AFFILIATIONS

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Creating an Automated Annual MDL Verification Process

Using technology to improve the required process for verifying method detection limits on an annual basis

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SINCE 1933

01. Introduction

USEPA published the *Definition and Procedure for the Determination of the Method Detection Limit, Revision 2* in 2016 to update the requirements necessary to establish initial MDLs and ongoing data collection and verification in the laboratory. To make this process simpler, the OCWD laboratory uses various software technologies to automate the process. The OCWD Laboratory and Information Services departments worked together to make an in-house LIMS-MDL web tool. After approximately 5 years of using the LIMS-MDL web tool, continuous improvements were made to better assign and track the annual verifications. The OCWD Lab uses a Quality Management System (QMS) software to assign MDL verifications to the primary Lab analyst. The workflow allows QA staff to check statuses, review reports, and track changes to updated values.

02. Key Objectives

- Establish a clear workflow process for lab staff (see *Figure A*)
- Easily calculate an MDL verification from an existing LIMS database
- Generate reports for traceability
- Improve communication between QA staff and Lab analysts
- Decrease the time it takes for Lab analysts and QA staff to review and report their MDL verifications for each analyte, analytical method, and analytical instrument
- Ensure compliance with federal and state regulatory limits

Figure A
This workflow diagram displays the major steps in the annual MDL verification process.

03. Methodology

- LIMS & MDL Calculation Tool
- QMS & MDL Workflow
- Comparison of Limits

Related literature

2016 TNI V1M4 1.5.2.4
EPA 821-R-16-006

04. LIMS & MDL Calculation Tool

The LIMS-MDL tool helps analysts easily review data related to the MDL calculation and generate reports from data collected in the past 24 months.

- Web tool was created in-house and connected to the OCWD LIMS database
- Analysts can search by date range, analytical method, instrument ID, and analyte
- Analysts can review selected data (analyte, analysis date, QC standard ID, analysis method, related LIMS worksheet ID, related qualifiers)
- Over time, OCWD developed the report to have the LIMS worksheet ID as a link that displays comments related to the batch (see *Figure B*) to allow easy review of gross errors
- A full summary report is generated for each method, analyte, and instrument, and saved in a PDF format (see *Figure C*)
- The full summary report lists who calculated the value, when it was calculated, the analysis date range, analytical method, analyte, analytical instrument used, MDL spike levels, MDLs values, MDLb values, and a final comparison of the MDLs versus the MDLb
- A report comparing all related limits is generated to ensure compliance with LOQs, DLRs, and MCLs (see *Figure H*)

Figure B
The MDL tool displays QC sample data that will be part of the calculation and contains a hyperlink for analysts to immediately view additional comments and sample details if a qualifier was applied that requires further review.

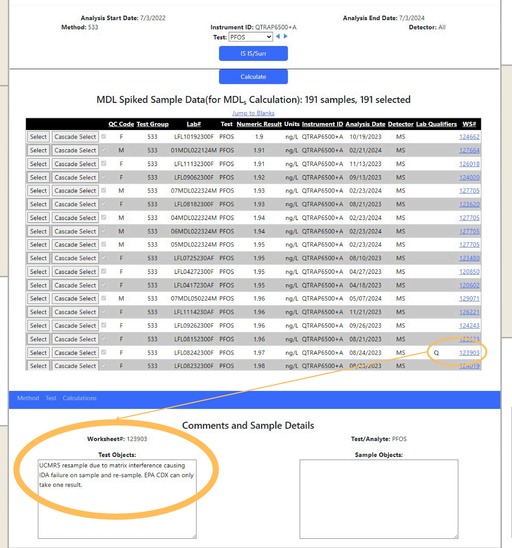
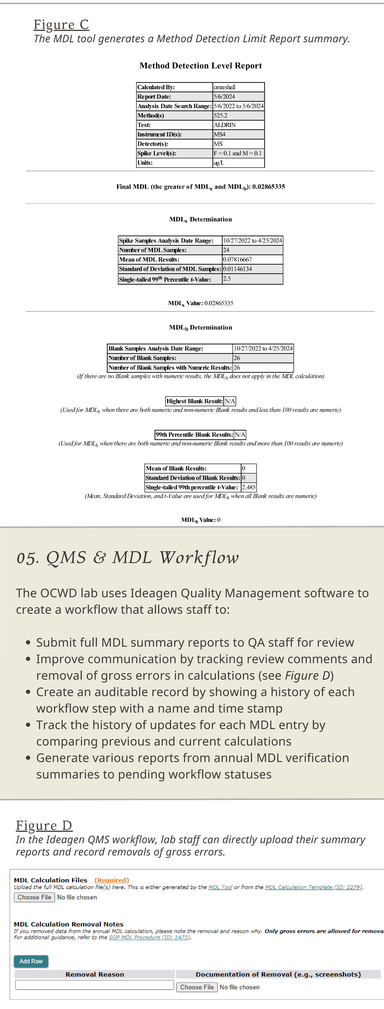


Figure C
The MDL tool generates a Method Detection Limit Report summary.



05. QMS & MDL Workflow

The OCWD lab uses Ideagen Quality Management software to create a workflow that allows staff to:

- Submit full MDL summary reports to QA staff for review
- Improve communication by tracking review comments and removal of gross errors in calculations (see *Figure D*)
- Create an auditable record by showing a history of each workflow step with a name and time stamp
- Track the history of updates for each MDL entry by comparing previous and current calculations
- Generate various reports from annual MDL verification summaries to pending workflow statuses

Figure D
In the Ideagen QMS workflow, lab staff can directly upload their summary reports and record removals of gross errors.

06. Comparison of Limits

- QA staff uses a spreadsheet to compare and verify the annual MDL calculated by the tool against the lab's published MDL and reporting limit (see *Figure E*).
- The spreadsheet will flag results if verifications are out of limits (50 -200% of the lab's published MDL) or above the reporting limit. Any verifications out of limits are flagged in the QMS-MDL workflow and a corrective action report is automatically generated (see *Figure F*).
- MDL verification results uploaded into the LIMS database are tagged with their effective date and expiration date (if applicable). This allows the laboratory to keep track of historical changes (see Figure G).
- All annual MDL verification results are uploaded into the LIMS database to generate a report that also shows other laboratory, state, or federal regulatory limits such as DLRs and MCLs. This report allows lab staff to see all limits in comparison to each other and is a helpful reference (see *Figure H*).

Figure E
A spreadsheet verifying the annual MDL has conditional formatting to easily see when the lab's published MDL needs to be updated.

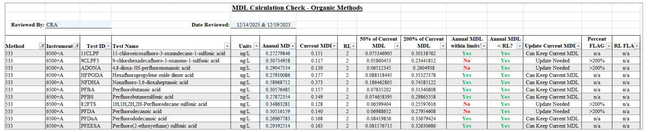
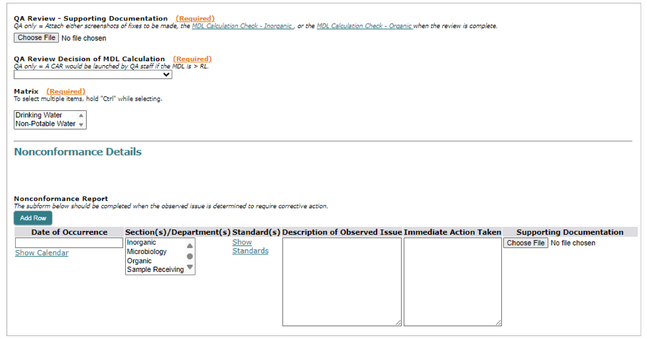


Figure F
QA staff fills out the Ideagen QMS workflow with review comments and the comparison spreadsheet to report the status of each annual MDL verification. If necessary, a nonconformance report is filled out to launch a corrective action report workflow.



07. Conclusion

Implementing these tools and software reduced human error and significantly decreased the time and effort it takes for all laboratory staff to complete the annual MDL verification. The workflow process is regularly evaluated and improved to meet changing regulatory requirements.

Figure G
This OCWD LIMS report summarizes the MDL data for each method, analyte, matrix, and instrument.

Limits As Of	Test Group	Test ID	MDL Matrix	MDL Instrument ID	MDL	MDL Units	MDL Prep Type	MDL Calculated	MDL Effective
04/26/2024	X200.8	Be	DW+NPW	ICPMS	0.16	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Al	DW+NPW	ICPMS	1.9	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	V	DW+NPW	ICPMS	0.17	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Cr	DW+NPW	ICPMS	0.33	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Mn	DW+NPW	ICPMS	0.28	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Co	DW+NPW	ICPMS	0.25	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Ni	DW+NPW	ICPMS	0.21	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Cu	DW+NPW	ICPMS	0.31	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Zn	DW+NPW	ICPMS	1.71	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	As	DW+NPW	ICPMS	0.23	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Se	DW+NPW	ICPMS	0.3	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Sr	DW+NPW	ICPMS	0.34	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Mo	DW+NPW	ICPMS	0.18	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Ag	DW+NPW	ICPMS	1.34	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Cd	DW+NPW	ICPMS	0.23	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Sb	DW+NPW	ICPMS	0.19	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Ba	DW+NPW	ICPMS	0.14	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Gd	DW+NPW	ICPMS	0.1	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Hg	DW+NPW	ICPMS	0.4	ug/L	Digested	11/01/2023	12/01/2023
04/26/2024	X200.8	Tl	DW+NPW	ICPMS	0.42	ug/L	Digested	11/01/2023	12/01/2023

Figure H
A report can be generated by staff using the OCWD LIMS to view the lab's published MDL, reporting limit, warning flags (action level), and state MCL.

Limits As Of	Test Group	Test ID	MDL Matrix	MDL Instrument ID	MDL Prep Type	MDL	MDL Units	MDL Calculated	RL	Action Level	MCL
04/26/2024	533	PFBA	DW+NPW	QTRAP 6500+	Cartridge	0.4428	ng/L	12/01/2023	2		
04/26/2024	533	PFHPA	DW+NPW	QTRAP 6500+	Cartridge	0.24137	ng/L	12/01/2023	2		
04/26/2024	533	PFHxA	DW+NPW	QTRAP 6500+	Cartridge	0.234	ng/L	12/01/2023	2		
04/26/2024	533	PFBS	DW+NPW	QTRAP 6500+	Cartridge	0.6115	ng/L	12/01/2023	2	375	
04/26/2024	533	PFMBA	DW+NPW	QTRAP 6500+	Cartridge	0.378	ng/L	12/01/2023	2		
04/26/2024	533	PFEESA	DW+NPW	QTRAP 6500+	Cartridge	0.387	ng/L	12/01/2023	2		
04/26/2024	533	NFDHA	DW+NPW	QTRAP 6500+	Cartridge	0.3359	ng/L	12/01/2023	2		
04/26/2024	533	4:2FTS	DW+NPW	QTRAP 6500+	Cartridge	0.4625	ng/L	12/01/2023	2		
04/26/2024	533	PFHxA	DW+NPW	QTRAP 6500+	Cartridge	0.5686	ng/L	12/01/2023	2		
04/26/2024	533	PFHxS	DW+NPW	QTRAP 6500+	Cartridge	0.39876	ng/L	12/01/2023	2		
04/26/2024	533	HFPODA	DW+NPW	QTRAP 6500+	Cartridge	0.4579	ng/L	12/01/2023	2	7.5	10
04/26/2024	533	PFHpA	DW+NPW	QTRAP 6500+	Cartridge	0.214	ng/L	12/01/2023	2		
04/26/2024	533	PFHxS	DW+NPW	QTRAP 6500+	Cartridge	0.4327	ng/L	12/01/2023	2	2.2	10
04/26/2024	533	ADONA	DW+NPW	QTRAP 6500+	Cartridge	0.4758	ng/L	12/01/2023	2		
04/26/2024	533	6:2FTS	DW+NPW	QTRAP 6500+	Cartridge	0.4156	ng/L	12/01/2023	2		
04/26/2024	533	PFOA	DW+NPW	QTRAP 6500+	Cartridge	0.552	ng/L	12/01/2023	2	5	4

08. Future Considerations

As the OCWD laboratory is continually improving, the following are future considerations to better the annual MDL verification process:

- Migrate the MDL tool to the OCWD in-house built LIMS rather than being a web-based tool.
- Add LIMS capability to categorize outlier QC results into those used in ongoing QC calculations (like MDL) and gross errors that will not be included.
- Create the comparison spreadsheet as an automated report in the OCWD LIMS.