Streamlining and Transparently Automating Complex Waste Determinations at Los Alamos National Laboratory-17286

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ABSTRACT

Environmental programs at Los Alamos National Laboratory (LANL) generate a large amount of sampling activities that can result in waste that needs to be characterized and properly disposed. Since 2011, sampling results are managed in the cloud-based Environmental Information Management (EIM) database, which contains over 16 million current and historical data records. In many cases, the database's analytical records are used to characterize and dispose waste from environmental operations. Three factors contribute to streamlining of the waste disposition operations: (1) if possible, use of the existing analytical data for waste characterization to avoid additional laboratory analysis; (2) reduction in time spent on data evaluation for various waste acceptance criteria; and (3) choice of the proper and least expensive disposal alternative. Use of the existing analytical data, when allowed by law, creates some paradoxical problems: when chemical analysis is requested with the purpose of characterizing waste, it creates only 100 to 400 analytical records. However, use of exiting analytical data at LANL may lead to evaluation of tens of thousands of analytical records, with many records for each single analyte. This occurs because data were collected for environmental characterization and not waste characterization. To streamline data analysis for waste disposition using existing data, LANL has created a Waste Data Summary (WDS) module in the site's EIM database.

Recognizing that waste determination is performed by groups outside the environmental program at LANL, the WDS allows for logically guided data selection for a specific waste determination (solids, liquids, radiological, etc.) and reduces potentially thousands of rows of data into simple formatted data reports that are easy to comprehend and process. This allows the waste evaluators to review data using multiple approaches to make their own determination on the most appropriate disposal method.

There are four basic principles of WDS operation: (1) The highest detected analytical result is evaluated for the selected samples (or the lowest undetected result if there are no detected results); (2) All approved disposal pathways are evaluated; (3) Any failures of the Waste Acceptance Criteria are visibly highlighted to focus the attention of the evaluator; and (4) The decision of the disposal path is left to the trained waste evaluator (WDS does not choose or suggest any disposal paths).

The summary results are presented as the set of short data reports. These reports can be divided into two groups: general comparison reports and disposal pathway specific forms. The general comparison forms show all Resource Conservation and Recovery Act (RCRA) analytes with pass/fail evaluation and with preference for toxicity characteristic leaching procedure (TCLP) results (or 20x rule) for solid samples, the potential RCRA hazard codes assignment for detected analytes, and all rad results. The detected chemical and radioactivity results are compared to the background values and to Soil Screening and Soil Action limits (SSL/SAL limits).

Disposal pathway specific forms follow Waste Acceptance Criteria requirements for all disposal pathways available at LANL. The programming of the WDS tries to maximize existing data by analyte substitutions (like using gross alpha for necessary alpha emitting isotopes) or by making calculations when analytical results do not agree with legal requirements (like total chlordane in the RCRA regulations, which is most often analyzed and reported as individual isomers).

All forms may be annotated by the waste evaluator to provide additional information to support decision making. Upon final decision of a disposal path, the complete dataset used in the evaluation and the WDS forms with annotations is "frozen" as an un-editable PDF export to document the data used in the waste disposal determination.

The streamlined process results in less work for waste evaluators and reduces overall labor and analytical costs. By comparison, a full review of a 10,000 record parent dataset may take a waste evaluator over a week to review, whereas with the WDS module, the task can be accomplished in less than one hour with clear, reproducible results. These results can be reviewed and checked at any time by quality assurance personnel, thus ensuring transparency in the decision making process. LANL believes this approach has broad applicability to other sites where waste determination is based on review of existing data collected for more generalized environmental purposes.

INTRODUCTION

WDS (Waste Data Summary) is a software module designed to take a set of analytical data from the cloud-based Environmental Information Management (EIM) system and assess that data based on Los Alamos National Laboratory (LANL) waste determination criteria and provide waste coordinators with sufficient information to make informed disposal decisions. The WDS is a replacement and enhancement for the existing LANL process that was performed with a series of Excel spreadsheets embedded with thousands of lines of macro code to perform the needed analyses. LANL desired a more robust and transparent process that was integrated with the source analytical data to ensure the most accurate and repeatable results for informing such important disposal determinations.

The WDS software is designed to perform simple statistics, compare the data to lists of limits, and provide a conservative summary of the chemical concentrations in the data. The data generated is normally from wastes (like soil cuttings from drilling a well or purge well water), although it can be applied to other types of samples as well. The WDS process produces over two dozen different summary reports that the LANL waste coordinators can use to determine appropriate disposal actions. The logic behind WDS is not particularly complicated, but there are numerous complex and prescribed rules to follow, both in general, as well as for specific parameters and reports. Following WDS generation and review in EIM, a subset of the data can be input into a different software system at LANL called the Waste Compliance and Tracking System (WCATS), where the final determination for the waste will be decided and the regulatory and formal reports will be generated. Although WCATS is the formal system of record for the waste disposal determination, data from EIM and results of the WDS analysis are also permanent records that support that environmental decision.

The WDS process, although built to LANL requirements, is sufficiently generic that it is applicable to other DOE sites facing similar waste determination needs.

WASTE DETERMINATION SUMMARY BUSINESS PROCESS

The overall waste determination business process is designed to be straightforward for the waste coordinator, whose job it is to evaluate the waste data results against a prescribed set of criteria. Then using the results of the analysis, coupled with domain expertise and knowledge of the operations that generated the waste, make a determination of the appropriate disposal path. The process of waste data analysis is shown in Figure 1 below.

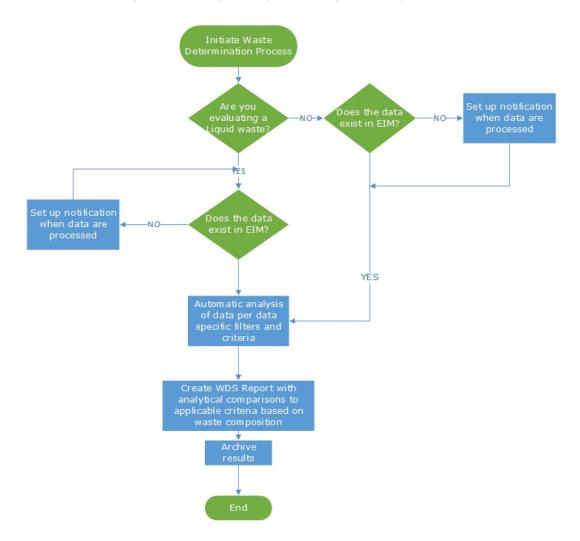


Figure 1 Overall waste analysis business process

There are four basic principles of WDS operation: (1) The highest detected analytical result is evaluated for the selected samples (or the lowest undetected result if there are no detected results); (2) All approved disposal pathways are evaluated; (3) Any failures of the Waste Acceptance Criteria are visibly highlighted to focus the attention of the evaluator; and (4) The decision of the disposal path is left to the trained waste evaluator (WDS does not choose or suggest any disposal paths).

From the user perspective, the process has been simplified to automatically guide the user through the various results and comparisons to enable them to rapidly draw accurate conclusions.

From the software configuration perspective, the complexity lies in the large number of rules, conditions, special cases, parameter substitutions and regulatory limits that have to be accurately applied to a wide range of complex analytical data sets.

APPROACH

LANL collaborated with Locus Technologies to start this process with an existing but complicated set of rules and reports codified in a large and complex Excel spreadsheet with macros developed over approximately 10 years. The original application was developed internally at LANL by an expert chemist and was continuously modified as analytical results presented variations not anticipated in the original design or when waste acceptance criteria was modified by statute or receiving facilities. It was also created to be highly automated to provide the users with a succinct set of reports for their use in the evaluation process. As with all automated programs, transparency was lost as the automation became more pervasive. Additionally, the original application was run on downloaded data sets from outside data systems, potentially generating issues when data are updated, corrected, validated or otherwise reviewed during normal data QA/QC processes.

A project team comprising of programing and technical experts from LANL and Locus Technologies was created to improve the process in multiple ways and set out the following approach:

- Revisit and review requirements for the application
- Embed the application in the same database as the source data
- Create a simplified work flow to users addressing existing data and anticipated data
- Enable easy access to the most recent underlying data so the user can immediately review any questionable item
- Clearly document the special conditions, parameter substitutions, and other "automated" calculations and regulatory limits so users and LANL application owners have transparency and reproducibility in the WDS process.
- Enable report archiving for long term information stewardship
- Reduce reliance on individual internal experts and "institutionalize" the process with professional support

Revisit and Review Requirements

To obtain the best application, a strong set of user requirements are essential. Often when transitioning from "home built" applications to something more

rigorous, there are often no documented requirements for how application operates. Typically, home grown "Excel" programs grow organically over time to encompass each new requirement, which result in a large, diverse body of coding that is almost impossible to dissect and replicate. The project team correctly realized the need to deconstruct the requirements one by one and started the process with a fresh look at what needed to happen, and laboriously went through the process in a series of all-day working meetings with domain experts to understand both the user perspective and the detailed evaluation rules hidden within the thousands of lines of code. This is arguably the most time and cost consuming part of any development or configuration process in software development. However, it is time well spent, as the actual programming of the requirements is far easier when developers have a clear set of specifications to follow. In this case, the requirements development took over a month and resulted in almost 200 pages of details for what was formerly a "black box" process.

The project team worked off a shared set of draft requirements with audit tracking to ensure nothing was lost in emails and all issues or corrections/questions were visible to be addressed.

Imbed the Application in EIM Database

From the onset of the process, it was determined the application would be a specific module of LANL's existing EIM system. This would allow LANL to streamline the number of supported applications and centralize regulatory reporting and analysis in a single system. It would also streamline obtaining data for the WDS process and enable LANL waste coordinators to work independently as their schedules allowed. It also provided LANL management more direct access and visibility of the process for overall review and quality assurance purposes. The need to track down individual decision "spreadsheets" from various locations was replaced with a simple system login and list of archived reports for review and permanent recordkeeping. Anyone with sufficient permissions can access the information at any time, thus eliminating the need to go through a discovery process to find the relevant information from a variety of sources.

Figure 2 shows the on-demand ability for anyone with permissions to review any completed WDS report. Figure 3 also shows the on-demand ability for anyone with permissions to review any "in process" or draft report.

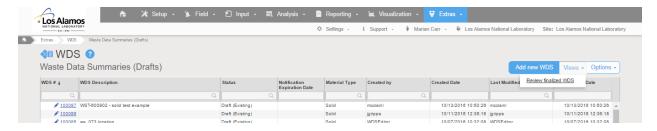


Figure 2 View of ability to review finalized WDS reports

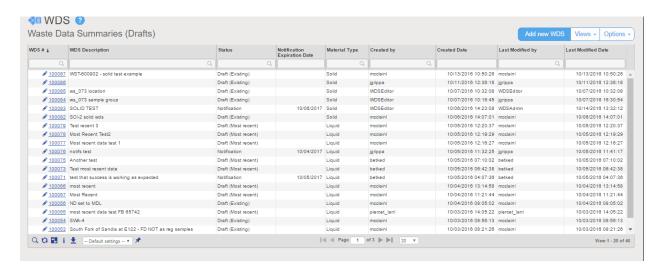


Figure 3. View of the selection screen for users and managers to review any of the in process WDS reports, providing access and transparency to the process

Simplify Work Flow

Before the new WDS process was added to the EIM database, the work flow was cumbersome and involved multiple steps. As shown in the work flow in Figure 4, users had to ensure use of the recent up to date spreadsheet and request a set of data from others at LANL to prepare the waste determination analysis. This introduced errors or delays in two ways: (1) using out of date analysis tools; and (2) depending on others to manually query and deliver the requested data set. The original "before" view of the Automated Waste Determination (AWD) process is shown in Figure 5. Any questions on the calculations was dependent on a single individual reviewing the lines of code and troubleshooting the issue. If that individual was not available, the analysis was delayed.

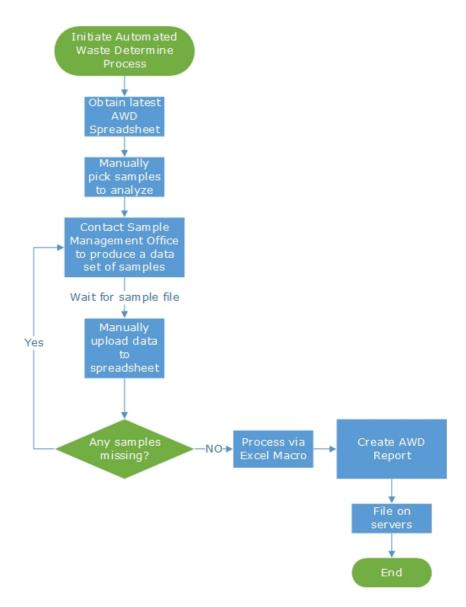


Figure 4. Original Automatic Waste Determination Process at LANL

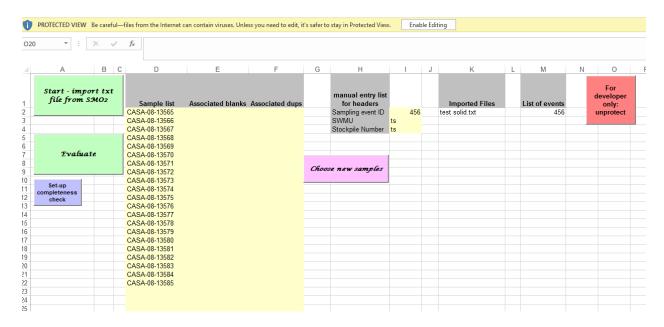


Figure 5 Original Work flow to create a waste determination report (AWD) at LANL

In the new WDS process, the user follows a simple work flow and answers a set of question screens to identify the type of analyses to be initiated, and select the relevant data sets. The process is simplified by guiding a user through the steps and allowing them to select and review data by sampling plans or other filters already in the database, where all status of samples are known.

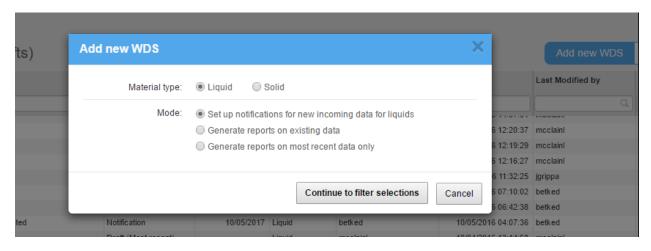


Figure 6. Start of the process, selecting the basic information for the scope of the report and the data used in the report.

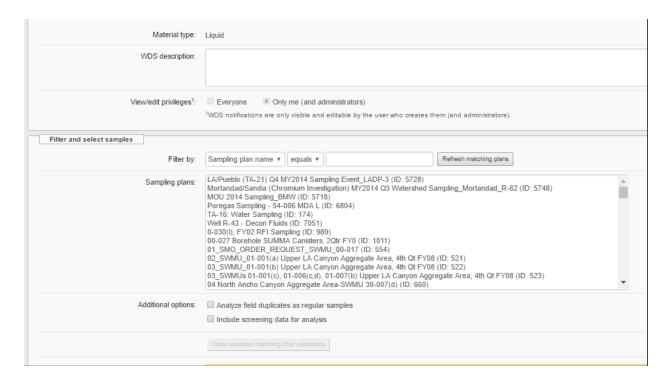


Figure 7. Selecting data to prepare a WDS report, including simplifying the process by selecting by sampling program

A waste coordinator is able to create new data summaries by selecting whether the WDS is for a solid or liquid matrix. Depending on the status of data in process, the user can determine if nightly email notifications are required, set data criteria filters in the system, or if perform WDS analysis on an entire dataset or only the most recent data for a given parameter.

Following selection of those high level choices, the user is then presented with a filter screen which allows the user to provide the filters to search the EIM database for the data to be analyzed. These include filtering by sampling plans, locations, location groups, and sample groups. After setting these master filters, a list of samples associated with those filters is presented, and the user may select any or all of those samples to be included in the downstream WDS analysis.

Enable Easy Access to Underlying Data

Because the WDS is integrated with the source database, users have access to all the underlying data that was used in the determination. The user has instant access the complete data sets and all the applicable information associated with the data including data validation status and track the data back to upload within the

EIM database. As shown in Figure 8, the user can select to see a "Total list of all data" associated with a specific WDS set of reports.

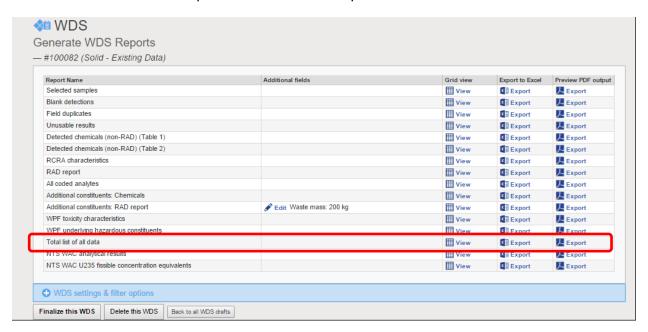


Figure 8 Screen shot of WDS menu for selecting Total list of all data report

In Figure 9, a data retrieval view shows all the relevant analytical data results associated with the samples that comprise the WDS within the grid. This data can also be exported into Excel or CSV file for further investigation as needed.

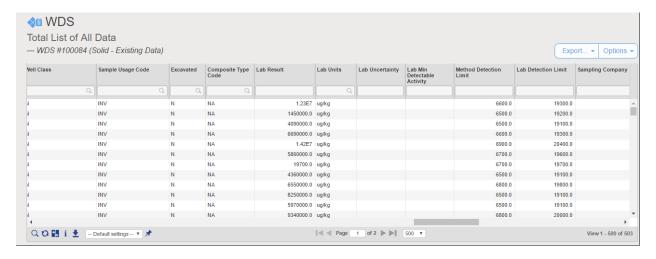


Figure 9 Detailed view of analytical data associated with a selected WDS

Document Special Conditions, Parameter Substitutions, and Other "Automated" Calculations

The complexity of waste acceptance criteria and land disposal requirements coupled with complex analytical data sets is a challenge for LANL. The majority of available characterization data (past and present) was collected for environmental investigation, reporting, and management purposes. This means the analytical methods were specific to the intended purpose of the sampling collection and were not focused on characterization of the samples for waste or land disposal. The simple answer would be to re-sample all the waste using waste characterization methods and use those data. However, this was cost prohibitive given the volumes of waste present at the LANL facility.

The special conditions analysis was designed based on chemistry to ensure data analyses using environmental data was sufficiently conservative and technically defensible to allow accurate determination of waste disposal options.

Table 1 Special Conditions, Parameter Substitutions, and Other Automated Calculations

Condition Name	Description	Purpose
Blank Detections	Produce report showing where chemical parameters were detected in laboratory blanks	Identify any chemical parameters that may be false positives due to laboratory contamination
Field Duplicates	Shows all results from paired REG-DUP samples as associated in the FIELD_SAMPLE_QC_PARTNER table, and will include a calculated Relative Percent Difference (RPD) with PASS/FAIL logic	Identify any chemical parameters that may be false positives due to field contamination
Unusable Results	Shows all results that have failed data validation or found to be not usable	Ensure only valid data are used in the WDS process
Filter Status results and action limits	Set of rules to address how to handle differences in filter status for combinations of analytical results and regulatory limits	Address the issue with mis-matched results when filter status of results or limits does not match

Condition Name	Description	Purpose
Special Parameter handling	Parameters which require special calculations to compare against disposal criteria include: pH, Radium, Aroclors, Xylenes, BHC, Chlordane, Endosulphans, Dichloropropene[cis/trans-1,3-], Nitrates, Phenols, PAHs, Trihalomethanes, Methylphenols, Nitrosodiphenylamine[N-],Total Toxic Organics (TTO), and	Address the differences in the actual data vs the waste disposal criteria that may say one parameter name, and not call out the various isomers or alternate names as are found in the data
	Nitrosodiphenylamine[N-],Total	

Example of Handling a Summed Aggregate Parameter

Often, the regulations for waste determination will list an individual limit associated with a total concentration for a set of isomers or similar compounds (like total toxic organics), but lab analysis for characterization may list the concentrations for those individual compounds separately. In this case, WDS needs to calculate "summed aggregate parameters", which are simply the calculated estimates of these totals. Due to differences, each individual summed aggregate parameter has guidelines on how to properly perform this estimate coded into WDS.

In the example below, the handling of Total Aroclor is described.

- Total Aroclor is a summed aggregate parameter and is always calculated as the sum of the other 7 Aroclors (Aroclor-1016, Aroclor-1221, Aroclor-1232, Aroclor-1242, Aroclor-1248, Aroclor-1254, Aroclor-1260) taken from the same sample.
- If one or more Aroclors are missing for a sample, still perform the sum, but add a comment that "Only X Aroclors out of 7 are present."
- There is currently no "Total Aroclor" parameter in the EIM database.
- If all 7 Aroclors are undetected for an individual sample, the total Aroclor result should carry a detect flag of 'N'.
- If any single Aroclor is detected, the detection flag will be 'Y' for the sample.

This is an example of addressing a parameter that is a sum of various isomers in the analytical data; one or more isomers may be present in the data, added and notated for the final analysis. There are other similar examples exist for parameters with multiple isomers. Any detection of any isomer will have the total indicated as detected for the waste determination.

Special Handling for Alpha/Beta Emitters

Radiological parameters provide additional layer of complexity by needing to determine if they are Alpha or Beta emitters. If a radiological parameter is not represented in the dataset, the program must first determine whether the missing parameter is an alpha emitter or a beta emitter. This is done by referencing the parameters DECAY_MODE in a static look up table

- DECAY_MODEs of Alpha_Transuranic and Alpha are alpha emitters, and modes of Beta_Without_Gamma and Beta are beta emitters.
- If a parameter is an "Alpha and Beta" emitter (or Gamma_only), no calculation is performed and the value would be listed as missing and FAIL for the WDS summary report.
- Once the program has determined the decay mode of the parameter (alpha or beta), then the program checks if there is a GROSSA or GROSSB parameter for that sample in the database.
 - If there is not a matching GROSS parameter (alpha emitter=GROSSA, beta emitter=GROSSB), then the value is listed as missing and FAIL for the analysis.
 - If there is a matching GROSS parameter, then the program calculates an adjusted value for that particular parameter, by subtracting the sum of all other detected emitters of that type (alpha or beta) from the GROSS parameter of that type and report that result for the missing parameter and compare PASS/FAIL.
 - Example: if the dataset is missing the Am-241 result and there is GROSSA and the other alpha emitters, in order to calculate the amount of Am-241 in the sample, subtract the value of the other alpha emitters (plutonium isotopes, U-235/236, U-234, U-238) from the GROSSA result if they are detected.
- In cases where a GROSSA or GROSSB subtraction is performed, a comment is added stating "Value determined using GROSSA" or "Value

determined using GROSSB" depending on the analyses to provide documented logic for program calculations to enhance transparency. There are also exceptions to consider based on method or isotope.

- Exceptions: if both U-235 and U-235/236 exist in the sample (both from Alpha spectroscopy method-HASL-300: ISOU), use only U-235/236 for any subtraction calculations (as above).
- Also, if either U-235 or U-235/236 are present (regardless of method), the other does not need to be calculated, the line will be listed empty with no values, and no pass or fail comparisons are performed.

Enable Record Archiving

A key requirement was an archived and immutable complete report of all analyses and data sets used in the WDS process. Once a WDS is complete, it becomes final in the database and can no longer be edited or modified. This ensures accountability for the decisions and leaves a clear audit trail. The program allows users to download a PDF version of the reports created by the WDS module, or it allows a link to the documentation to be entered in other programs for easy future access. Figure 10 shows the view of a finalized and archived WDS with detailed information about the filters and settings used, and a link to the archived PDF reports resulting from the analysis.

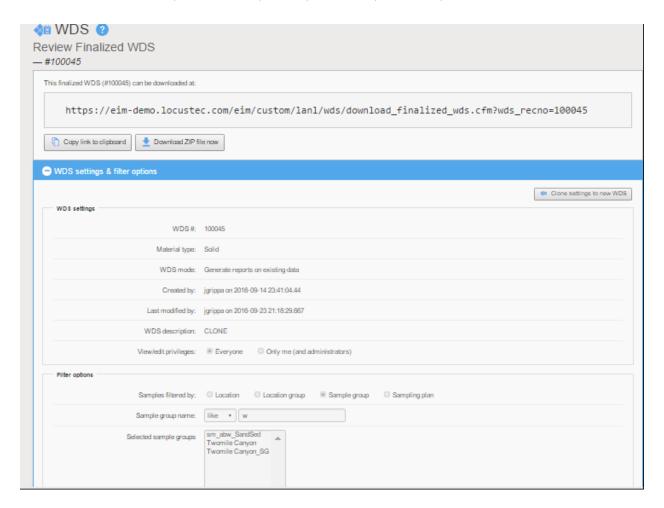


Figure 10 View of a Finalized WDS with links to download the archived PDF Reports

Institutionalize the Process

When LANL introduced a single unified environmental data management system, it streamlined a formerly complex approach to handling environmental information and created an efficient way of handling and reporting environmental data. As the new environmental data management system became institutionalized, the LANL managers sought to identify any remaining critical environmental data handling processes outside the system, and move them into a more formal and documented process. The AWD process, outlined in this paper, was one such process. Recognizing that data submitted to regulators or data used in environmental decision making required a high degree of QA/QC and transparency, LANL decided to move the AWD process to the EIM environmental data management system. Once the EIM system was integrated with normal daily operations at LANL, the

move to expand its charter was simple. Users were eager to have more advanced and reliable tools for making waste determinations, and were supportive of embedding the process into a data system well established at LANL. Having a vendor supported software allows the waste coordinators to perform work without relying on a single individual for support.

CONCLUSION

LANL and Locus Technologies worked together to simplify, streamline and consolidate LANL's existing AWD process to create the new WDS process. Since the EIM database stores all of LANL's environmental monitoring data, having WDS integrated with this system simplifies the analyses for waste coordinators to perform chemical summary profiles. Analyses can be performed on-demand and are continuously updated due to the direct connection with the source database.

Over the process of creating WDS, the AWD excel macros were carefully evaluated for continuing usefulness to the waste coordinators. The functionality which was deemed to be essential was clearly described in the scope of work, which will be maintained as part of the ongoing documentation for the WDS system. This process allowed LANL to streamline the WDS process, while making the functionality and coding easier to maintain, as well as making the process more transparent to all stakeholders.

The improvements to the waste analysis process at LANL should allow waste coordinators to retrieve the chemical data summary information to determine the appropriate disposal path for waste generated at the facility. This will assist in decreasing the holding duration of wastes generated at LANL, thus driving down costs for maintenance and storage, and ultimately, help to reduce the amount of on-site stored waste.