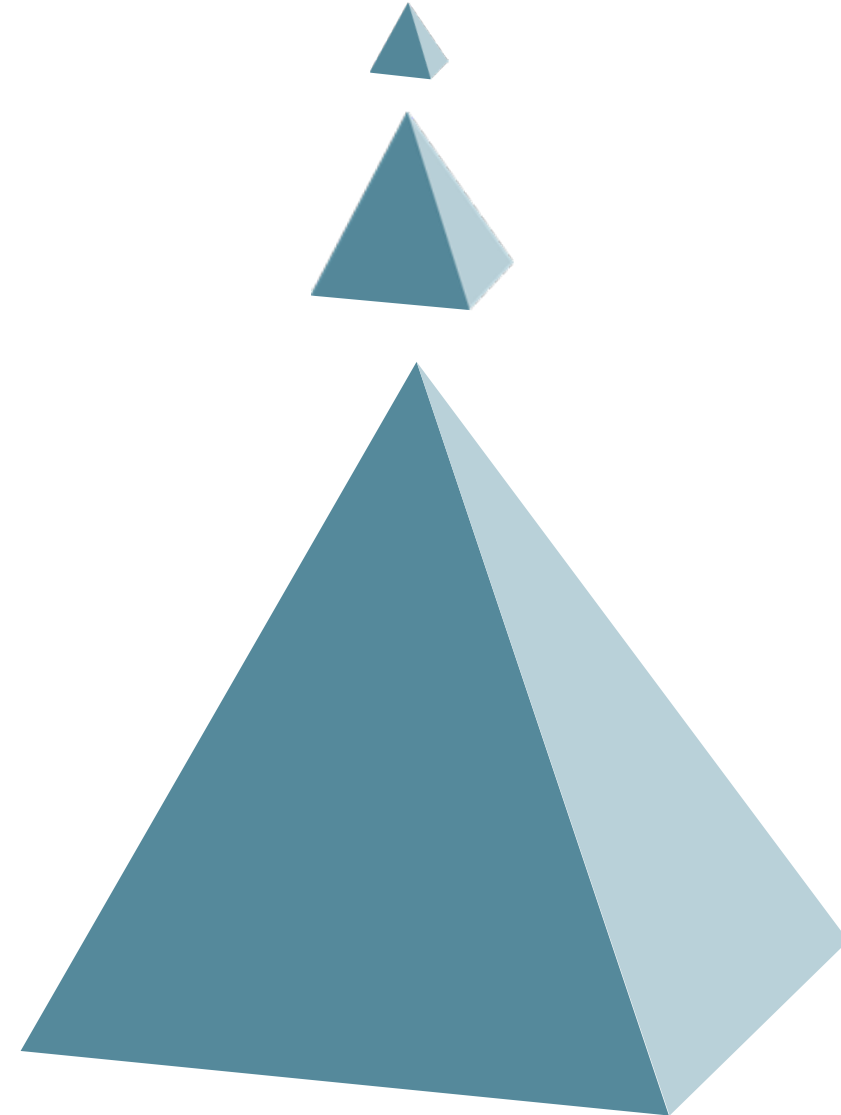
- Above + prep QC

STAGE 2B

- Above + calibration

STAGE 4

- Above + raw data



- Individual sample results marked with a *qualifier*

ANALYTE	RESULT	UNIT	FINAL QUALIFIER
PFHxA	1.2	ng/L	J+

- May be summarized in a written report
- Typically, EDD is populated with qualifiers

Common/Conventional Qualifiers

- **J, J-, J+, K, L, and UJ**
 - **Estimated** – with or without bias
- **U or UJ**
 - **Not Detected or Not Detected-ish**
- **N or NJ**
 - **Tentative** – ID criteria not met or not supported
- **R**
 - **Rejection** – result is not usable
 - “Oh, shoot!”

EQuIS™ DATA QUALIFICATION MODULE

- Performs specified checks on analytical data
- Applies qualification to results automatically

WHAT IS DQM DESIGNED TO DO? – 1 PROJECT TO A BOX

- Single project eQAPP
- Limited scope
 - Specific methods
 - Specific analyte list
 - Specific matrices
 - Specific limits

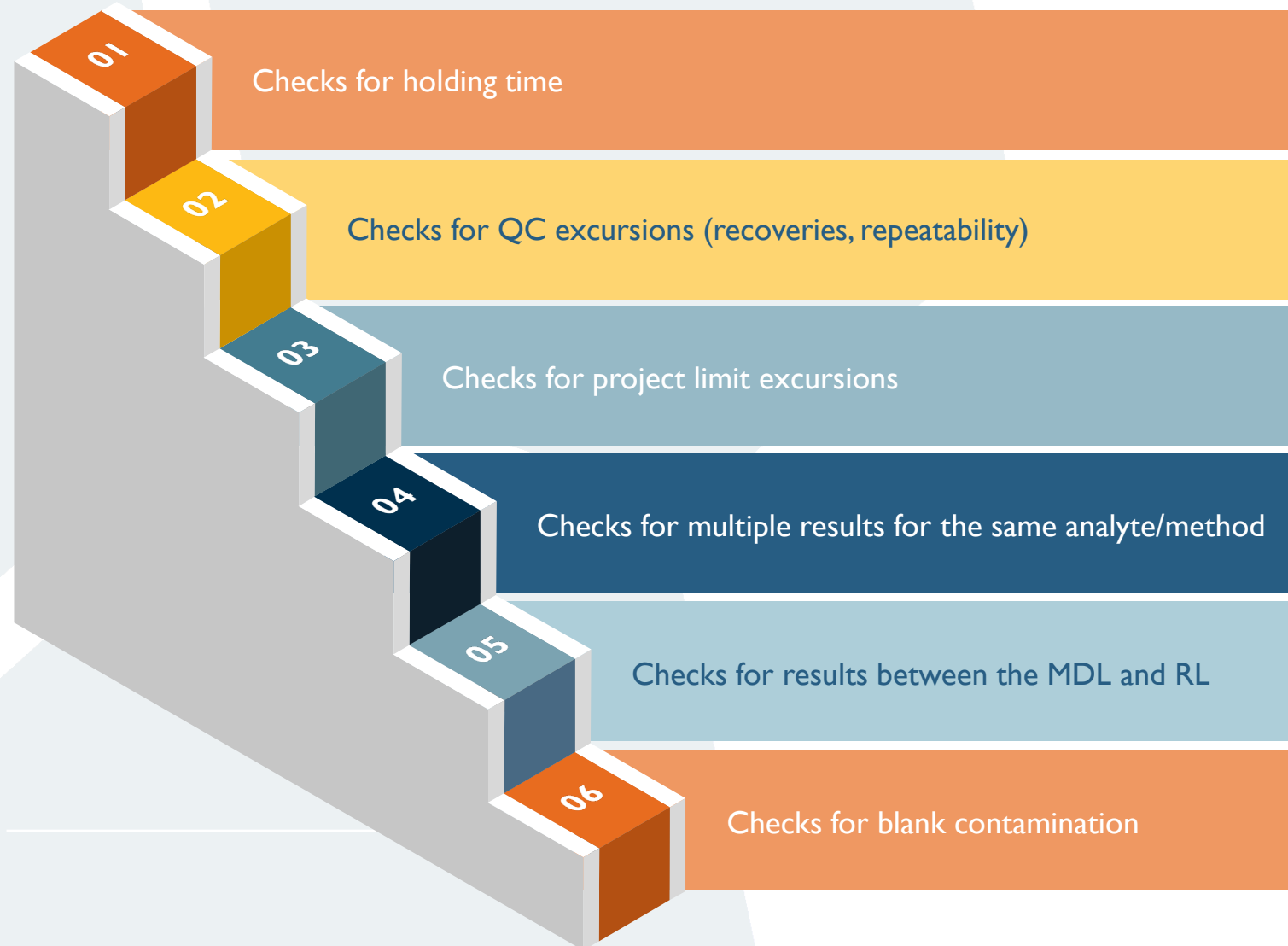


HOW DO WE NEED TO USE IT AT DDMS? – 1 great big box

- Any project
- Any analyte
- Any matrix
- Default rules
- Default limits



WHAT IS DQM DESIGNED TO DO?



Earthsoft is working on adding more checks, and improving existing ones

Example: Preservative verification added to holding time check in 7.21.1

Event Summary Review Exceptions by Check Review All Results Review Samples and Results by Sample Event Status Errors

Enter new value into yellow textbox and click button to update all filtered records.

DQM CHECK: **Spike Recovery - Multiple Rules** 1

Update Apply Remark Update Apply RC Update Apply Q Check to include in Apply Q Update

Total Number of Exceptions: 27
Number of Exceptions from Selected Check: 5 2

Exceptions by Check: 5 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Method	Matrix	FR	Test Type	Analysis Date
The Blank Spike Recovery exceeds the UCL High bias	SPR1	J				J	Sodium 1H,1H,2H,2H-Perfluorooctane Sulfonate (62) (6.2FTS)	ABCD12345-BS1	9/16/2021 12:36:00 PM	LCS	E537	SQ	T	INITIAL	9/22/2021 12:33:00 PM
The Blank Spike Recovery exceeds the UCL High bias	SPR1	J				J	Perfluorohexanoic Acid (PFHxA)	ABCD12345-BS1	9/16/2021 12:36:00 PM	LCS	E537	SQ	T	INITIAL	9/22/2021 12:33:00 PM
The Blank Spike Recovery is less than the LCL but greater than the Lower Cutoff. Low bias	SPR4	J				J	Perfluorobutanoic acid (PFBA)	ABCD12345-BS1	9/16/2021 12:36:00 PM	LCS	E537	SQ	T	INITIAL	9/22/2021 12:33:00 PM

Update Apply Remark Update Apply RC Update Apply Q Check to include in Apply Q Update

ASSOCIATED RESULTS 5

Total Number of Associated Results: 360
Number of Results from Selected Check: 31 3

Associated Results: 29 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Method	Matrix	FR	Test Type	Analysis Date
Associated Result from: The Blank Spike Recovery exceeds the UCL. High bias	SPR1	J				J	Perfluorohexanoic Acid (PFHxA)	EXCAV-14-K_20210913	9/13/2021 6:50:00 PM	FD	E537	SO	T	INITIAL	9/22/2021 6:52:00 PM
Associated Result from: The Blank Spike Recovery is less than the LCL but greater than the Lower Cutoff. Low bias	SPR4	UJ	U		U	UJ	Perfluorobutanoic acid (PFBA)	EXCAV-1_20210913	9/13/2021 3:00:00 PM	N	E537	SO	T	INITIAL	9/22/2021 3:09:00 PM
Associated Result from: The Blank Spike Recovery is less than the LCL but greater than the Lower Cutoff. Low bias	SPR4	J				J	Perfluorobutanoic acid (PFBA)	EXCAV-10_20210913	9/13/2021 2:05:00 PM	N	E537	SO	T	INITIAL	9/22/2021 4:16:00 PM

Save Event

Complete Event

ABCD12345

Event Summary

Review Exceptions by Check

Review All Results

Review Samples and Results by Sample

Event Status

Errors

2

Update Apply Remark

Update Apply RC

Update Apply Q

ve percent difference between paired results.

RPDF1

J

Check to include in Apply Q Update

Enter new value into yellow textbox and click button to update all filtered records.

ALL RESULTS

Total Number of Results 741

All Results: 11 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					N-deuteriomethylperfluoro-1-octanesulfonamidoacetic acid	EXCAV-14_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					N-deuterioethylperfluoro-1-octanesulfonamidoacetic acid	EXCAV-14_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (62)	EXCAV-14_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-decane sulfonate (82)	EXCAV-14_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Perfluoro[2,3,4-13C3]Butanesulfonic Acid (M3Pfts)	EXCAV-14_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Perfluoropentanoic Acid (PFPeA)	EXCAV-14-K_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					N-deuteriomethylperfluoro-1-octanesulfonamidoacetic acid	EXCAV-14-K_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					N-deuterioethylperfluoro-1-octanesulfonamidoacetic acid	EXCAV-14-K_20210913
Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-13C2]-octane sulfonate (62)	EXCAV-14-K_20210913
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Results were qualified as estimated (J) due to a high relative percent difference between paired results.	RPDF1	J					Perfluoro[2,3,4-13C3]Butanesulfonic Acid (M3Pfts)	EXCAV-14-K_20210913

WHAT IS DQM NOT DESIGNED TO DO?



WHAT IS DQM NOT DESIGNED TO DO?



Inconsistency. Inconsistency is a real sticking point for PFAS.

- Analyte nomenclature can vary significantly by method and lab
 - Database headaches when trying to query and compare data
- Competing sample and result types
 - LCS vs LFB vs OPR vs LLOPR
 - SUR vs IS vs EIS vs Labeled Compounds/Analog
- Tedious analyte associations between surrogates/labeled compounds and target analytes
 - 1 surrogate to 1 target analyte frequently the case
- List of target analytes and control limits frequently changing

- DQM is an additional chance to lock down and tighten vocabulary
 - Target analytes
 - Surrogates and labeled compounds
 - Error log is sometimes the quickest way to catch nomenclature woes

Event Summary	Review Exceptions by Check	Review All Results	Review Samples and Results by Sample	Event Status	Errors	
	Source of Error	Error Message			Error_Type	EddDataRow
▶	EarthSoft.DQM.SurrogateRecovery	Surrogate Recovery LCL--UCL is missing or not numeric; at sys_sample_code=EXCAV-1_20220113 and analytic_method='E537' and cas_rm='13C8PFNA'			DQM Setting Missing	
	EarthSoft.DQM.SurrogateRecovery	Surrogate Recovery LCL--UCL is missing or not numeric; at sys_sample_code=EXCAV-1_20220113 and analytic_method='E537' and cas_rm='M2-6:2FTS'			DQM Setting Missing	
	EarthSoft.DQM.SurrogateRecovery	Surrogate Recovery LCL--UCL is missing or not numeric; at sys_sample_code=EXCAV-1_20220113 and analytic_method='E537' and cas_rm='M2-8:2FTS'			DQM Setting Missing	
	EarthSoft.DQM.SurrogateRecovery	Surrogate Recovery LCL--UCL is missing or not numeric; at sys_sample_code=EXCAV-1_20220113 and analytic_method='E537' and cas_rm='M3PFBS'			DQM Setting Missing	

DQM is flexible and targeted! DQM allows the user to define how sample types and result types are handled.

- LCS, LFB, OPR, and LLOPR → Can be classified and reviewed exactly like a blank spike
 - Ensures batch spike recovery excursions are “seen” no matter what
- SUR, IS, EIS, LC (Labeled Compounds) → Can be classified and reviewed exactly like a surrogate spike
 - Ensures sample-specific spike recovery excursion are “seen” no matter what

HOW DQM HELPS – COMPETING SPIKE TYPES

Enter new value into yellow textbox and click button to update all filtered records.

DQM CHECK: **Spike Recovery - Multiple Rules**

SUCCESS!

Total Number of Exceptions: 27

Number of Exceptions from Selected Check: 5

Exceptions by Check: 5 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Result Type	Method
The Blank Spike Recovery exceeds the UCL. High bias	SPR1	J				J	Sodium 1H,1H,2H,2H-Perfluorooctane Sulfonate (6:2) (6:2FTS)	BBCD12345-BS1	10/16/2021 3:36:00 PM	LFB	SC	E537
The Blank Spike Recovery exceeds the UCL. High bias	SPR1	J				J	Perfluorohexanoic Acid (PFHxA)	BBCD12345-BS1	10/16/2021 3:36:00 PM	LFB	SC	E537
The Blank Spike Recovery is less than the LCL but greater than the Lower Cutoff. Low bias	SPR4	J				J	Perfluorobutanoic acid (PFBA)	BBCD12345-BS1	10/16/2021 3:36:00 PM	LFB	SC	E537
The Blank Spike Recovery is less than the LCL but greater than the Lower Cutoff. Low bias	SPR4	J				J	Perfluoroheptanoic acid (PFHpA)	BBCD12345-BS1	10/16/2021 3:36:00 PM	LFB	SC	E537
The Blank Spike Recovery exceeds the UCL. High bias	SPR1	J				J	Sodium 1H,1H,2H,2H-Perfluorodecane Sulfonate (8:2) (8:2FTS)	BBCD12345-BS1	10/16/2021 3:36:00 PM	LFB	SC	E537

HOW DQM HELPS – COMPETING SUR TYPES

Enter new value into yellow textbox and click button to update all filtered records.

Update Apply Remark

Update Apply RC

Update Apply Q

Check to include in Apply Q Update

DQM CHECK: **Surrogate Recovery**

SUCCESS!

Total Number of Exceptions:27

Number of Exceptions from Selected Check:22

Exceptions by Check: 22 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Result Type	Method
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C2-Perfluorotetradecanoic acid	CBCD12345-BLK1	11/16/2021 3:36:00 PM	LB	EIS	E537
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C2-Perfluorotetradecanoic acid	CBCD12345-BS1	11/16/2021 3:36:00 PM	OPR	EIS	E537
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C2-Perfluorododecanoic acid	CBCD12345-MS1	11/16/2021 3:36:00 PM	MS	EIS	E537
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C2-Perfluorotetradecanoic acid	CBCD12345-MS1	11/16/2021 3:36:00 PM	MS	EIS	E537
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C4-Perfluoroheptanoic acid	CBCD12345-MS1	11/16/2021 3:36:00 PM	MS	EIS	E537

DQM allows analyte-specific associations to surrogates.

- Methods using one surrogate per target analyte
 - A recovery failure in the surrogate affects *only* the associated target analyte
- This is *huge!* For most non-PFAS methods, a surrogate failure is intended to qualify every target analyte reported for the sample
- With DQM, we have the flexibility to handle surrogates either way

HOW DQM HELPS – SURROGATE ASSOCIATIONS

Enter new value into yellow textbox and click button to update all filtered records.

DQM CHECK: **Surrogate Recovery**

Update Apply Remark

Update Apply RC

Update Apply Q

Check to include in Apply Q Update

Total Number of Exceptions: 1
Number of Exceptions from Selected Check: 1

Exceptions by Check: 1 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Result Type	Method	Me
The Surrogate Recovery is less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR7	J				J	13C2-Perfluorododecanoic acid	EXCAV-3_20220113	1/13/2022 8:10:00 AM	N	SUR	E537	



ASSOCIATED RESULTS

1 SUR to 1 TRG

Total Number of Associated Results: 1
Number of Results from Selected Check: 1

Associated Results: 1 records (filtered)

Apply Remark	Apply RC	Apply Q	Lab Q	Val Q	Inter Q	DQM Q	Analyte	Sample	Sample Date	Samp Type	Result Type	Method	Me
Associated Result from: Associated Non-Detected Result of a Surrogate Recovery less than the LCL but greater than the Lower Surrogate Cutoff. Low bias	SURR4	UJ	U		U	UJ	Perfluorododecanoic Acid (PFDoA)	EXCAV-3_20220113	1/13/2022 8:10:00 AM	N	TRG	E537	

When new guidance is published (again), when the lab limits are updated (again), it is simple to update DQM

- When new recovery limits are published for 40 target analytes, plus the 40 labeled compounds . . .
 - Would you rather update an eQAPP spreadsheet (DQM), or vet every spike recovery manually?
- PFAS methods and guidance are changing readily right now. It's the name of the game.

HOW DQM HELPS – UPDATING LIMITS

	A	B	C	E	F	G	M	N	O	P	Q
1	#dqm_qapp_code	matrix_code	analytic_method	result_type_code	cas_rn	chemical_name	lcs_rec_lower_cutoff	lcs_recovery_lcl	lcs_recovery_ucl	lcs_rec_upper_cutoff	lcs_dup_rpd_cl
2	#Text(40)	Text(10)	Text(20)	Text(10)	Text(15)	Text(255)	Text(19)	Text(19)	Text(19)	Text(19)	Text(19)
23	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	106-46-7	1,4-dichlorobenzene	10	45	110	110	20
24	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	95-95-4	2,4,5-trichlorophenol	10	44	110	110	20
25	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	88-06-2	2,4,6-trichlorophenol	10	43	110	110	20
26	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	121-14-2	2,4-dinitrotoluene	10	49	124	124	20
27	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	95-48-7	2-methylphenol	10	46	110	110	20
28	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	15831-10-4	3&4-methylphenol	10	45	117	117	20
29	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	87-68-3	Hexachloro-1,3-butadiene	10	34	110	110	20
30	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	118-74-1	Hexachlorobenzene	10	52	115	115	20
31	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	67-72-1	Hexachloroethane	10	43	113	113	20
32	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	98-95-3	Nitrobenzene	10	41	112	112	20
33	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	87-86-5	Pentachlorophenol	10	38	135	135	20
34	DQM_Starter_Standard	WG	SW-846 1311/8270D	SC	110-86-1	Pyridine	10	24	118	118	20
35	DQM_Starter_Standard	SO	SW8270				10	40	120	120	40
36	DQM_Starter_Standard	SO	SW8270		108-95-2	Phenol	10	40	105	105	40
37	DQM_Starter_Standard	SO	SW8270		51-28-5	2,4-Dinitrophenol	10	50	120	120	30
38	DQM_Starter_Standard	SO	SW8270		95-57-8	2-Chlorophenol	10	40	105	105	40
39	DQM_Starter_Standard	SO	SW8270		59-50-7	4-Chloro-3-methylphenol	10	45	110	110	30
40	DQM_Starter_Standard	WG	SW8260				10	70	130	130	20
41	#Note 1) The more specific control limits (e.g., those that include a CAS_RN) override the less specific control limits.										
42	#Note 2) The RESULT_TYPE_CODE is not used by the DQM code, but is helpful to organize this EDD file.										
43	#Note 3) By default the DQM_QAPP_CODE used for surrogate associations is the selected QAPP code another DQM_QAPP_CODE can be selected on the										
44	#Note 4) Remember that all of these control limits, including the associations below, need to be reviewed to assure that they meet your specific project										
45	#Note 5) The MATRIX_CODE in the associations below is just a placeholder because use that is a required column. The DQM code applies the association										
46	DQM_Starter_Standard	WG		TRG	108-95-2	Phenol					
47	DQM_Starter_Standard	WG		TRG	58-90-2	2,3,4,6-Tetrachlorophenol					
48	DQM_Starter_Standard	WG		TRG	95-95-4	2,4,5-Trichlorophenol					
49	DQM_Starter_Standard	WG		TRG	88-06-2	2,4,6-Trichlorophenol					
50	DQM_Starter_Standard	WG		TRG	120-83-2	2,4-Dichlorophenol					
51	DQM_Starter_Standard	WG		TRG	105-67-9	2,4-Dimethylphenol					
52	DQM_Starter_Standard	WG		TRG	51-28-5	2,4-Dinitrophenol					
53	DQM_Starter_Standard	WG		TRG	95-57-8	2-Chlorophenol					
54	DQM_Starter_Standard	WG		TRG	95-48-7	2-Methylphenol					
55	DQM_Starter_Standard	WG		TRG	88-75-5	2-Nitrophenol					
56	DQM_Starter_Standard	WG		TRG	106-44-5	3+4-Methylphenol					
57	DQM_Starter_Standard	WG		TRG	534-52-1	4,6-Dinitro-2-methylphenol					
58	DQM_Starter_Standard	WG		TRG	59-50-7	4-Chloro-3-methylphenol					
59	DQM_Starter_Standard	WG		TRG	100-02-7	4-Nitrophenol					
60	DQM_Starter_Standard	WG		TRG	65-85-9	Benzoic Acid					

You should consider DQM when your project . . .

- Requires or benefits from validation (naturally)
- Has clear, defined data quality objectives
- Has high sample through-put (sudden cavalcade of data or long-term, routine sampling)
- Projects with “confident” laboratory EDDs available in an EQuIS format
- Has access to capable hands (DQM eQAPP Setup)



"Any questions?"

ICEDM, SEPT 2022

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