Pacific Northwest
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PNNL-35029

Online Analytics for Remedy Support at DOE Environmental Management Sites

September 2023

Christian D. Johnson
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U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Richland, Washington 99354

Summary

Environmental data is important for managing environmental restoration/waste site remediation, planning of monitoring efforts, addressing climate resilience, and engaging with stakeholders and regulators. A major challenge is how to manage the many different types and the large volume of environmental data in a way that allows practitioners and site managers to understand data implications and support decisions. The Suite Of Comprehensive Rapid Analysis Tools for Environmental Sites (SOCRATES, https://www.pnnl.gov/projects/socrates) is a web application that provides data access, visualization, and rapid analytics to help make sense of environmental data, support remedy decisions, and communicate information. Development of SOCRATES has been funded through the DOE Richland Operations Office (RL) to support communication and decision making for the Hanford Site, thus is only tied into Hanford environmental data. However, the capabilities of SOCRATES are more broadly applicable to DOE-EM sites engaged in environmental remediation and management. This report describes the work to develop mechanisms for bringing non-Hanford data into SOCRATES so that other DOE-EM sites could make use of the visualization and analysis capabilities to support communication and decision making related to managing environmental restoration/waste site remediation, optimization/exit strategies for pump-and-treat systems, planning monitoring efforts, addressing climate resilience, and/or engaging with stakeholders and regulators. The background, approach, data transfer formats, examples, and next steps (including deployment) for this new software, referred to as SOCRATES-EM, are described in this report.

Acknowledgments

This work was funded by the U.S. Department of Energy Office of Environmental Management Headquarters, who are gratefully acknowledged in this important endeavor to better utilize environmental data to make progress with cleanup remedies.

The work performed included contributions from members of the PNNL CATALYST team, including Joshua Wassing, Joseph Loftus, Eric Engel, Marcus Perry, Tycko Franklin, Ekman Kaur, Alex Buchko, Yusuf Afzal, John Garza, Frank Lopez, Hung Luu, Ben Farias Dela Mora, Jesus Fernandez, Derek Trom, and John Wilburn.

Acronyms and Abbreviations

3D	three-dimensional
API	application programming interface
AWS	Amazon Web Services
CAS	Chemical Abstracts Service
COPC	contaminant of potential concern
CR	carriage return
CRATES	Charting, Reporting, And TEmporal visualizationS
CRS	coordinate reference system
CSV	comma-separated value
DOE	U.S. Department of Energy
EC2	elastic cloud compute
EM	Office of Environmental Management
EPA	U.S. Environmental Protection Agency
EPSG	European Petroleum Survey Group
GALEN	Groundwater AnaLytics for the Environment
GFM	geologic framework model
IaaS	infrastructure as a service
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LF	line feed
LM	Office of Legacy Management
NIST	National Institute of Standards and Technology
NQA	Nuclear Quality Assurance
ORIGEN	Online Retrieval Interface for GEologic iNformation
PaaS	platform as a service
PGDP	Paducah Gaseous Diffusion Plant
PLATO	PLume Analysis TOol
PNNL	Pacific Northwest National Laboratory
PORTS	Portsmouth Gaseous Diffusion Plant
RDS	relational database service
REST	representational state transfer
RL	Richland Operations Office
S3	simple storage service
SOCRATES	Suite Of Comprehensive Rapid Analysis Tools for Environmental Sites
SRS	Savannah River Site
USGS	U.S. Geological Survey
VPC	virtual private cloud
WIPP	Waste Isolation Pilot Plant

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1.0 Introduction

Environmental data is important for managing environmental restoration/waste site remediation, planning of monitoring efforts, addressing climate resilience, and engaging with stakeholders and regulators. A major challenge is how to manage the many different types and the large volume of environmental data in a way that allows practitioners and site managers to understand data implications and support decisions. Specifically, across the U.S. Department of Energy (DOE) Office of Environmental Management (EM) complex of sites (and extending to DOE Office of Legacy Management [LM] sites) there is a need to interpret and analyze environmental data to assess operation and optimization of pump-and-treat systems, determine remediation endpoints/exit strategies, communicate conceptual models and cleanup risks/priorities, evaluate monitoring/sampling data to identify data gaps, and apply remote sensing data for characterization and change alerts.

The Suite Of Comprehensive Rapid Analysis Tools for Environmental Sites (SOCRATES, https://www.pnnl.gov/projects/socrates) is a web application that provides data access, visualization, and rapid analytics to help make sense of Hanford Site environmental data, support remedy decisions, and communicate information. SOCRATES includes a suite of modules for visualizing and analyzing the site 3D geological context/conceptual site model, groundwater levels and flow direction, water quality/contaminant concentrations, plume trends/dynamics, remediation system performance, waste site risks/priorities, and remote sensing data. Development of SOCRATES has been funded through the DOE Richland Operations Office (RL) to support communication and decision making for the Hanford Site, thus is only tied into Hanford environmental data. Developed by the Pacific Northwest National Laboratory (PNNL) for DOE-RL under a NQA-1[1] compliant quality program, SOCRATES includes capabilities that meet specific Hanford needs related to pump-and-treat data, geologic framework data visualization, plume analysis, and more.

The capabilities of SOCRATES are more broadly applicable to DOE-EM sites engaged in environmental remediation and management. Multiple sites, including Idaho National Laboratory (INL), the Waste Isolation Pilot Plant (WIPP), Savannah River (SRS), Los Alamos National Laboratory (LANL), Paducah Gaseous Diffusion Plant (PGDP), and the Portsmouth Gaseous Diffusion Plant (PORTS) have expressed interest in understanding SOCRATES and the potential applications and benefits for working with their environmental data. To expand application to other EM sites, the SOCRATES framework needs features for connecting to non-Hanford data sources (where the intent would be segregation of a site's data in a separate instance/deployment of the software).

[1] Nuclear Quality Assurance (NQA-1) is a national consensus standard established and maintained by the American Society of Mechanical Engineers (ASME) for quality assurance in the nuclear industry.

1.1 Objectives

The overall objective of this work was to develop mechanisms whereby non-Hanford data could be brought into SOCRATES so that other DOE-EM sites could make use of the visualization and analysis capabilities to support communication and decision making related to managing environmental restoration/waste site remediation, operation/optimization/exit strategies for pump-and-treat systems, planning monitoring efforts, addressing climate resilience, and/or engaging with stakeholders and regulators.

The specific goals of this work were to 1) define the data transfer approach and the data content/format, 2) implement and demonstrate functionality for bringing in non-Hanford groundwater well, chemistry, and water level data, and 3) implement and demonstrate functionality for bringing in non-Hanford data to depict the subsurface geology in three dimensions.

This work will result in a new version of SOCRATES that extends applicability across DOE-EM sites, supporting environmental data evaluation, remedy decision-making, and communication. This proposed work is focused on making a SOCRATES framework that is data-source agnostic, allowing other DOE-EM sites to leverage existing functionality. This new version is referred to as "SOCRATES-EM" to distinguish it as the application with a generic data ingestion workflow. SOCRATES-EM will be separate from the SOCRATES deployment for the Hanford Site. The approach for SOCRATES-EM deployment is to have separate instances for each site that uses the software and/or to use role-based access control to limit access to a site's data.

2.0 Overview of SOCRATES-EM

As noted above, SOCRATES-EM is a web application that provides data access, visualization, and rapid analytics to help make sense of site environmental data, support remedy decisions, and communicate information. SOCRATES-EM promotes technical communication through sharing, reproducibility, and availability. The software also provides a consistent, technically defensible approach to support decisions about exit strategies, remedy optimization, adaptive remedy decisions, and monitoring plan decisions. SOCRATES-EM is a platform (or framework) for working with site environmental data, for which access is controlled either through separate deployments for each site and/or role-based access control.

SOCRATES-EM is comprised of a suite of modules for visualizing and analyzing the site 3D geological context to frame the conceptual site model, water quality, contaminant concentrations, plume trends and dynamics, remediation system performance, and groundwater levels and flow direction. The modules relevant to SOCRATES-EM (Figure 1) are ORIGEN, CRATES, PLATO, and GALEN, which are described in the sections below. ORIGEN is for working with geologic framework models and wells, while the other three modules are for working with groundwater chemistry and water level data, in addition to well information. The modules can be accessed via the dashboard landing page (Figure 2), which also lists any saved sessions for reference or loading.

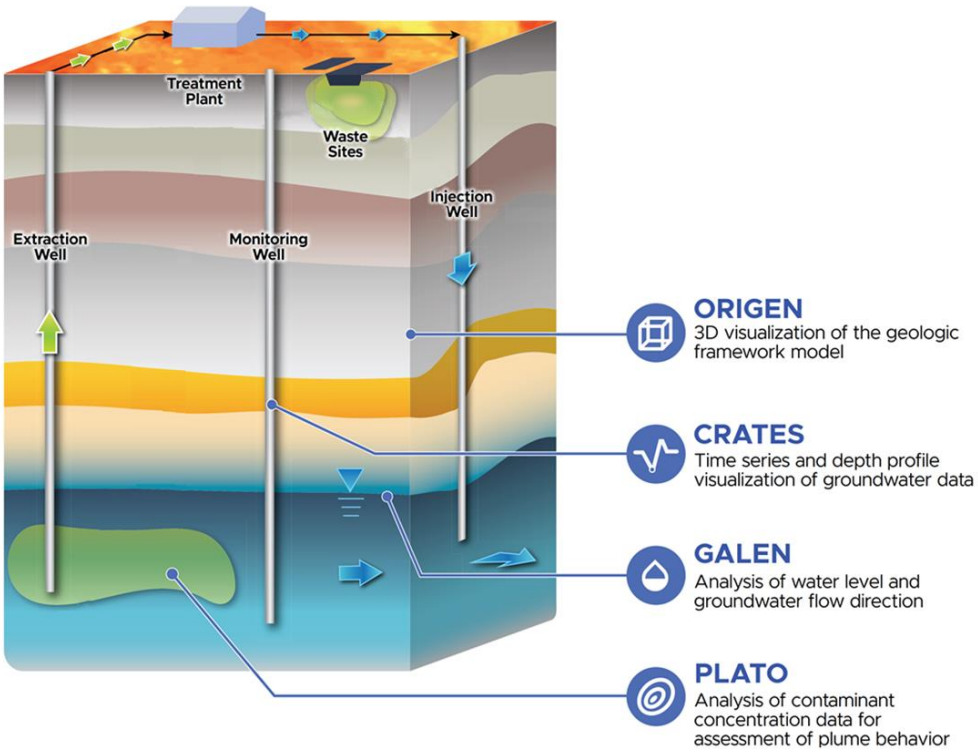

Figure 1. Modules comprising SOCRATES-EM. The SOCRATES application for the Hanford site includes additional pump-and-treat, waste site, and remote sensing modules that are not currently available in SOCRATES-EM.

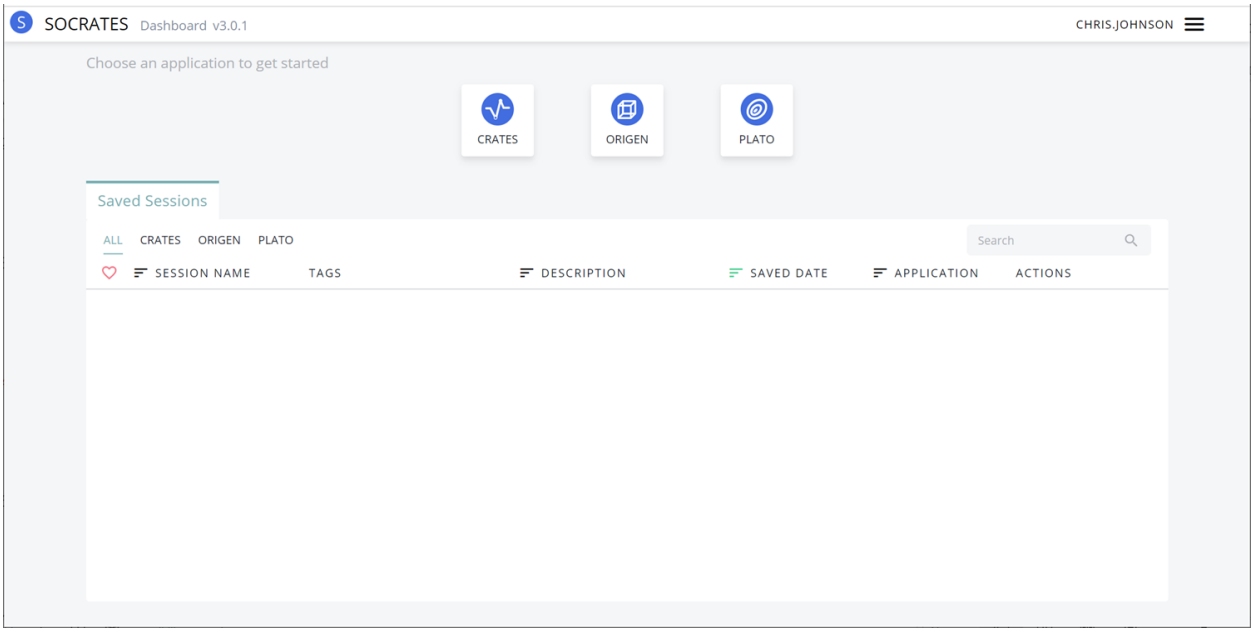

Figure 2. SOCRATES-EM dashboard (landing page after logging in) showing links to open the modules and to access saved sessions. The GALEN module is pending final touches.

2.1 ORIGEN (Online Retrieval Interface for GEologic iNformation)

Three-dimensional geological models represent the interpretation of rock and sediment structure in the subsurface, providing information that can support the management of groundwater remedies, water supply assessments, and subsurface storage. The ORIGEN module is a viewer to access and communicate about site geology, with features to create cross sections and access information on stratigraphic thicknesses and well construction information (Figure 3). A site provides a geologic framework model in the form of a set of surfaces that represent the top surfaces of each geologic unit (the data required is described more in Section 5.0).

ORIGEN allows a section of a site geologic framework model (GFM) to be displayed in an interactive three-dimensional (3D) viewer and to be interrogated for key information. Wells, and optionally well screens, can be displayed in the 3D view to provide context for understanding the subsurface and a site conceptual model. The 3D GFM itself can be interrogated to obtain the depths to the different geologic unit surfaces at an arbitrary user-selected location. When the user searches for or selects a well, available information on the well construction and lithology are depicted. Vertical poly-line cross sections through the 3D model can also be created, with an option for zooming in on the z-axis. If a cross section definition includes a well, then the well and well screen are also depicted in the cross section. The cross section can be exported as a nicely formatted image for sharing or inclusion in a report.

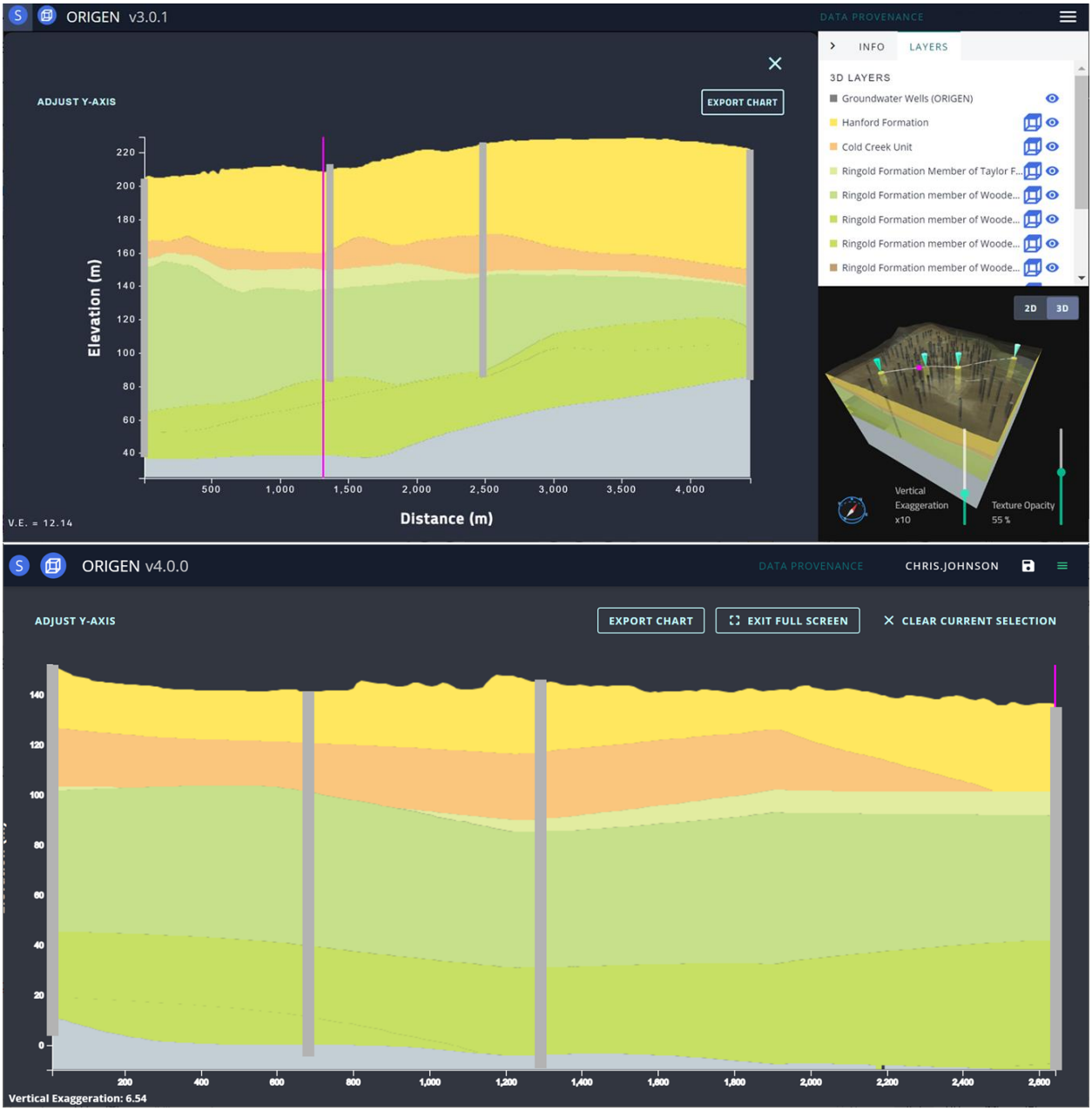

Figure 3. Screenshots of ORIGEN showing the 3D view and the cross section view.

2.2 CRATES (Charting, Reporting, And TEmporal visualizationS)

Although the visualization of groundwater data can be straightforward, it is often complicated by the existence of disparate data sources and data qualifiers describing the quality of the data. CRATES provides visualization of groundwater concentration data, streamlining data visualization, and supporting environmental management, remedy decisions, and technical communication. CRATES enables the user to easily identify well locations for plotting user-specified groundwater parameters/constituents of interest. Data can be plotted as a time series

(Figure 4) or, when depth information is available, as a depth profile (Figure 5). CRATES can be used for assessing monitoring data, to identify missing data or invalid data. CRATES can also be used for remedy performance assessment to assess questions about completion of a remedy, remedy effectiveness, or impacts of boundary conditions based on trends at individual wells and/or collectively for multiple wells. The user can specify the parameters, wells, and time frame of interest, with options to show and hide samples with filtered/unfiltered or reject/suspect attributes. Data can also be viewed in a table and both the table and the plot can be exported.

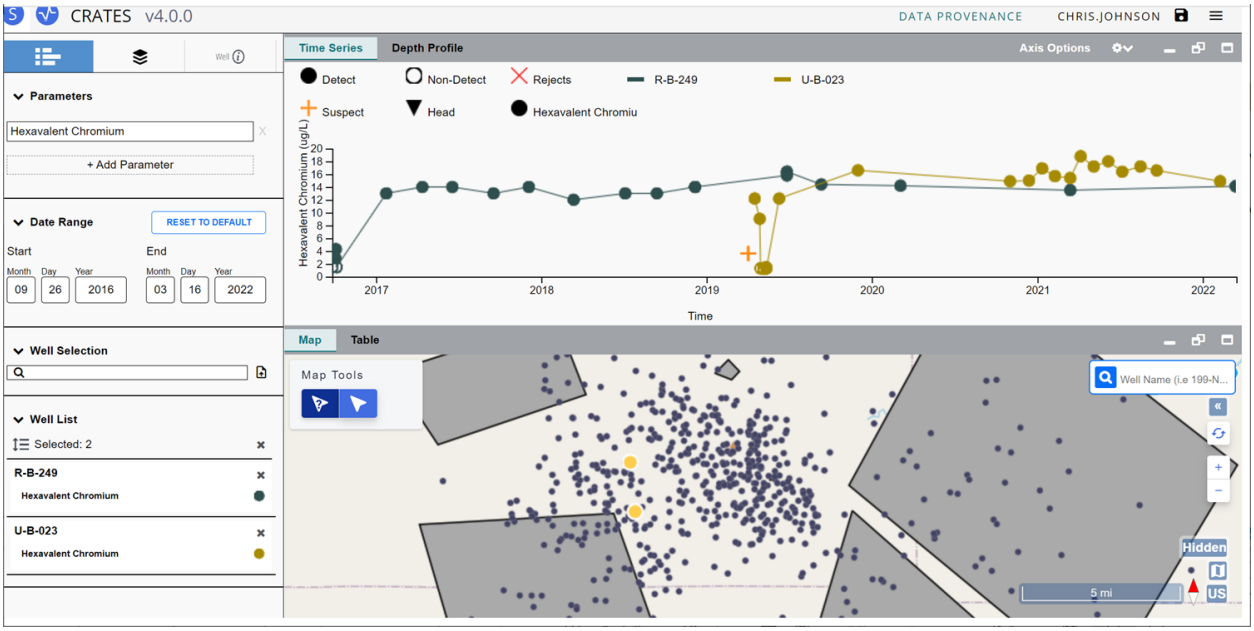

Figure 4. Screenshot of CRATES depicting the map and the time series plot.

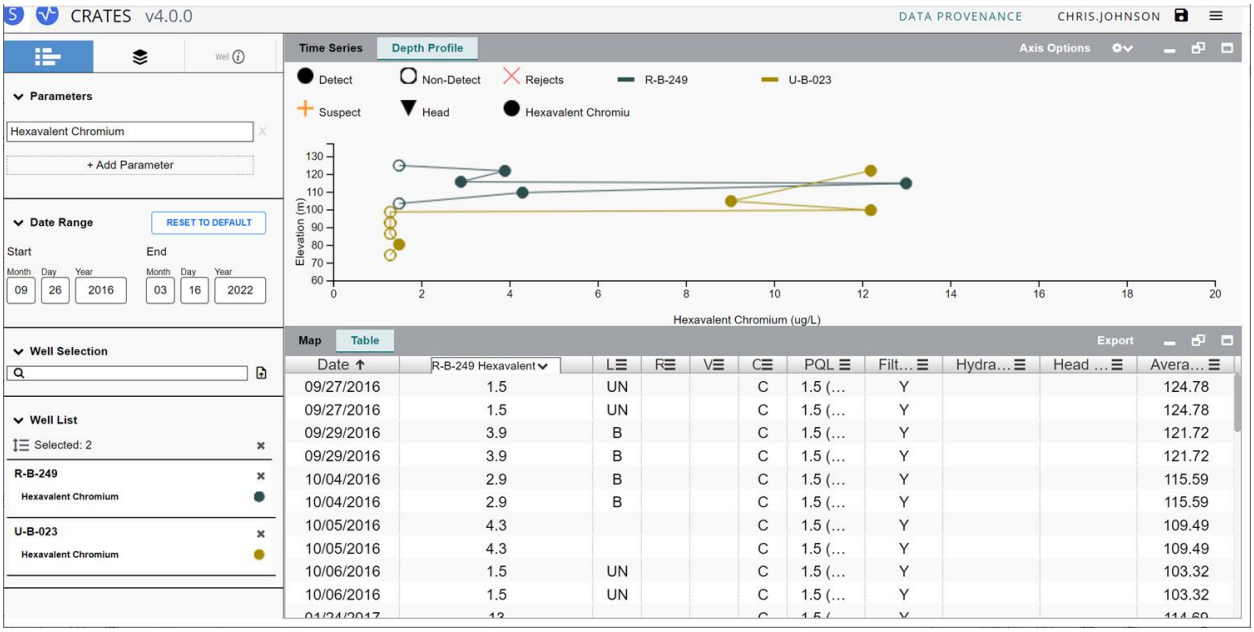

Figure 5. Screenshot of CRATES depicting the data table and the depth profile plot.

2.3 PLATO (PLume Analysis TOol)

PLATO analyzes groundwater data to assess contaminant plume behavior, providing a consistent framework to quantify groundwater contaminant plume dynamics that support remedial decisions about remedy performance assessment, remedy optimization, and monitoring needs. The PLATO analyses also allow assessment of plume attenuation, which is a key quantity for determining an exit strategy for pump-and-treat systems. PLATO implements data-driven, quantitative analyses based on standard statistical methods and published guidance from the U.S. Environmental Protection Agency and U.S. Geological Survey (EPA, 2002; Truex et al., 2015, 2017; Truex and Johnson, 2016).

PLATO enables rapid visualization (Figure 6) of groundwater concentration data, providing filters for well selection based on well attributes such as type, location, and geologic unit interrogated. In addition, PLATO allows rapid selection of wells with groundwater samples from the same time periods. This is accomplished by organizing well data based on temporal coverage, with histograms providing a visual indication of the consistency in sampling times.

PLATO provides two modes of analysis, single well and multi-well. In the single-well analysis, concentration data can be assessed with linear and exponential trends to see the regression statistics, plotted trend lines, confidence intervals, and prediction intervals for a single well. The multi-well analysis provides the same type of analyses and results, but for a group of wells (i.e., to represent the behavior of a plume. For both modes, analysis uses average concentrations in each time interval (bin) within the selected time window, where the time intervals can be 1-6 months or 1-6 years in size. The multi-well analysis also allows selection of either equal weighting or area-based weighting to reflect plume contaminant mass.

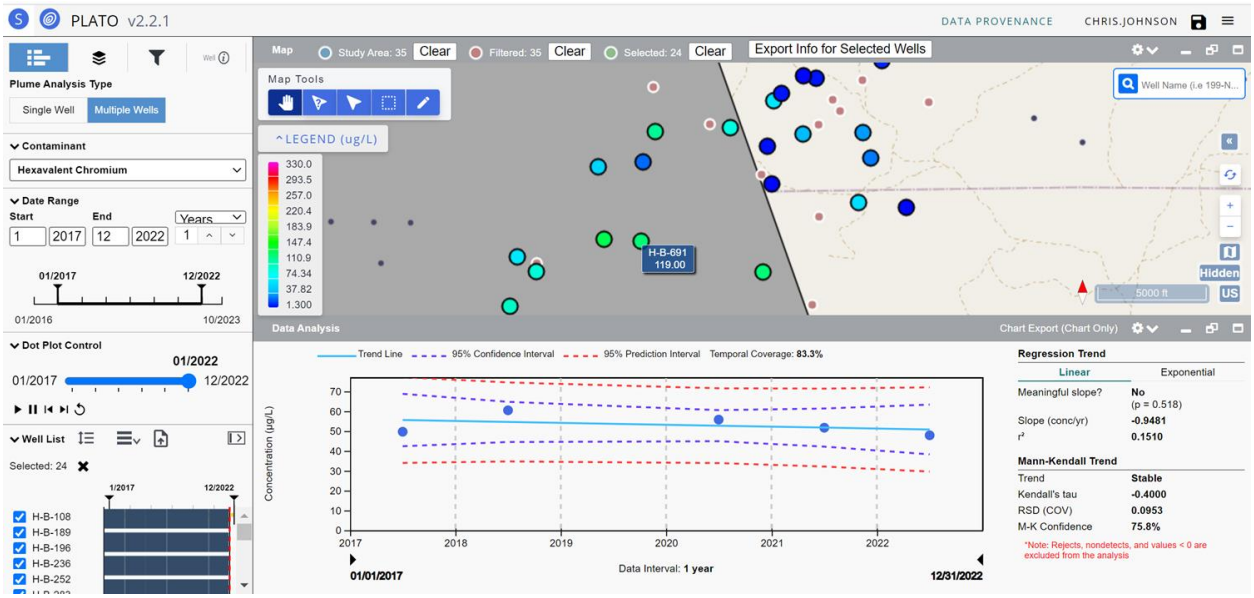

Figure 6. Screenshot of PLATO depicting a multi-well trend analysis plot and statistics for groundwater concentration data.

2.4 GALEN (Groundwater AnaLytics for the Environment)

GALEN is intended to provide access to multiple sources of water level data through a single access portal. It includes tools for visualization and analysis of groundwater level and flow direction over time, key elements in supporting site characterization and enhancing remediation system design and performance monitoring. GALEN enables rapid visualization of groundwater level data, providing filters for well selection based on well attributes such as type, location, and geologic unit interrogated.

Visualization and analysis of aquifer hydraulic head data facilitates understanding of groundwater plume behavior in terms of the migration path and rate of travel. Seasonal or other temporal changes in water levels can also be assessed for implications on groundwater plumes. Data is presented in summary form, plotted as a time series, and tabulated in a table (Figure 7). Time series data can be displayed as the original data values or using several data smoothing options (e.g., running median, Gaussian) to better see the overall trend. Data from manual water level measurements versus data collected via sensors, such as water level/pressure transducers.

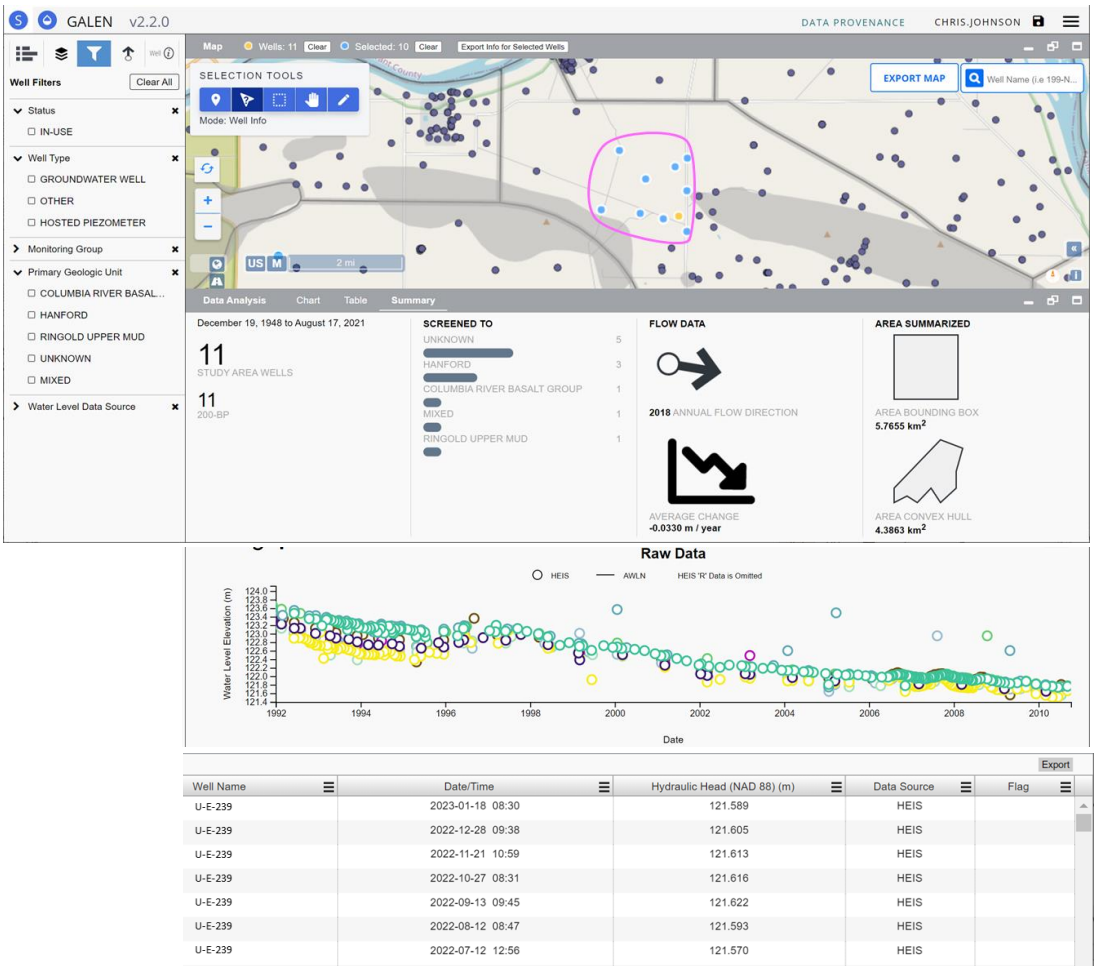

Figure 7. Screenshots of GALEN depicting the map, summary information, time series plot, and data table.

3.0 Technology Behind SOCRATES-EM

SOCRATES-EM is hosted using the Amazon Web Services[2] (AWS) cloud infrastructure, taking advantage of serverless architecture (Figure 8) to provide robust performance and easy maintenance. Serverless functionality is essentially "code as infrastructure" and avoids having physical or virtual machines.

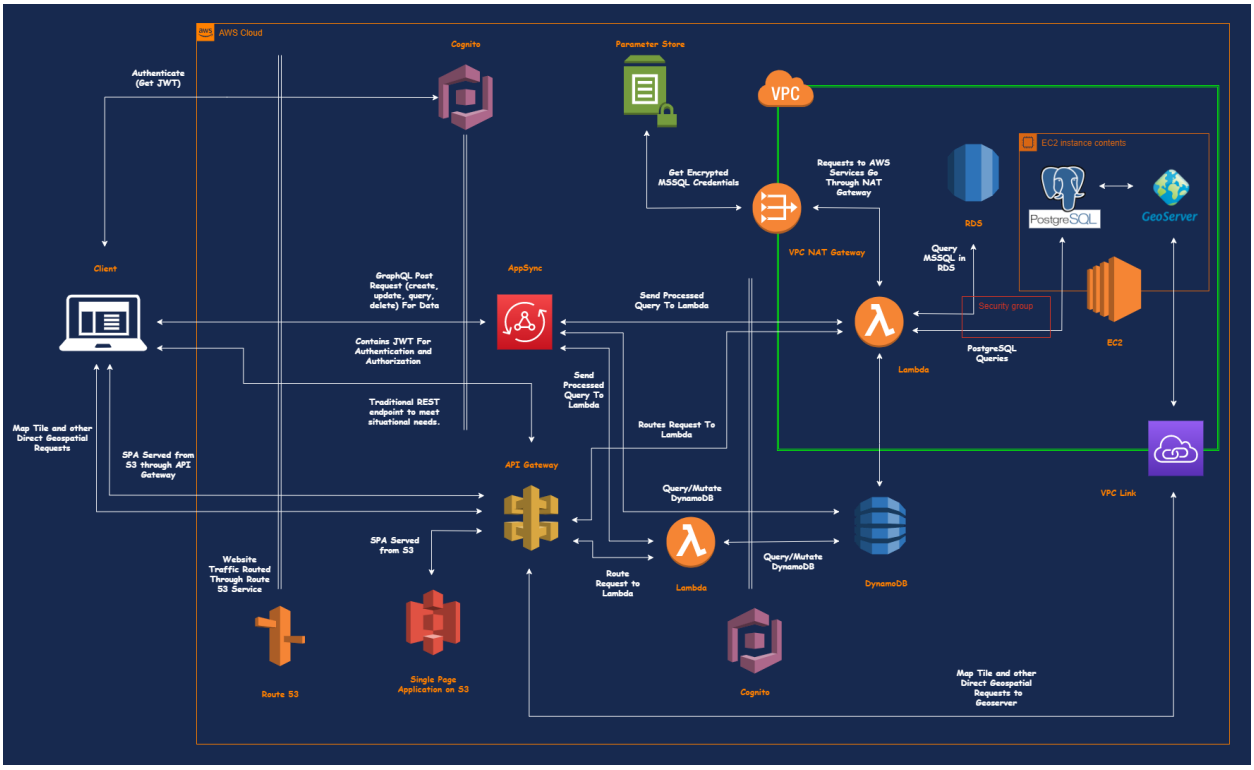

Figure 8. AWS serverless architecture used for SOCRATES-EM.

AWS components used for SOCRATES-EM include the following.

- Route 53 – AWS service responsible for managing registered domains and routing rules.
- Cognito – AWS service for user authentication/authorization and role-based access.
- S3 – AWS simple storage service for storage of files (including the data ingested into SOCRATES, which is described in Section 5.0)
- AppSync – AWS service allowing connections between client requests and data for the application.
- API Gateway – AWS service for routing https calls from Route 53 (i.e., from the client) to AWS services.

[2] https://aws.amazon.com/

- Lambda – AWS service for function code that can perform a variety of data ingestion, fetching, and calculation operations.
- Parameter Store – AWS service for encrypting information, such as database credentials.
- DynamoDB – AWS service for a NoSQL key/value pair database.
- Aurora – AWS service for a Postgres database that used for geospatial and other data.
- RDS – AWS relational database service for a SQL Server database.
- Fargate – AWS serverless compute engine that is an alternative to a virtual machine for calculations, Geoserver[3], etc.
- EC2 – AWS elastic cloud compute virtual machine for running servers, calculations, etc.
- VPC – AWS virtual private network service for segregation/protection of other services, such as virtual machines.

Implementation of SOCRATES-EM on AWS means that a shared responsibility model for cyber security is employed. In this model, the cloud provider (i.e., AWS) is responsible for protecting the infrastructure and all services offered. PNNL's responsibility, as the application developer, is determined by the cloud services selected and their specific agreements, as well as their documentation. PNNL has implemented native security tools and processes to help meet NIST 800-53 R4[4] and industry best practices[5]. All cloud projects are monitored by PNNL cyber security via AWS GuardDuty and other alerts. Security for infrastructure as a service (IaaS), such as AWS EC2, is configured and managed by PNNL. Security for platform as a service (PaaS) elements, such as the AWS RDS, requires PNNL management of users and access levels. SOCRATES-EM operates in a close to 100% serverless environment and uses very limited IaaS.

[3] https://geoserver.org/

[4] https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.800-53r4.pdf

[5] https://d1.awsstatic.com/whitepapers/AWS_Cloud_Best_Practices.pdf

4.0 Approach for SOCRATES-EM

The approach for implementation of SOCRATES-EM was to first define Hanford-specific elements or assumptions that would need to be reworked, define the data sources and data formats for ingestion into SOCRATES-EM, build out CRATES, build out the initial structure for PLATO and GALEN, build out ORIGEN, finalize PLATO, finalize GALEN, perform testing and documentation. Adding example data was part of the build-out phases to have data for testing and demonstrating the functionality. Data for a fictitious site and for actual EM-Sites were targeted for inclusion. All of these items were completed except for finalizing GALEN and obtaining a full set of actual EM site data, which are part of the next steps described in Section 7.0.

The SOCRATES web application for the Hanford site was leveraged to develop the SOCRATES-EM application that is data source agnostic. There are two primary areas of focus for this transition: the backend code/infrastructure, and the method for bringing data into the application. A third area pertains to deployment for site adoption.

4.1 Reconfiguring the SOCRATES Framework for non-Hanford Data

Initial planning reviewed the codebase and existing approaches to determine areas that needed to be made more generic and areas where processing or cost efficiency could be improved. The backend required stripping out Hanford-specific items based on assumptions about the data and reconfiguration of services to be more amenable to generic data. Data fetching calls were switched form a GraphQL query approach to a REST[6] endpoint approach. The Geoserver map server functionality was transitioned from implementation on an AWS EC2 virtual machine to using the AWS Fargate service and the Aurora Postgres database. AWS lambdas were reconfigured to allow for new data sources and data processing workflows. AWS SQL Server database tables were transitioned to the more cost-effective Dynamo database.

4.2 Adding data to SOCRATES-EM

The other significant transition item was the approach for ingesting data. The Hanford Site SOCRATES application is tied directly into a database snapshot for well, chemistry, and water level data, and geologic framework models are manually added to the SOCRATES backend database. Clearly, this approach needed revision to allow non-Hanford data to be used in SOCRATES-EM. Two approaches were considered, as depicted in Figure 9. In one approach, a site would have (or would set up) a data service (endpoint), from which specific data could be fetched through a network request. A data service can be very convenient for pulling in data, particularly when there are routine updates such as new chemistry results. A data service is less pertinent for data that changes infrequently (i.e., yearly at most). Additionally, setting up a data service will typically require a process of cyber security reviews and guardrails to mitigate

[6] REST (Representational state transfer) is a software architectural style defining how computer systems communicate. See https://en.wikipedia.org/wiki/REST.

potential misuse of the data connection. The other approach is for a site to upload data via files formatted in a defined structure. Files with appropriate names and file structures (described in Section 5.0) can easily be uploaded to an AWS S3 bucket, where file uploading triggers an AWS Lambda function to parse the data and add it to the SOCRATES-EM database, making it available in the application web interface. The second approach of uploading files was selected for the initial implementation of SOCRATES-EM. As sites set up data services in the future, they can be incorporated as data sources.

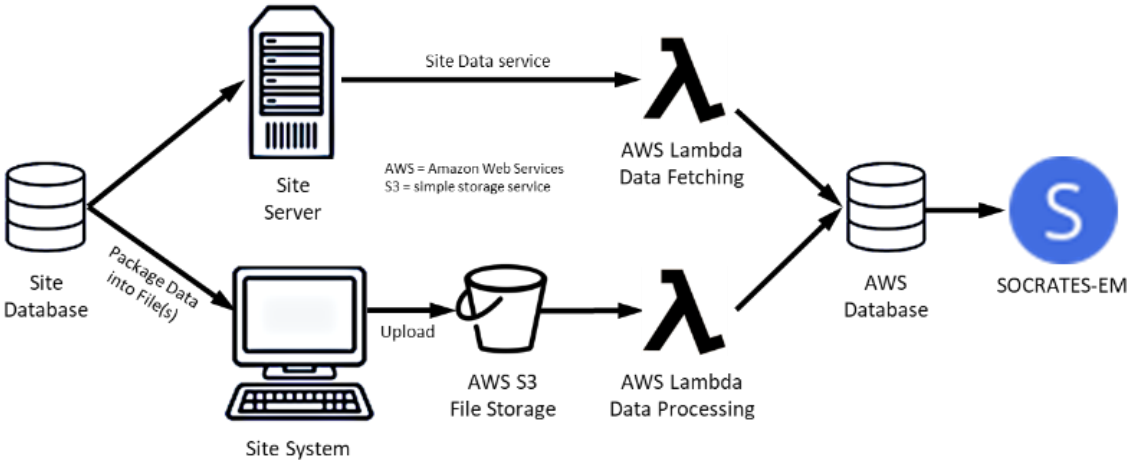

Figure 9. Processing workflow options to bring site data into SOCRATES-EM.

4.3 Deployment Options

SOCRATES-EM is a web-based single-page application built on AWS services (Section 3.0), and thus requires hosting. The hosting costs are associated with the AWS framework and will vary depending on site usage, but are generally quite reasonable. The highest cost service is the RDS SQL Server database, but this service has been replaced in SOCRATES-EM with the more cost-effective Aurora database.

Deployment has two primary options, hosting within a site's existing AWS capabilities or hosting at PNNL paid for by the site. The distinction between the two options is who controls the AWS account and does maintenance. System security can be similar in both cases. So, the choice is mainly based on site preferences. In either case, there are some initial costs for setting up the AWS account and connecting all the necessary AWS services. Once configured, the primary maintenance activities would be user management via AWS Cognito and ingestion of new data. As long as the data adheres to established formats, the data updates are mostly automated (aside from map layers). In the initial protype release of SOCRATES-EM, PNNL is hosting the application with data from a fictitious site (and LANL data expected early in FY24, as noted in Section 7.1). As PNNL works with EM sites for adoption, part of the discussion will be the preferred deployment option.

5.0 Formatting Data for Ingestion

Data is ingested into SOCRATES-EM via comma-separated value (CSV) format files[7] of specified names and with specified fields. As described above, data is ingested by adding the files to an S3 bucket and processing with a serverless lambda function to store the data in the SOCRATES-EM database. Some of the data will be a single (or very infrequent) upload, while other data types may involve multiple ingestion events to append new data.

It is important to note a few items regarding the format of the CSV data files. A CSV file stores tabular data in plain text as a set of comma-separated values (fields or columns), with each row in the file comprising a separate data record. Except where noted in the sections below, CSV files for SOCRATES-EM consist of one row with field names (the "header" row), followed by one or more rows of data records. Field values may be required or optional. When a field is not required to have a value and there is no value for that field for a given record, then a placeholder value of "null" is expected in that field. That is, a value of "null" should be used instead of a blank field represented by successive commas. Double quotes are recommended around a field value when a field value contains spaces, commas, or other punctuation characters. The CSV file is expected to use MS-DOS-style lines that end with carriage return/line feed (CR/LF) characters, in contrast to UNIX-style lines that end in only a LF character. Line end characters are optional for the last line.

The sections below describe the data file formats and fields for the following kinds of information that can be accessed, visualized, and analyzed in SOCRATES-EM:

- Site location
- Groundwater wells
- Lithologic units
- Geologic framework model
- Contaminants of potential concern
- Groundwater chemistry data
- Water level data

5.1 Site Location

The "Site_Center.csv" file consists of a header row and a single data value row. The data specifies both the coordinates for the center of the site and the initial zoom for map views, which are used to set the initial view of the site on SOCRATES-EM maps. An example of the file is shown in Figure 10. All fields are required. Coordinates must be in the EPSG 3857 pseudo-Mercator coordinate reference system (CRS)[8]. The most appropriate initial zoom depends on the site size,

[7] CSV files for SOCRATES-EM has similarities with, but differs from, the RFC 4180 technical standard for the MIME type "text/csv" (Shafranovich, 2005).

[8] EPSG codes, originally developed by the European Petroleum Survey Group, are maintained by the International Association of Oil & Gas Producers (IOGP, https://www.iogp.org/). EPSG 3857 is the "WGS 84 / Pseudo-Mercator" CRS that is used for web mapping applications. Information on EPSG is available via websites such as https://epsg.io/3857 or https://epsg.org/crs_3857/WGS-84-Pseudo-Mercator.html.

but is probably in the range of 20-40 (a zoom factor of 30 was used for the nominal 38,000 m width of the fictitious example site discussed in Section 6.0).

```
easting_3857,northing_3857,initial_zoom
-11925398.81,5385136.886,30
```

Figure 10. Listing of an example "Site_Center.csv" file, showing the required header line and example coordinates and zoom level.

5.2 Groundwater Well Information

Much of the capabilities of SOCRATES-EM are centered around groundwater data, which is typically obtained as point data via wells. Thus, groundwater well information is key for visualizing, interpreting, and analyzing the groundwater data. Table 1 lists the fields for a well record as part of the "Well_Information_GW.csv" data file.

Some key notes about select fields:

- The easting and northing values can be in a CRS appropriate for the site. However, the easting_3857 and northing_3857 values need to be in the EPSG 3857 pseudo-Mercator CRS, in meters.
- The well_type value should consist of one of the following options: GROUNDWATER WELL, AQUIFER TUBE, PIEZOMETER, BORING, PROPOSED SITE, or CANCELLED SITE.
- The status field value should consist of one of the following options: AWAITING DRILLING, DRILLING CANCELLED, CANDIDATE FOR DECOMMISSIONING, IN-USE, or DECOMMISSIONED.
- See the discussion in Section 5.3 related to defining the geology (primary lithologic unit) intersected by the well screen.

Table 1. Fields for the "Well_Information_GW.csv" data file.

Field Name	Description	Required?	Format	Example
well_name	Well name	Yes	string	U-C-234
well_id	Unique alphanumeric identifier for the well	Yes	string	R2234
easting	Coordinate in the X direction	Yes	number	-107.2166171
northing	Coordinate in the Y direction	Yes	number	43.57566071
easting_3857	EPSG 3857 pseudo-mercator coordinate in the X direction (m)	Yes	number	-11935299.224
northing_3857	EPSG 3857 pseudo-mercator coordinate in the Y direction (m)	Yes	number	5400007.819

Field Name	Description	Required?	Format	Example
mgmt_area	Name of management area for this well		string	Central
operable_unit	Name of operable unit for this well		string	OU-1
other_area_name	Name of other area associated with this well		string	null
sort_name	Well name that can be used for sorting	Yes	string	U-C-234
well_type	Type of well (see notes)	Yes	string	GROUNDWATER WELL
well_status	Status of well (see notes)	Yes	string	IN-USE
drill_date	Date well was drilled		date/time string	1998-09-26 00:00
DrillDepth	Total depth drilled (ft)		number	350.35
NominalHeadElev	Representative recent average hydraulic head elevation (m)		number	121.6253
headStartDate	Start date for averaged value in NominalHeadElev		date/time string	2/7/2019
headEndDate	End date for averaged value in NominalHeadElev		date/time string	11/8/2019
elevation	Ground surface elevation at well (m)	Yes	number	196.787
well_depth	Total depth of the well (ft)	Yes	number	350.35
depth_type	Source of well depth (e.g., drilled depth, constructed depth, etc.)		string	drilled
ScreenTopElev	Elevation for the top of the primary well screen (m)		number	100.0
ScreenBotElev	Elevation for the bottom of the primary well screen (m)		number	95.0
CasingTopElev	Elevation for the top of the primary well casing (m)		number	196.787
CasingBotElev	Elevation for the bottom of the primary well casing (m)		number	90.0
AEA	Is this well part of an Atomic Energy Act monitoring program?		"AEA" or null	null
CERCLA	Is this well part of a CERCLA monitoring program?		"CERCLA" or null	CERCLA
RCRA	Is this well part of a RCRA monitoring program?		"RCRA" or null	null
DOH	Is this well part of a state Department of Health monitoring program?		"DOH" or null	null

Field Name	Description	Required?	Format	Example
DEQ	Is this well part of a state Department of Environmental Quality monitoring program?		"DEQ" or null	DEQ
ManualWL	Does this well have manual water level data?		"manual" or null	manual
SensorWL	Does this well have water level data from sensors?		"sensor" or null	null
OtherWL	Other water level flag		"other" or null	null
WL_ID	Unique alphanumeric identifier for the sensor water level source		string	null
Geology	Name of primary lithologic unit at the elevation of the well screen (can also be “Unknown” or “Mixed”)	Yes	string	Mixed
HasWL	Does this well have water level data?		true, false, or null	true
HasChem	Does this well have groundwater chemistry data?		true, false, or null	true
CasingInfo	Delimited description of well casing segment(s), including size, top/bottom elevations, material, and presence of manual perforations		string	"4 in.,196.8 - 124.2 m; SS;No Perf.; ~4 in.,119.7 - 119.6 m; SS;No Perf.;"
ScreenInfo	Delimited description of well screen(s), including size, top/bottom elevations, and material		string	"4 in.,124.2 - 119.7 m; SS"
LithologyInfo	Delimited description of lithology at this well (must be consistent with lithology definitions), including name and top/bottom elevations		string	"196.0 - 133.5 m,SF ~133.5 - 120.7 m,BCF ~120.7 - 117.3 m,TB"

5.3 Lithologic Units

Information on the lithologic (geologic) units at the site is important for the context of groundwater sample collection and the geologic framework that is part of the basis for the conceptual site model. The “LithologicUnits.csv” file described in Table 2 is how the lithologic/geologic unit names, lithologic unit description, and integer identifier (e.g., numbered 1 to n for the “n” units) are defined.

Table 2. Fields for the "LithologicUnits.csv" data file.

Field Name	Description	Required?	Format	Example
LithID	Unique numerical identifier	Yes	integer	0
FullName	Full name of lithologic unit	Yes	string	"Torque Basalt"
ShortName	Abbreviated name	Yes	string	TB
Description	Short description of the lithologic unit	Yes	string	"Ancient competent basalt"

In addition to the actual lithologic layers, the "LithologicUnits.csv" is recommended to include definition of two other lithologic data categories, "Mixed" and "Unknown" (see Figure 11), which are used in describing the primary lithologic unit intersected by a well screen. The "Mixed" lithologic type describes a well screen that intersects multiple lithologic units. Where either the well construction/screen or lithologic information is unavailable, the "Unknown" lithologic type should be used for the geology field in a well record.

```
9,Mixed,Mix,Mixture of multiple lithologic units
10,Unknown,Unk,No lithologic information
```

Figure 11. Recommended additional items for inclusion in the "LithologicUnits.csv" file, where "Mixed" is for well screens that span multiple lithologic units and "Unknown" is where lithology or well construction information is not available.

5.4 Geologic Framework Model

A GFM for visualization in ORIGEN is described through multiple files, including a master file and a list of files, one for the top surface of each geologic unit. The master file (Figure 12) is a flavor of a CSV file, but with key-value pairs instead of a header row and multiple records. The master file defines the name of the GFM (it is useful to include a version identifier with the name), how many geologic units there are (numfiles), the number of rows and columns in the grid of geologic unit data (i.e., number of data values in each geologic layer file is assumed to be the same and is equal to the product nrow × ncol), the value that represents "no data" (i.e., where the geologic unit is not present), the elevation to use as the floor of the geologic framework model (i.e., a flat plane below the bottommost geologic layer), the EPSG number of the coordinate reference system used for the easting and northing values, and the units (m or ft) for both the easting/northing and elevation data. Note that, currently, only data in EPSG 3857 pesudo-Mercator can be ingested. Following these first 9 key-value pairs, is a list of numfiles number of records identifying the files containing the data for the top surface of each lithologic layer. Each of these records consists of the lithologic id (consistent with the actual lithologic units defined in the "LithologicUnits.csv" file discussed in Section 5.3) and the CSV file name that contains the data for that geologic unit.

```
gfmname,"Hattie GFM v. 1.0"
numfiles,7
nrow,951
ncol,1401
nodata,-999.0
floor,-100.0
epsg,3857
unitsXY,m
unitsZ,m
0,"0_torque_basalt.csv"
1,"1_ginger.csv"
⋮
```

Figure 12. Example "gfm.csv" master file that describes the geologic framework data.

The individual geologic unit files specified in the "gfm.csv" master file are typical CSV files with a header row and the record format specified in Table 3. The data include northing and easting (both in the EPSG 3857 CRS) and either an elevation value or the "no data" value.

Table 3. Fields for the CSV files used to describe the geologic framework units.

Field Name	Description	Required?	Format	Example
easting	EPSG 3857 pseudo-Mercator coordinate in the X direction (units specified in master file)	Yes	number	-11952000.0
northing	EPSG 3857 pseudo-Mercator coordinate in the Y direction (units specified in master file)	Yes	number	5407000.0
elevation	Elevation at the specified X and Y coordinates (units specified in master file)	Yes	number	94.4879

5.5 Contaminants of Potential Concern

Most sites have chemical contaminants of potential concern (COPCs), i.e., contaminants specified as targets or potential targets for remediation. The "COPC_List.csv" data file (Table 4) provides a method to specify a short list of COPCs that are available in PLATO. The records in this file describe each COPC contaminant and associated information on cleanup standards. Consider using the list of chemicals and parameters in Appendix A for names and CAS registry numbers[9].

[9] A CAS Registry Number is a unique and unambiguous identifier for a specific substance. See https://www.cas.org/cas-data/cas-registry.

Table 4. Fields for the "COPC_List.csv" data file.

Field Name	Description	Required?	Format	Example
chemical	Chemical or parameter name	Yes	string	"Carbon tetrachloride"
chemical_id	Unique alphanumeric identifier for the chemical/parameter	Yes	string	56-23-5
method_category	Equal to COPC	Yes	string	COPC
concentration_units	Units for measured value	Yes	string	ug/L
regulatory_limit	Relevant cleanup concentration	Yes	number	5.0
gw_regulatory_limit_type	Type of regulatory limit	Yes	string	MCL
regulatory_ref	Reference for the regulatory limit	Yes	string	"40CFR141-Safe Drinking Water Act Maximum Contaminant Level"

5.6 Groundwater Chemistry Data

Table 5 shows the data fields expected for ingesting analytical data into SOCRATES-EM via the "Analytical_Results_GW.csv" data file.

Some key notes about select fields:

- The laboratory, review, and validation qualifiers can be those used by a site, with a few exceptions that are required. To indicate that a result is below the method detection limit (i.e., the value is non-detect), use a "U" laboratory qualifier (which can be combined with other qualifiers). For a result is estimated, which may be due to a variety of reasons, use a "J" laboratory qualifier. A review or validation qualifier of "R" is used to indicate a rejected result. A review or validation qualifier of "Y" indicates a suspect result.
- If a result has an average elevation value for the sample collection location, the data can be displayed in the depth profile plot in CRATES. If avg_elevation is provided, then avg_depth, elevation_top, elevation_bottom, std_samp_intv_units, sample_depth_top, sample_depth_bot, and sample_depth_units should all be provided to describe the sample collection vertical location.
- The media and matrix are expected (assumed) to be "water" and "groundwater", respectively.
- The method_category may be one of INORGANIC, ORGANIC, PHYSICAL, RAD, or UNKNOWN. The method_class is a more specific categorization of the method, such as biological, dioxins, pesticides, wet-chemistry, etc.
- CAS registry numbers are well defined, but some parameters do not have CAS numbers. Consider using the list of chemicals and parameters in Appendix A.

Table 5. Fields for the "Analytical_Results_GW.csv" data file.

Field Name	Description	Required?	Format	Example
well_id	Unique alphanumeric identifier for the well	Yes	string	R2234
well_name	Well name	Yes	string	U-C-234
samp_date_time	Date and time of sample collection	Yes	date/time string	2020-09-29 09:48:00
date_sampled	Date of sample collection	Yes	date string	9/29/2020
chemical	Chemical or parameter name	Yes	string	"1,1,1-Trichloroethane"
chemical_id	Unique alphanumeric identifier for the chemical/parameter	Yes	string	71-55-6
concentration	Measured value	Yes	number	0.25
concentration_units	Units for measured value	Yes	string	ug/L
lq	Laboratory qualifier	Yes	string	UZ
rq	Review qualifier	Yes	string	H
vq	Validation qualifier		string	null
reject	Is result rejected?	Yes	true or false	false
detect	Is result a detection? (i.e., does not have a "U" lab. qualifier)	Yes	true or false	false
collection_purpose	Identifier denoting the reason for sample collection (e.g., R = routine)		string	R
filtered_flag	Was sample filtered?		true, false, or null	false
avg_elevation	Nominal elevation of sample		number	97.5
avg_depth	Nominal depth of sample		number	325.74475
elevation_top	Top elevation for sample collection interval		number	100.0
elevation_bottom	Bottom elevation for sample collection interval		number	95.0
std_samp_intv_units	Units for sample collection elevations		string	m
sample_depth_top	Top depth for sample collection interval		number	317.54265
sample_depth_bot	Bottom depth for sample collection interval		number	333.94685
sample_depth_units	Units for sample collection depths		string	ft
pql	Practical quantitation limit or similar		string	0.25 (MDL)
std_reporting_limit	Reporting limit value		number	0.25

Field Name	Description	Required?	Format	Example
reporting_limit_type	Type of reporting limit (e.g., PQL, MDL, etc.)		string	MDL
std_required_detection_limit	minimum level of detection required		number	null
std_mda	Minimum detectable activity		number	null
std_counting_error	Variability of the measurement as two times the standard deviation		number	null
std_total_anal_error	Counting error plus a laboratory-specific uncertainty estimate		number	null
dilut_factor	Dilution factor for analyzed sample		number	1
method_name	Analysis method name		string	EPA 8260
method_category	Broad category of the analysis method		string	ORGANIC
method_class	More specific categorization of the method		string	semi-volatiles
tic_flag	Flag for a tentatively identified compound (i.e., constituent that was identified in the analysis but was not on the target constituent list)		yes or null	null
media	Sample material phase (water)		string	Water
matrix	Groundwater		string	Groundwater
samp_mthd	Method used to collect sample		string	submersible pump/low-flow
samp_num	Unique alphanumeric identifier for the sample		string	BX4821-9
otherdocnum	Reference number for other related document		string	null
sampleplandocnum	Reference number for sample plan		string	SAP-481, R3
reviewdocnum	Reference number for data review document		string	LDR-129
samp_site_sort_name	Well name that can be used for sorting	Yes	string	U-C-234
hydraulic_head	Hydraulic head elevation value (m) for the sample event		number	121.967
head_source	Data source for hydraulic head data		string	manual e-tape
elevation	Ground surface elevation at well (m)	Yes	number	196.787

5.7 Water Level Data

Water level (hydraulic head) data useful for understanding groundwater flow direction is specified in the "Hydraulic_Head_GW.csv" data file described in Table 6. Note that sensor water level data should be aggregated (averaged) to daily values.

Table 6. Fields for the Hydraulic_Head_GW.csv data file.

Field Name	Description	Required?	Format	Example
well_id	Unique alphanumeric identifier for the well	Yes	string	R2234
well_name	Well name	Yes	string	U-C-234
hyd_head_date_time	Date and time of water level measurement	Yes	date/time string	2016-02-03 10:52:00
hyd_head_m_navd88	Water level (hydraulic head) measurement value (m)	Yes	number	121.732
depth_to_water_mp	Depth to water from the measurement point		number	246.2
depth_to_water_mp_units	Units for the depth_to_water_mp value		string	ft
depth_to_water_rp	Depth to water from the reference point		number	245.94
depth_to_water_rp_units	Units for the depth_to_water_rp value		string	ft
ElevationM	Elevation for the water level measurement point (m)	Yes	number	196.774
flag	Data quality flag	Yes	string	null
method	Method by which water level measurement was taken		string	"E-tape (laminated steel)"
SourceDB	Type of measurement (i.e., manual, sensor, or other)	Yes	string	manual

5.8 Map Layers

Beyond groundwater well locations, map layers provide important information for reference in the plan view map. For example, SOCRATES for the Hanford Site includes map layers with operable unit boundaries, basalt outcrops, waste sites, contaminant plumes, and water level contours. SOCRATES-EM, like SOCRATES for Hanford, does not have facilities for automatic ingestion of map layers. Rather, map layers must be provided in either a geodatabase format or as a GeoJSON file[10]. The map layers can then be manually added to the Geoserver instance for SOCRATES-EM.

[10] See https://geojson.org/

6.0 Example non-Hanford Data

Two approaches were pursued for data with which to illustrate the ability to ingest and work with non-Hanford data: arbitrary example data and data from a DOE-EM partner site.

An arbitrary location in central Wyoming away from cities was selected as the location for a fictitious site (Figure 13). Adhering to the data formats described in Section 5.0, a set of well, analytical chemistry, lithology, geologic framework, and water level data for this fictitious site were generated. Additionally, some random polygons in a map layer were added manually to the SOCRATES-EM map layer server. The chemistry and geologic data in this fictitious example are randomly distributed, versus representing an actual plume. However, the data adequately illustrate ORIGEN 3D geology visualization and the CRATES/PLATO functionality for chemical data visualization and analysis.

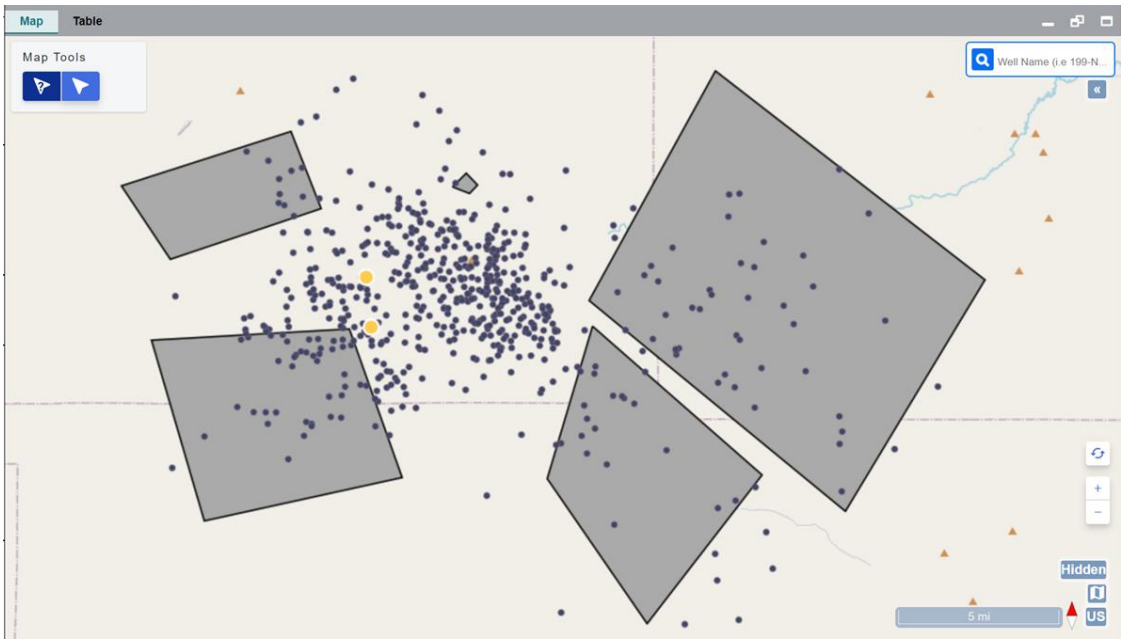

Figure 13. Fictitious site used to illustrate module functionality in SOCRATES-EM.

During the development of SOCRATES-EM in FY23, multiple sites were engaged through presentations, demonstrations, and discussion as potential partner sites for showing example data in the initial SOCRATES-EM prototype. The sites (INL, WIPP, SRS, LANL, PGDP, and PORTS) expressed interest in understanding SOCRATES and the potential applications and benefits for working with their environmental data. Many sites have some kind of groundwater chemistry database, but the discussions highlighted how SOCRATES provides an integration of data and features for assessment, analysis, and communication. The interactive 3D visualization features of ORIGEN garnered the most interest as a tool for visualizing well and geologic data to support conceptual site model application and communication amongst site staff and regulators and stakeholders.

The ability of sites to partner with example data varied depending on things like ability of contractors to provide data (i.e., is such a function within their contract scope) and the current priorities at the site. Paducah and Portsmouth both use the PEGASIS[11] database framework, so analytical data is generally readily available. Paducah also has a pump and treat system where SOCRATES-EM assessment of plume dynamics may be helpful as that remedy progresses. However, it was LANL that followed up their interest to provide some example data. LANL provided plume maps for their chromium plumes in technical area TA-05 (Figure 14). LANL also has analytical data in their Intellus-NM[12] database. As with the other sites, LANL is quite interested in the interactive 3D geologic model visualization capabilities of ORIGEN, but receipt of the geologic model files is still pending in September 2023. Once received (expected in October 2023), they will be easy to load, providing a second GFM for visualization. The LANL GFM will be paired with well and chemistry data from Intellus-NM to have a second example for SOCRATES-EM that represents an actual DOE-EM site.

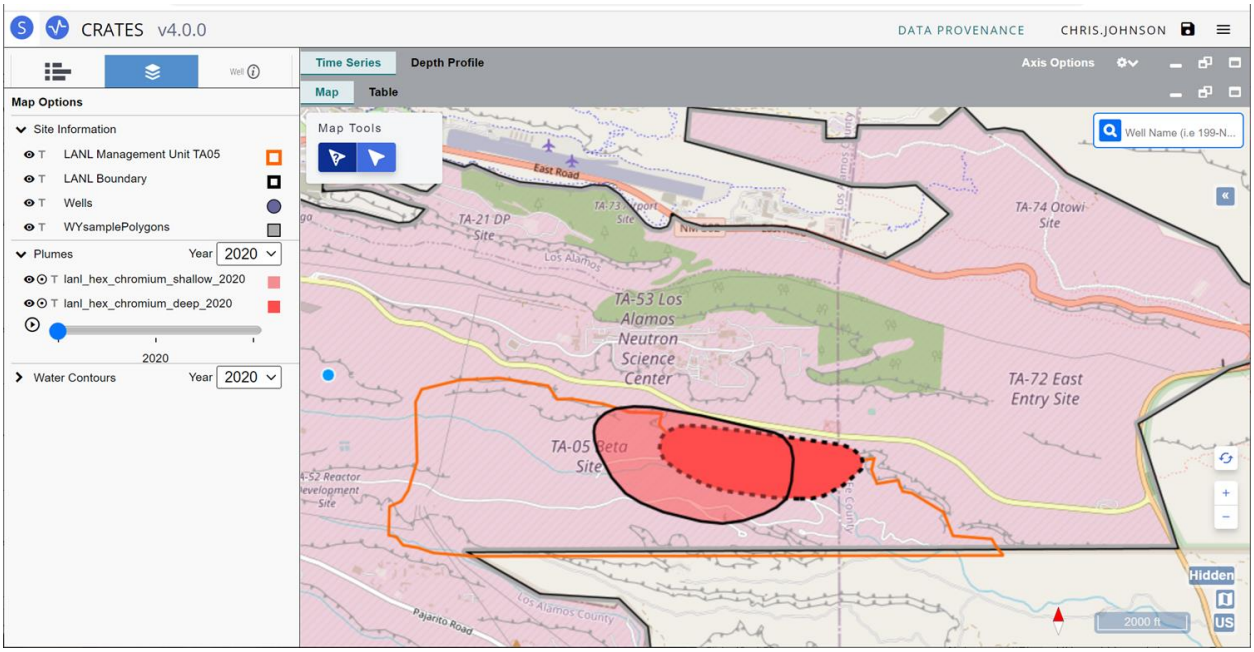

Figure 14. Screenshot of CRATES showing the map pane with the LANL site, the technical area TA-05 boundary, and the shallow and deep chromium groundwater plumes for 2020.

[11] https://pegasis.ports.pppo.gov/Pegasis/Default.aspx and https://pegasis.pad.pppo.gov/

[12] https://www.intellusnm.com/

7.0 Next Steps for Refinement and Deployment

The work in FY23 has resulted in the development of the prototype SOCRATES-EM web application with one full example data set. Additional work to supplement the data, refine the functionality, and promote adoption of the software are part of the next steps in FY24 using remaining funding carried over from FY23.

7.1 Refinement of Data and Functionality

The following data and development items are expected to be addressed in Q1 FY24.

- Once the remaining geologic, well, and groundwater chemistry data for LANL is received, the data will be ingested to provide a second set of example data, but for an actual DOE-EM site. Data is expected in October 2023, but is dependent on delivery by the site.
- GALEN water level and flow direction data for the fictitious site in Wyoming is not currently accessible in SOCRATES-EM. Early in FY24, the finishing touches will be completed to make that data available.
- The use of U.S. Geological Survey (USGS) REST endpoints for bringing in river stage gage data as additional reference information for use in GALEN and CRATES will be investigated. The USGS REST endpoint is available and described at https://waterservices.usgs.gov/rest/DV-Test-Tool.html. This information is generally of lower priority, but implementing this connection would be a great demonstration of how data ingestion via a data service (i.e., the first approach discussed in Section 4.2) would work.
- Availability of the water level and flow direction data via GALEN, will allow implementation of the Well Pair analysis mode in PLATO. This mode allows assessment of contaminant attenuation along a plume flow path (i.e., based on flow direction), which is a third approach for attenuation assessment when considering plume dynamics and pump-and-treat exit strategies.
- Work will be done to allow data to be ingested in standard State Plane, UTM, or Lat/Lon CRS instead of constraining coordinates to the EPSG 3857 pseudo-Mercator CRS.
- Work will be conducted to add the ability to automatically ingest GeoJSON or geodatabase map layer files using a processing workflow along the lines of that in Figure 15.

Figure 15. Proposed workflow for automated processing of map layers for visualization in SOCRATES-EM.

7.2 Deployment

Engagement with EM sites will take place to facilitate adoption/deployment of SOCRATES-EM. Given their level of interest in the application, LANL will be the first site targeted for deployment within their own AWS infrastructure or as an instance hosted by PNNL. As described in Section 4.0, deployment has those two options, with data being segregated for each site and the site specifying who is authorized to have access.

Discussion with the other sites will also encourage adoption and deployment. As mentioned previously, discussion with INL, WIPP, SRS, PGDP, and PORTS sites has taken place in FY23 and additional demonstration and interactions in FY24 will be undertaken about SOCRATES-EM to help sites support communication and decision making. Discussions will also consider the potential for the site to set up REST endpoints as an alternate approach for transfer of data into SOCRATES-EM.

8.0 References

EPA. 2002. *Calculation and Use of First-Order Rate Constants for Monitored Natural Attenuation Studies*. EPA/540/S-02/500, U.S. Environmental Protection Agency, National Risk Management Research Laboratory, Cincinnati, Ohio.

Shafranovich, Y. 2005. "Common Format and MIME Type for CSV Files." RFC 4180, Internet Engineering Task Force. doi:10.17487/RFC4180.

Truex, M.J., and C.D. Johnson. 2016. *Approach for Pump-and-Treat Performance Assessment at the Hanford Site*. PNNL-25875, Pacific Northwest National Laboratory, Richland, Washington.

Truex M.J., C.D. Johnson, D. Becker, M.H. Lee, and M.J. Nimmons. 2015. *Performance Assessment for Pump-and-Treat Closure or Transition*. PNNL-24696, Pacific Northwest National Laboratory, Richland, Washington.

Truex, M.J., C.D. Johnson, T. Macbeth, D.J. Becker, K. Lynch, D. Giaudrone, A. Frantz, and H. Lee. 2017. "Performance Assessment of Pump-and-Treat Systems." *Groundwater Monitoring and Remediation*, 37(3):28-44. https://doi.org/10.1111/gwmr.12218.

Appendix A – List of Chemicals

The following lists many chemicals/analytes and other measured parameters. The chemical_id is the CAS registry number, where available. Non-CAS number chemical_id values are arbitrary, so a site could use a different identifier, if desired. However, it is vital that identifiers be used consistently.

chemical	chemical_id
(2S)-propane-1,2-diol	4254-15-3
(m+p)-Xylene	179601-23-1
(o+p)-Xylene	136777-61-2
1-(1H-pyrrol-2-yl)ethanone	1072-83-9
1-(o-Chlorophenyl)thiourea	5344-82-1
1,1,1,2-Tetrachloroethane	630-20-6
1,1,1-Trichloroethane	71-55-6
1,1,2,2-Tetrachloroethane	79-34-5
1,1,2,2-tetrafluoropropane	40723-63-5
1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1
1,1,2-Trichloroethane	79-00-5
1,1'-Biphenyl	92-52-4
1,1-Dichloroethane	75-34-3
1,1-Dichloroethene	75-35-4
1,1-Dichloropropene	563-58-6
1,1-Dimethylhydrazine	57-14-7
1,1-Dimethylindane	4912-92-9
1,2,3,3-Tetrachloro-propene	20589-85-9
1,2,3,4,6,7,8-Heptachlorodibenzodioxin	35822-46-9
1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4
1,2,3,4,7,8,9-Heptachlorodibenzofuran	55673-89-7
1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227-28-6
1,2,3,4-Tetrachlorobenzene	634-66-2
1,2,3,5-Tetrachlorobenzene	634-90-2
1,2,3,5-Tetramethylbenzene	527-53-7
1,2,3,6,7,8-Hexachlorodibenzofuran	57117-44-9
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	57653-85-7
1,2,3,7,8,9-Hexachlorodibenzofuran	72918-21-9
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	19408-74-3
1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	40321-76-4
1,2,3-Trichlorobenzene	87-61-6
1,2,3-Trichloropropane	96-18-4
1,2,3-Trimethylbenzene	526-73-8
1,2,4,5-Tetrachlorobenzene	95-94-3
1,2,4,5-Tetramethylbenzene	95-93-2

chemical	chemical_id
1,2,4-Trichlorobenzene	120-82-1
1,2,4-Trimethylbenzene	95-63-6
1,2-Benzenedicarboxylic acid butyl 2-ethylhexyl ester	85-69-8
1,2-Benzenedicarboxylic acid, 3-nitro-	603-11-2
1,2-Benzenedicarboxylic acid, butyl, 2-methylpropylester	17851-53-5
1,2-Benzenedicarboxylic acid, diheptyl ester	3648-21-3
1,2-Benzisothiazole	272-16-2
1,2-Dibromo-3-chloropropane	96-12-8
1,2-Dibromoethane	106-93-4
1,2-Dichlorobenzene	95-50-1
1,2-Dichloroethane	107-06-2
1,2-Dichloroethene (Total)	540-59-0
1,2-Dichloropropane	78-87-5
1,2-Dichlorotetrafluoroethane	76-14-2
1,2-Dimethylhydrazine	540-73-8
1,2-Diphenylhydrazine	122-66-7
1,2-Propanediol	57-55-6
1,3,5-Trichlorobenzene	108-70-3
1,3,5-Trimethylbenzene	108-67-8
1,3-Dichlorobenzene	541-73-1
1,3-Dichloropropane	142-28-9
1,3-Dichloropropene	542-75-6
1,3-Isobenzofurandione	85-44-9
1,4-Dichloro-2-butene	764-41-0
1,4-Dichlorobenzene	106-46-7
1,4-Dinitrobenzene	100-25-4
1,4-Dioxane	123-91-1
1,4-Naphthoquinone	130-15-4
1,6-Hexanediol	629-11-8
10-Dodecen-1-ol	35237-63-9
11-Bromoundecanoic acid	5/1/2834
11H-Dibenzo[b,e][1,4]d	13450-73-2
13-Docosenamide, (Z)-	112-84-5
1-acetyl-1H-imidazole	2466-76-4
1-Acetyl-2-thiourea	591-08-2
1-Adamantanol	768-95-6
1-Butanol	71-36-3
1-Butenyl-benzene	1005-64-7
1-Butoxy-2-propanol	5131-66-8
1-Butynol	L60
1-Chloro-1,1-difluoroethane	75-68-3
1-Chloro-2,3-epoxypropane	106-89-8
1-Chlorohexane	544-10-5
1-Decene	872-05-9

chemical	chemical_id
1-Decyn-4-ol	27907-00-2
1-Ethyl-2,3-Dimethylbenzene	933-98-2
1-Ethyl-2,4-Dimethylbenzene	874-41-9
1-Ethyl-3,5-Dimethylbenzene	934-74-7
1H-Benzotriazole	95-14-7
1-Heptanol	111-70-6
1-Hexanol	111-27-3
1-Methyl-2-pyrrolidinone	872-50-4
1-Methyl-4-propylbenzene	1074-55-1
1-Methylnaphthalene	90-12-0
1-Naphthyl-2-thiourea	86-88-4
1-Naphthylamine	134-32-7
1-Octadecanol	112-92-5
1-Pentanol	71-41-0
1-Penten-3-ol, 2-methyl	7/5/2088
1-Phenyl-2-methyl-1-propene	768-49-0
1-Propanol	71-23-8
2-(2-ethoxyethoxy)ethanol	111-90-0
2-(2-methyl-4-chlorophenoxy) propionic acid	93-65-2
2(3H)-Furanone, dihydro-5-propyl-	105-21-5
2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl	2051-24-3
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	40186-72-9
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	35694-08-7
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	52663-79-3
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	42740-50-1
2,2',3,3',4,4',5,6-Octachlorobiphenyl	52663-78-2
2,2',3,3',4,4',5-Heptachlorobiphenyl	35065-30-6
2,2',3,3',4,4',6,6'-Octachlorobiphenyl	33091-17-7
2,2',3,3',4,4',6-Heptachlorobiphenyl	52663-71-5
2,2',3,3',4,4'-Hexachlorobiphenyl	38380-07-3
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	52663-77-1
2,2',3,3',4,5,5',6'-Octachlorobiphenyl	52663-75-9
2,2',3,3',4,5,5',6-Octachlorobiphenyl	68194-17-2
2,2',3,3',4,5,5'-Heptachlorobiphenyl	52663-74-8
2,2',3,3',4,5,6,6'-Octachlorobiphenyl	52663-73-7
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	40186-71-8
2,2',3,3',4,5,6'-Heptachlorobiphenyl	38411-25-5
2,2',3,3',4,5,6-Heptachlorobiphenyl	68194-16-1
2,2',3,3',4,5',6-Heptachlorobiphenyl	40186-70-7
2,2',3,3',4',5,6-Heptachlorobiphenyl	52663-70-4
2,2',3,3',4,5'-Hexachlorobiphenyl	52663-66-8
2,2',3,3',4,5-Hexachlorobiphenyl	55215-18-4
2,2',3,3',4,6,6'-Heptachlorobiphenyl	52663-65-7
2,2',3,3',4,6'-Hexachlorobiphenyl	38380-05-1

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2,2',3,3',4,6-Hexachlorobiphenyl	61798-70-7
2,2',3,3',4-Pentachlorobiphenyl	52663-62-4
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	2136-99-4
2,2',3,3',5,5',6-Heptachlorobiphenyl	52663-67-9
2,2',3,3',5,5'-Hexachlorobiphenyl	35694-04-3
2,2',3,3',5,6,6'-Heptachlorobiphenyl	52663-64-6
2,2',3,3',5,6'-Hexachlorobiphenyl	52744-13-5
2,2',3,3',5,6-Hexachlorobiphenyl	52704-70-8
2,2',3,3',5-Pentachlorobiphenyl	60145-20-2
2,2',3,3',6,6'-Hexachlorobiphenyl	38411-22-2
2,2',3,3',6-Pentachlorobiphenyl	52663-60-2
2,2',3,3'-Tetrachlorobiphenyl	38444-93-8
2,2',3,4,4',5,5',6-Octachlorobiphenyl	52663-76-0
2,2',3,4,4',5,5'-Heptachlorobiphenyl	35065-29-3
2,2',3,4,4',5,6,6'-Octachlorobiphenyl	74472-52-9
2,2',3,4,4',5,6'-Heptachlorobiphenyl	60145-23-5
2,2',3,4,4',5,6-Heptachlorobiphenyl	74472-47-2
2,2',3,4,4',5',6-Heptachlorobiphenyl	52663-69-1
2,2',3,4,4',5'-Hexachlorobiphenyl	35065-28-2
2,2',3,4,4',5-Hexachlorobiphenyl	35694-06-5
2,2',3,4,4',6,6'-Heptachlorobiphenyl	74472-48-3
2,2',3,4,4',6'-Hexachlorobiphenyl	59291-64-4
2,2',3,4,4',6-Hexachlorobiphenyl	56030-56-9
2,2',3,4,4'-Pentachlorobiphenyl	65510-45-4
2,2',3,4,5,5',6-Heptachlorobiphenyl	52712-05-7
2,2',3,4',5,5',6-Heptachlorobiphenyl	52663-68-0
2,2',3,4,5,5'-Hexachlorobiphenyl	52712-04-6
2,2',3,4',5,5'-Hexachlorobiphenyl	51908-16-8
2,2',3,4,5,6,6'-Heptachlorobiphenyl	74472-49-4
2,2',3,4',5,6,6'-Heptachlorobiphenyl	74487-85-7
2,2',3,4,5,6'-Hexachlorobiphenyl	68194-15-0
2,2',3,4,5,6-Hexachlorobiphenyl	41411-61-4
2,2',3,4,5',6-Hexachlorobiphenyl	68194-14-9
2,2',3,4',5,6'-Hexachlorobiphenyl	74472-41-6
2,2',3,4',5,6-Hexachlorobiphenyl	68194-13-8
2,2',3,4',5',6-Hexachlorobiphenyl	38380-04-0
2,2',3,4,5'-Pentachlorobiphenyl	38380-02-8
2,2',3,4,5-Pentachlorobiphenyl	55312-69-1
2,2',3,4',5-Pentachlorobiphenyl	68194-07-0
2,2',3',4,5-Pentachlorobiphenyl	41464-51-1
2,2',3,4,6,6'-Hexachlorobiphenyl	74472-40-5
2,2',3,4',6,6'-Hexachlorobiphenyl	68194-08-1
2,2',3,4,6'-Pentachlorobiphenyl	73575-57-2
2,2',3,4,6-Pentachlorobiphenyl	55215-17-3

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2,2',3,4',6-Pentachlorobiphenyl	68194-05-8
2,2',3',4,6-Pentachlorobiphenyl	60233-25-2
2,2',3,4'-Tetrachlorobiphenyl	36559-22-5
2,2',3,4-Tetrachlorobiphenyl	52663-59-9
2,2',3,5,5',6-Hexachlorobiphenyl	52663-63-5
2,2',3,5,5'-Pentachlorobiphenyl	52663-61-3
2,2',3,5,6,6'-Hexachlorobiphenyl	68194-09-2
2,2',3,5,6'-Pentachlorobiphenyl	73575-55-0
2,2',3,5,6-Pentachlorobiphenyl	73575-56-1
2,2',3,5',6-Pentachlorobiphenyl	38379-99-6
2,2',3,5'-Tetrachlorobiphenyl	41464-39-5
2,2',3,5-Tetrachlorobiphenyl	70362-46-8
2,2',3,6,6'-Pentachlorobiphenyl	73575-54-9
2,2',3,6'-Tetrachlorobiphenyl	41464-47-5
2,2',3,6-Tetrachlorobiphenyl	70362-45-7
2,2',3-Trichlorobiphenyl	38444-78-9
2,2',4,4',5,5'-Hexachlorobiphenyl	35065-27-1
2,2',4,4',5,6'-Hexachlorobiphenyl	60145-22-4
2,2',4,4',5-Pentachlorobiphenyl	38380-01-7
2,2',4,4',6,6'-Hexachlorobiphenyl	33979-03-2
2,2',4,4',6-Pentachlorobiphenyl	39485-83-1
2,2',4,4'-Tetrachlorobiphenyl	2437-79-8
2,2',4,5,5'-Pentachlorobiphenyl	37680-73-2
2,2',4,5,6-Pentachlorobiphenyl	68194-06-9
2,2',4,5',6-Pentachlorobiphenyl	60145-21-3
2,2',4,5'-Tetrachlorobiphenyl	41464-40-8
2,2',4,5-Tetrachlorobiphenyl	70362-47-9
2,2',4,6,6'-Pentachlorobiphenyl	56558-16-8
2,2',4,6'-Tetrachlorobiphenyl	68194-04-7
2,2',4,6-Tetrachlorobiphenyl	62796-65-0
2,2',4-Trichlorobiphenyl	37680-66-3
2,2',5,5'-Tetrachlorobiphenyl	35693-99-3
2,2',5,6'-Tetrachlorobiphenyl	41464-41-9
2,2',5-Trichlorobiphenyl	37680-65-2
2,2',6,6'-Tetrachlorobiphenyl	15968-05-5
2,2',6-Trichlorobiphenyl	38444-73-4
2,2'-Dichlorobiphenyl	13029-08-8
2,2-Dichloropropane	594-20-7
2,3,3',4,4',5,5',6-Octachlorobiphenyl	74472-53-0
2,3,3',4,4',5,5'-Heptachlorobiphenyl	39635-31-9
2,3,3',4,4',5,6-Heptachlorobiphenyl	41411-64-7
2,3,3',4,4',5',6-Heptachlorobiphenyl	74472-50-7
2,3,3',4,4',5'-Hexachlorobiphenyl	69782-90-7
2,3,3',4,4',5-Hexachlorobiphenyl	38380-08-4

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2,3,3',4,4',6-Hexachlorobiphenyl	74472-42-7
2,3,3',4,4'-Pentachlorobiphenyl	32598-14-4
2,3,3',4,5,5',6-Heptachlorobiphenyl	74472-51-8
2,3,3',4',5,5',6-Heptachlorobiphenyl	69782-91-8
2,3,3',4,5,5'-Hexachlorobiphenyl	39635-35-3
2,3,3',4',5,5'-Hexachlorobiphenyl	39635-34-2
2,3,3',4,5,6-Hexachlorobiphenyl	41411-62-5
2,3,3',4,5',6-Hexachlorobiphenyl	74472-43-8
2,3,3',4',5,6-Hexachlorobiphenyl	74472-44-9
2,3,3',4',5',6-Hexachlorobiphenyl	74472-45-0
2,3,3',4,5'-Pentachlorobiphenyl	70362-41-3
2,3,3',4,5-Pentachlorobiphenyl	70424-69-0
2,3,3',4',5-Pentachlorobiphenyl	70424-68-9
2',3,3',4,5-Pentachlorobiphenyl	76842-07-4
2,3,3',4,6-Pentachlorobiphenyl	74472-35-8
2,3,3',4',6-Pentachlorobiphenyl	38380-03-9
2,3,3',4'-Tetrachlorobiphenyl	41464-43-1
2,3,3',4-Tetrachlorobiphenyl	74338-24-2
2,3,3',5,5',6-Hexachlorobiphenyl	74472-46-1
2,3,3',5,5'-Pentachlorobiphenyl	39635-32-0
2,3,3',5,6-Pentachlorobiphenyl	74472-36-9
2,3,3',5',6-Pentachlorobiphenyl	68194-10-5
2,3,3',5'-Tetrachlorobiphenyl	41464-49-7
2,3,3',5-Tetrachlorobiphenyl	70424-67-8
2,3,3',6-Tetrachlorobiphenyl	74472-33-6
2,3,3'-Trichlorobiphenyl	38444-84-7
2,3',4,4',5,5'-Hexachlorobiphenyl	52663-72-6
2,3,4,4',5,6-Hexachlorobiphenyl	41411-63-6
2,3',4,4',5',6-Hexachlorobiphenyl	59291-65-5
2,3,4,4',5-Pentachlorobiphenyl	74472-37-0
2,3',4,4',5-Pentachlorobiphenyl	31508-00-6
2',3,4,4',5-Pentachlorobiphenyl	65510-44-3
2,3,4,4',6-Pentachlorobiphenyl	74472-38-1
2,3',4,4',6-Pentachlorobiphenyl	56558-17-9
2,3,4,4'-Tetrachlorobiphenyl	33025-41-1
2,3',4,4'-Tetrachlorobiphenyl	32598-10-0
2,3',4,5,5'-Pentachlorobiphenyl	68194-12-7
2',3,4,5,5'-Pentachlorobiphenyl	70424-70-3
2,3,4,5,6-Pentachlorobiphenyl	18259-05-7
2,3,4',5,6-Pentachlorobiphenyl	68194-11-6
2,3',4,5',6-Pentachlorobiphenyl	56558-18-0
2',3,4,5,6'-Pentachlorobiphenyl	74472-39-2
2,3,4,5-Tetrachlorobiphenyl	33284-53-6
2,3,4',5-Tetrachlorobiphenyl	74472-34-7

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2,3',4,5'-Tetrachlorobiphenyl	73575-52-7
2,3',4,5-Tetrachlorobiphenyl	73575-53-8
2,3',4',5-Tetrachlorobiphenyl	32598-11-1
2',3,4,5-Tetrachlorobiphenyl	70362-48-0
2,3,4,6,7,8-Hexachlorodibenzofuran	60851-34-5
2,3,4,6-Tetrachlorobiphenyl	54230-22-7
2,3,4',6-Tetrachlorobiphenyl	52663-58-8
2,3',4,6-Tetrachlorobiphenyl	60233-24-1
2,3',4',6-Tetrachlorobiphenyl	41464-46-4
2,3,4,6-Tetrachlorophenol	58-90-2
2,3,4,7,8-Pentachlorodibenzofuran	57117-31-4
2,3,4'-Trichlorobiphenyl	38444-85-8
2,3,4-Trichlorobiphenyl	55702-46-0
2,3',4-Trichlorobiphenyl	55712-37-3
2',3,4-Trichlorobiphenyl	38444-86-9
2,3',5,5'-Tetrachlorobiphenyl	41464-42-0
2,3,5,6-Tetrachlorobiphenyl	33284-54-7
2,3',5',6-Tetrachlorobiphenyl	74338-23-1
2,3,5-Trichlorobiphenyl	55720-44-0
2,3',5-Trichlorobiphenyl	38444-81-4
2',3,5-Trichlorobiphenyl	37680-68-5
2,3,6-Trichlorobiphenyl	55702-45-9
2,3',6-Trichlorobiphenyl	38444-76-7
2,3,7,8-Tetrachlorodibenzofuran	51207-31-9
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6
2,3,7-Trimethyloctane	62016-34-6
2,3'-Dichlorobiphenyl	25569-80-6
2,3-Dichlorobiphenyl	16605-91-7
2,3-Epoxy-2-methylbutane	5076-19-7
2,4,4',5-Tetrachlorobiphenyl	32690-93-0
2,4,4',6-Tetrachlorobiphenyl	32598-12-2
2,4,4'-Trichlorobiphenyl	7012-37-5
2,4,5-T(2,4,5-Trichlorophenoxyacetic acid)	93-76-5
2,4,5-TP(2-(2,4,5-Trichlorophenoxy)propionic acid)Silvex	93-72-1
2,4,5-Trichlorobiphenyl	15862-07-4
2,4',5-Trichlorobiphenyl	16606-02-3
2,4,5-Trichlorophenol	95-95-4
2,4,6-Trichlorobiphenyl	35693-92-6
2,4',6-Trichlorobiphenyl	38444-77-8
2,4,6-Trichlorophenol	88-06-2
2,4-D(2,4-Dichlorophenoxyacetic acid)	94-75-7
2,4-DB(4-(2,4-Dichlorophenoxy)butanoic acid)	94-82-6
2,4'-Dichlorobiphenyl	34883-43-7
2,4-Dichlorobiphenyl	33284-50-3

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2,4-Dichloropentane	625-67-2
2,4-Dichlorophenol	120-83-2
2,4-Dimethylphenol	105-67-9
2,4-Dinitrophenol	51-28-5
2,4-Dinitrotoluene	121-14-2
2,5-Dichlorobiphenyl	34883-39-1
2,5-Dimethyl furane	625-86-5
2,6-bis(1,1-dimethylethyl)-4-methyl phenol	128-37-0
2,6-Dichlorobiphenyl	33146-45-1
2,6-Dichlorophenol	87-65-0
2,6-Dimethyl-undecane	17301-23-4
2,6-Dinitrotoluene	606-20-2
2,6-Nonadienal, (e,e)-	17587-33-6
2,7,10-Trimethyldodecane	74645-98-0
2-Acetylaminofluorene	53-96-3
2-Benzothiazolethiol	149-30-4
2-Bromo ethylhexane	1647-26-3
2-Butanol	78-92-2
2-Butanone	78-93-3
2-Butoxyethanol	111-76-2
2-Chloroethyl vinyl ether	110-75-8
2-Chloronaphthalene	91-58-7
2-Chlorophenol	95-57-8
2-Chlorotoluene	95-49-8
2-Cyclohexyl-4,6-dinitrophenol	131-89-5
2-Ethyl-1,3-Dimethylbenzene	4/4/2870
2-Ethyl-1,4-Dimethylbenzene	1758-88-9
2-Ethyl-1-hexanol	104-76-7
2-Ethylhexanoic acid	149-57-5
2-Ethyltoluene	611-14-3
2-Fluoro-4-nitrophenol	403-19-0
2-Fluoro-5-nitropyrimidine	62802-41-9
2-Fluoro-6-nitrophenol	1526-17-6
2-Heptanone	110-43-0
2-Hexanone	591-78-6
2-Hydroxy-2-methylpropanoic acid	594-61-6
2-Iminoimidazolidin-4-one	503-86-6
2-Methyl-2-(methylthio)propionaldehyde-o-(methylcarbonyl) ox	116-06-3
2-Methyl-2-Propanol	75-65-0
2-Methyl-4 chlorophenoxyacetic acid	94-74-6
2-Methylanthracene	613-12-7
2-Methylaziridine	75-55-8
2-Methylcyclohex-5-en	3718-56-7
2-Methyllactonitrile	75-86-5

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2-Methylnaphthalene	91-57-6
2-Methylphenol (cresol, o-)	95-48-7
2-Monochlorobiphenyl	2051-60-7
2-Naphthylamine	91-59-8
2-Nitroaniline	88-74-4
2-Nitrophenol	88-75-5
2-Nitropropane	79-46-9
2-Pentanol	6032-29-7
2-Pentanone	107-87-9
2-Picoline	109-06-8
2-Propanol	67-63-0
2-Propyn-1-ol	107-19-7
3,3',4,4',5,5'-Hexachlorobiphenyl	32774-16-6
3,3',4,4',5-Pentachlorobiphenyl	57465-28-8
3,3',4,4'-Tetrachlorobiphenyl	32598-13-3
3,3',4,5,5'-Pentachlorobiphenyl	39635-33-1
3,3',4,5'-Tetrachlorobiphenyl	41464-48-6
3,3',4,5-Tetrachlorobiphenyl	70362-49-1
3,3',4-Trichlorobiphenyl	37680-69-6
3,3',5,5'-Tetrachlorobiphenyl	33284-52-5
3,3',5-Trichlorobiphenyl	38444-87-0
3,3'-Dichlorobenzidine	91-94-1
3,3'-Dichlorobiphenyl	2050-67-1
3,3'-Dimethoxybenzidine	119-90-4
3,3'-Dimethylbenzidine	119-93-7
3,4,4',5-Tetrachlorobiphenyl	70362-50-4
3,4,4'-Trichlorobiphenyl	38444-90-5
3,4,5-Trichlorobiphenyl	53555-66-1
3,4',5-Trichlorobiphenyl	38444-88-1
3,4'-Dichlorobiphenyl	2974-90-5
3,4-Dichlorobiphenyl	2974-92-7
3,5-Dichlorobiphenyl	34883-41-5
3,5-Di-tert-butyl-2,6-	92375-27-4
3,5-Di-tert-butyl-4-hydroxybenzaldehyde	1620-98-0
3,6-Dimethyldecane	17312-53-7
3,7,7-trimethyl bicyclohep-3-ene	13466-78-9
3+4 Methylphenol (cresol, m+p)	65794-96-9
3-Bromocyclohexene	1521-51-3
3-Chloro-3-methyl-1-butene	2190-48-9
3-Chloropropionitrile	542-76-7
3-Hydroxy-3-methyl-2-butanone	115-22-0
3-Hydroxydecanoic acid	33044-91-6
3-Methylcholanthrene	56-49-5
3-Methylphenol (cresol, m-)	108-39-4

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3-Monochlorobiphenyl	2051-61-8
3-Nitroaniline	99-09-2
3-Octyne, 5-methyl-	62108-33-2
3-Penten-2-one, 3,4-dimethyl	16983-60-1
3-tert-Butyl-4-methoxyphenol	88-32-4
4,4'-DDD (Dichlorodiphenyldichloroethane)	72-54-8
4,4'-DDE (Dichlorodiphenyldichloroethylene)	72-55-9
4,4'-DDT (Dichlorodiphenyltrichloroethane)	50-29-3
4,4'-Dichlorobiphenyl	2050-68-2
4,4'-Methylenebis(2-chloroaniline)	101-14-4
4,6-Dinitro-2-methylphenol	534-52-1
4-Aminobiphenyl	92-67-1
4-Bromophenylphenyl ether	101-55-3
4-Chloro-3-methylphenol	59-50-7
4-Chloroaniline	106-47-8
4-Chlorophenylphenyl ether	7005-72-3
4-Chlorotoluene	106-43-4
4-Fluoroaniline	371-40-4
4-Fluorobromobenzene	460-00-4
4-Heptanone, 3-methyl-	15726-15-5
4-Hexen-3-ol	4798-58-7
4-Hydroxy-2-butanone	590-90-9
4'-Hydroxyacetanilide	103-90-2
4-Methyl-2-pentanol	108-11-2
4-Methyl-2-pentanone	108-10-1
4-Methylphenol (cresol, p-)	106-44-5
4-Monochlorobiphenyl	2051-62-9
4-Nitroaniline	100-01-6
4-Nitrophenol	100-02-7
4-Nitroquinoline-1-oxide	56-57-5
4-Nonanol	5932-79-6
5-(Aminomethyl)-3-isoxazolol	2763-96-4
5-Methyl-3-hexanol	623-55-2
5-Nitro-o-toluidine	99-55-8
7,12-Dimethylbenz[a]anthracene	57-97-6
7H-Dibenzo[c,g]carbazole	194-59-2
7-Methylindan-1-one	39627-61-7
Absorbable Organic Halides	AOX
Acenaphthene	83-32-9
Acenaphthylene	208-96-8
Acetic acid, methyl ester	79-20-9
Acetone	67-64-1
Acetonitrile	75-05-8
Acetophenone	98-86-2

chemical	chemical_id
Acrolein	107-02-8
Acrylamide	79-06-1
Acrylonitrile	107-13-1
Actinium-228	14331-83-0
Adipic acid, 2-ethylhexyl ester	4337-65-9
Aldrin	309-00-2
Aliphatic Petroleum Hydrocarbons >nC10-nC12	ALIPHHC>NC10-12
Aliphatic Petroleum Hydrocarbons >nC12-nC16	ALIPHHC>NC12-16
Aliphatic Petroleum Hydrocarbons >nC16-nC21	ALIPHHC>NC16-21
Aliphatic Petroleum Hydrocarbons >nC21-nC34	ALIPHHC>NC21-34
Aliphatic Petroleum Hydrocarbons nC8-nC10	ALIPHHC_NC8-10
Alkalinity	ALKALINITY
Allyl alcohol	107-18-6
Allyl chloride	107-05-1
Alpha	ALPHAHI
alpha,alpha-Dimethylphenethylamine	122-09-8
Alpha-BHC	319-84-6
Alpha-Chlordane	5103-71-9
Aluminum	7429-90-5
Americium-241	14596-10-2
Amitrole	61-82-5
Ammonia	7664-41-7
Ammonium ion	14798-03-9
Amyl acetate (mixed isomers)	628-63-7
Amylene Hydrate	75-85-4
Aniline	62-53-3
Anthracene	120-12-7
Antimony	7440-36-0
Antimony-125	14234-35-6
Aramite	140-57-8
Aroclor-1016	12674-11-2
Aroclor-1221	11104-28-2
Aroclor-1232	11141-16-5
Aroclor-1242	53469-21-9
Aroclor-1248	12672-29-6
Aroclor-1254	11097-69-1
Aroclor-1260	11096-82-5
Aroclor-1262	37324-23-5
Aroclor-1268	11100-14-4
Aromatic Petroleum Hydrocarbons >nC10-nC12	AROMAHC>NC10-12
Aromatic Petroleum Hydrocarbons >nC12-nC16	AROMAHC>NC12-16
Aromatic Petroleum Hydrocarbons >nC16-nC21	AROMAHC>NC16-21
Aromatic Petroleum Hydrocarbons >nC21-nC34	AROMAHC>NC21-34
Aromatic Petroleum Hydrocarbons nC8-nC10	AROMAHC_NC8-10

chemical	chemical_id
Arsenic	7440-38-2
Arsenic, filtered	H37
Auramine	492-80-8
Azinphos Methyl	86-50-0
Azobenzene	103-33-3
Barium	7440-39-3
Barium-133	13981-41-4
Barium-140	14798-08-4
Benz[c]acridine	225-51-4
Benzene	71-43-2
Benzenethiol	108-98-5
Benzidine	92-87-5
Benzo(a)anthracene	56-55-3
Benzo(a)pyrene	50-32-8
Benzo(b)fluoranthene	205-99-2
Benzo(ghi)perylene	191-24-2
Benzo(k)fluoranthene	207-08-9
Benzo[j]fluoranthene	205-82-3
Benzoic acid	65-85-0
Benzoic acid, 2-[(trimethylsilyl)oxy]-,trimethylsilyl ester	3789-85-3
Benzoic acid, 5-methyl	1000153-59-4
Benzophenone	119-61-9
Benzothiazole	95-16-9
Benzyl alcohol	100-51-6
Benzyl chloride	100-44-7
Beryllium	7440-41-7
Beryllium-7	13966-02-4
beta-1,2,3,4,5,6-Hexachlorocyclohexane (beta-BHC)	319-85-7
Bicarbonate	71-52-3
Bi-carbonate alkalinity	HCO3ALKALINITY
Bicyclo[2.2.1]heptane,	61177-16-0
Biochemical Oxygen Demand	BOD
Bis(2-chloro-1-methylethyl)ether	108-60-1
Bis(2-Chloroethoxy)methane	111-91-1
Bis(2-chloroethyl) ether	111-44-4
Bis(2-chloroisopropyl)	39638-32-9
Bis(2-ethylhexyl) phthalate	117-81-7
Bis(chloromethyl) ether	542-88-1
Bismuth	7440-69-9
Bismuth-212	14913-49-6
Bismuth-214	14733-03-0
Bisphenol A	80-05-7
Boron	7440-42-8
Bromacil (ACN)	314-40-9

chemical	chemical_id
Bromide	24959-67-9
Bromoacetone	598-31-2
Bromobenzene	108-86-1
Bromochloromethane	74-97-5
Bromodichloromethane	75-27-4
Bromoform	75-25-2
Bromomethane	74-83-9
Butane, 2-methoxy-2-methyl-	994-05-8
Butanoic Acid Methyl Ester	623-42-7
Butanoic acid, 2-ethyl	56554-54-2
Butylbenzylphthalate	85-68-7
Cadmium	7440-43-9
Calcium	7440-70-2
Calcium Carbonate	471-34-1
Carbazole	86-74-8
Carbethoxy malathion	121-75-5
Carbon disulfide	75-15-0
Carbon tetrachloride	56-23-5
Carbon-14	14762-75-5
Carbon-14 percent modern carbon	C14 PMC
Carbonate alkalinity	CO3ALKALINITY
Carbonate ion	3812-32-6
Carbophenothion	786-19-6
Cerium/Praseodymium-144	CE/PR-144
Cerium-141	13967-74-3
Cerium-144	14762-78-8
Cesium-134	13967-70-9
Cesium-137	10045-97-3
Chemical Oxygen Demand	COD
Chloral	75-87-6
Chlordane	57-74-9
Chloride	16887-00-6
Chlorine-36	13981-43-6
Chlorine-36/Chlorine atom ratio	CL36/CLRT
Chlornaphazine	494-03-1
Chloroacetaldehyde	107-20-0
Chloroalkyl ethers	B44
Chlorobenzene	108-90-7
Chlorobenzilate	510-15-6
Chlorodifluoromethane	75-45-6
Chloroethane	75-00-3
Chloroform	67-66-3
Chloromethane	74-87-3
Chloromethyl methyl ether	107-30-2

chemical	chemical_id
Chloroprene	126-99-8
Chromium	7440-47-3
Chromium-51	14392-02-0
Chrysene	218-01-9
cis-1,2-Dichloroethylene	156-59-2
cis-1,3-Dichloropropene	10061-01-5
Citrus red No. 2	6358-53-8
Cobalt	7440-48-4
Cobalt-57	13981-50-5
Cobalt-58	13981-38-9
Cobalt-60	10198-40-0
Coliform Bacteria	COLIFORM
Copper	7440-50-8
Crotonaldehyde	4170-30-3
Curium-242	15510-73-3
Curium-243/244	CM-243/244
Curium-244	13981-15-2
Cyanide	57-12-5
Cyanide amenable to chlorination	CATC
Cyanogen	460-19-5
Cyanogen bromide	506-68-3
Cyanogen chloride	506-77-4
Cyclobutene, 2-propeny	52097-85-5
Cyclohexane	110-82-7
Cyclohexane, octyl-	1795-15-9
Cyclohexanol, 2-methyl-5-(1-methylethyl)-, (1a,2b,5a)-	499-69-4
Cyclohexanone	108-94-1
Cyclotetrasiloxane, Octamethyl	556-67-2
Dalapon	75-99-0
Decamethylcyclopentasiloxane	541-02-6
Decane	124-18-5
Decane, 2,3,5-trimethyl	62238-11-3
Decanoic acid	334-48-5
Dehydroabietic acid, methyl ester	1235-74-1
delta Carbon-13 ratio relative to PDB (Pee Dee Belemnite)	DELTA-C13
delta Deuterium ratio relative to SMOW	DELTA-H2
delta Oxygen-18 ratio relative to SMOW	DELTA-O18
delta Sulfur-34 ratio relative to Canyon Diablo troilite	DELTA-S34
Delta-BHC	319-86-8
D-Glucose, 4-O-alpha-D-glucopyranosyl	69-79-4
Diacetone alcohol	123-42-2
Diallate	2303-16-4
Diazinon	333-41-5
Dibenz[a,h]acridine	226-36-8

chemical	chemical_id
Dibenz[a,h]anthracene	53-70-3
Dibenz[a,j]acridine	224-42-0
Dibenzo[a,e]pyrene	192-65-4
Dibenzo[a,h]pyrene	189-64-0
Dibenzo[a,i]pyrene	189-55-9
Dibenzofuran	132-64-9
Dibromochloromethane	124-48-1
Dibromomethane	74-95-3
Dibutyl Butylphosphonate	78-46-6
Dibutylphosphate	107-66-4
Dicamba	1918-00-9
Dichlorodifluoromethane	75-71-8
Dichlorofluoromethane	75-43-4
Dichloromethyl-benzene	98-87-3
Dichloroprop	120-36-5
Dichloropropanol	26545-73-3
Didodecyl phthalate	2432-90-8
Dieldrin	60-57-1
Diethyl arsine	692-42-2
Diethyl ether	60-29-7
Diethylphthalate	84-66-2
Diethylstilbesterol	56-53-1
Dihydrosafrole	94-58-6
Diisobutyl Phthalate	84-69-5
Dimethoate	60-51-5
Dimethyl phthalate	131-11-3
Dimethyldisulfide	624-92-0
Di-n-butylphthalate	84-74-2
Di-n-nonyl phthalate	84-76-4
Di-n-octylphthalate	117-84-0
Dinoseb(2-secButyl-4,6-dinitrophenol)	88-85-7
Dioctyl adipate	123-79-5
Diphenylamine	122-39-4
Diphenylamine+N-Nitrosodiphenylamine	DPA+NNDPA
Dissolved organic carbon	DOC
Dissolved oxygen	DO
Disulfoton	298-04-4
Dithiocarbamic acid	16696-88-1
D-limonene	5989-27-5
Dodecamethylcyclohexasiloxane	540-97-6
Dodecanamide	1120-16-7
Dodecane	112-40-3
Eicosane	112-95-8
Eicosane, 10-methyl-	54833-23-7

chemical	chemical_id
Elaidic Acid	112-79-8
Enanthoic Acid	111-14-8
Endosulfan I	959-98-8
Endosulfan II	33213-65-9
Endosulfan sulfate	1031-07-8
Endrin	72-20-8
Endrin aldehyde	7421-93-4
Endrin ketone	53494-70-5
Ethanol	64-17-5
Ethyl 4-ethoxybenzoate	23676-09-7
Ethyl acetate	141-78-6
Ethyl carbamate (Urethane)	51-79-6
Ethyl cyanide	107-12-0
Ethyl methacrylate	97-63-2
Ethyl methanesulfonate	62-50-0
Ethyl methylene phosphorodithioate	563-12-2
Ethyl thiocyanate	542-90-5
Ethylbenzene	100-41-4
Ethylene glycol	107-21-1
Ethylene oxide	75-21-8
Ethyleneimine	151-56-4
Ethylenethiourea	96-45-7
Europium-152	14683-23-9
Europium-154	15585-10-1
Europium-155	14391-16-3
Famphur	52-85-7
Fluoranthene	206-44-0
Fluorene	86-73-7
Fluoride	16984-48-8
Fluoroacetic acid	144-49-0
Formaldehyde	50-00-0
Formate	FORMATE
Free Cyanide	FREE-CN
Furfural	98-01-1
Gamma-BHC (Lindane)	58-89-9
gamma-Chlordane	5566-34-7
Glycidylaldehyde	765-34-4
Glycine	56-40-6
Gross alpha	12587-46-1
Gross beta	12587-47-2
Hardness	HARDNESS
Heneicosane	629-94-7
Heptachlor	76-44-8
Heptachlor epoxide	1024-57-3

chemical	chemical_id
Heptachlorodibenzofurans	38998-75-3
Heptachlorodibenzo-p-dioxins	37871-00-4
Heptacosane	593-49-7
Heptadecane	629-78-7
Heptadecane, 2,6,10,15-Tetramethyl	54833-48-6
Hexachlorobenzene	118-74-1
Hexachlorobutadiene	87-68-3
Hexachlorocyclopentadiene	77-47-4
Hexachlorodibenzofurans	55684-94-1
Hexachlorodibenzo-p-dioxin	34465-46-8
Hexachloroethane	67-72-1
Hexachlorophene	70-30-4
Hexachloropropene	1888-71-7
Hexacyanocolbaltate(III)	CO(CN)6
Hexadecane	544-76-3
Hexadecanoic acid (9CI)	57-10-3
Hexadecanoic acid, butyl ester	111-06-8
Hexamethylcyclotrisiloxane	541-05-9
Hexane	110-54-3
Hexavalent Chromium	18540-29-9
Hexyl methyl ketone	111-13-7
Hydrazine	302-01-2
Hydrogen sulfide	6/4/7783
Hydroxyl anion as CaCO3	OHALKALINITY
Hydroxylion	84625-61-6
icosan-1-ol	629-96-9
Ignitability	IGNITABILITY
Indeno(1,2,3-cd)pyrene	193-39-5
Iodine-129	15046-84-1
Iodine-129/Iodine-127 ratio	I129/127RT
Iodine-131	10043-66-0
Iodomethane	74-88-4
Iron	7439-89-6
Iron-59	14596-12-4
Iron-II Ion	FE(II)
Isobutyl alcohol	78-83-1
Isobutylene	115-11-7
Isodrin	465-73-6
Isophorone	78-59-1
Isopropylbenzene	98-82-8
Isosafrole	120-58-1
Kepone	143-50-0
Lauric-acid	143-07-7
Lead	7439-92-1

chemical	chemical_id
Lead-212	15092-94-1
Lead-214	15067-28-4
Lineatin	65035-34-9
Linoleic acid	60-33-3
Lithium	7439-93-2
Magnesium	7439-95-4
Maleic hydrazide	123-33-1
Malononitrile	109-77-3
Manganese	7439-96-5
Manganese-54	13966-31-9
m-Dinitrobenzene	99-65-0
Melphalan	148-82-3
Mercury	7439-97-6
Mesityl oxide	141-79-7
Methacrylonitrile	126-98-7
Methane	74-82-8
Methanethiol	74-93-1
Methanol	67-56-1
Methapyrilene	91-80-5
Metholonyl	16752-77-5
Methoxychlor	72-43-5
Methoxytrimethylsilane	1825-61-2
Methyl 2-hydroxyisobutyrate	2110-78-3
Methyl cyclohexane	108-87-2
Methyl methacrylate	80-62-6
Methyl methanesulfonate	66-27-3
Methyl parathion	298-00-0
Methyl tert-butyl ether	1634-04-4
Methyl tetrahydrofurfuryl ether	19354-27-9
Methylcyclopentane	96-37-7
Methylene chloride	75-09-2
Methylhydrazine	60-34-4
Methylthiouracil	56-04-2
Molybdenum	7439-98-7
Monobutyl phosphate	1623-15-0
Monopotassium phosphate	7778-77-0
m-Xylene	108-38-3
n,n-Diethylhydrazine	616-40-0
Naphthalene	91-20-3
n-Butylbenzene	104-51-8
n-Butyric Acid	107-92-6
n-Decanamide	2319-29-1
n-Dotriacontane	544-85-4
Neopentyl glycol	126-30-7

chemical	chemical_id
Neptunium-237	13994-20-2
n-Heptane	142-82-5
n-Heptyl Aldehyde	111-71-7
n-Hexacosane	630-01-3
n-Hexanoic Acid	142-62-1
Nickel	7440-02-0
Nickel-63	13981-37-8
Nicotinic acid	59-67-6
Niobium-94	14681-63-1
Nitrate	14797-55-8
Nitrite	14797-65-0
Nitrobenzene	98-95-3
Nitrogen in Nitrite and Nitrate	NO2+NO3-N
Nitrosopyrrolidine	930-55-2
n-Nitrosodiethanolamine	1116-54-7
n-Nitrosodiethylamine	55-18-5
n-Nitrosodimethylamine	62-75-9
n-Nitrosodi-n-butylamine	924-16-3
n-Nitrosodi-n-propylamine	621-64-7
n-Nitrosodiphenylamine	86-30-6
n-Nitrosomethylethylamine	10595-95-6
n-Nitrosomethylvinylamine	4549-40-0
n-Nitrosomorpholine	59-89-2
n-Nitroso-N-methylurethane	615-53-2
n-Nitrosonornicotine	16543-55-8
n-Nitrosopiperidine	100-75-4
n-Octadecane	593-45-3
nonadecane	629-92-5
Nonadecanoic acid	646-30-0
Nonaldehyde (pelargonic aldehyde)	124-19-6
Nonanoic acid	112-05-0
n-Phenylthiourea	103-85-5
n-Propylamine	107-10-8
n-Propylbenzene	103-65-1
n-Tetracosane	646-31-1
O,O,O-Triethyl phosphorothioate	126-68-1
O,O-Diethyl O-2-pyrazinyl phosphorothioate	297-97-2
Octachlorodibenzofuran	39001-02-0
Octachlorodibenzo-p-dioxin	3268-87-9
Octacosane	630-02-4
Octadecanoic acid	57-11-4
Octane, 2,6-dimethyl-	2051-30-1
Octanoic Acid	124-07-2
Octathiocane	10544-50-0

chemical	chemical_id
Oil and grease	OIL/GREASE
Oleic acid	112-80-1
Organic	198
Organic bromide	ORGANIC BR
Organic chloride	ORGANIC CL
Organic iodide	ORGANIC I
Osmium	4/2/7440
o-Toluidine	95-53-4
o-Toluidine hydrochloride	636-21-5
Oxidation Reduction Potential	EH
o-Xylene	95-47-6
p,p,p-Triphenyl-phosphine imide	2240-47-3
Paraldehyde	123-63-7
Parathion	56-38-2
p-Benzoquinone	106-51-4
p-Cymene	99-87-6
p-Dimethylaminoazobenzene	60-11-7
Pentachlorobenzene	608-93-5
Pentachlorodibenzofurans	30402-15-4
Pentachlorodibenzo-p-dioxins	36088-22-9
Pentachloroethane	76-01-7
Pentachloronitrobenzene (PCNB)	82-68-8
Pentachlorophenol	87-86-5
Pentacosane	629-99-2
Pentadecan-6-one	1001-45-2
Pentadecane	629-62-9
Pentanoic acid	109-52-4
Percent passing 1.5 inch sieve	PAS1.5IN
Percent passing 3 inch sieve	PAS3IN
Percent passing 3/4 inch sieve	PAS3/4IN
Percent passing 3/8 inch sieve	PAS3/8IN
Percent passing No. 10 sieve	PAS#10
Percent passing No. 100 sieve	PAS#100
Percent passing No. 140 sieve	PAS#140
Percent passing No. 20 sieve	PAS#20
Percent passing No. 200 sieve	PAS#200
Percent passing No. 4 sieve	PAS#4
Percent passing No. 40 sieve	PAS#40
Percent passing No. 60 sieve	PAS#60
Perchlorate anion	14797-73-0
pH Measurement	PH
Phenacetin	62-44-2
Phenanthrene	85-01-8
Phenol	108-95-2

chemical	chemical_id
Phenols	64743-03-9
Phenylenediamine	25265-76-3
Phorate	298-02-2
Phosphate	14265-44-2
Phosphine oxide, triphenyl-	791-28-6
Phosphorothioic Acid, O,O-diethyl O-(2-(ethylthio)ethyl...	8065-48-3
Phosphorus	7723-14-0
Phthalic acid esters	C31
Plutonium	7/5/7440
Plutonium-238	13981-16-3
Plutonium-239	15117-48-3
Plutonium-239/240	PU-239/240
Plutonium-241	14119-32-5
Plutonium-242	13982-10-0
Polychlorinated dibenzofurans	136677-10-6
Polychlorinated dibenzo-p-dioxins	136677-09-3
Potassium	9/7/7440
Potassium-40	13966-00-2
p-Phenylenediamine	106-50-3
Preludin	134-49-6
Pronamide	23950-58-5
Propane, 1,1-dichloro-	78-99-9
Protactinium-231	14331-85-2
p-Xylene	106-42-3
Pyrene	129-00-0
Pyridine	110-86-1
Pyrrolidin-2-one	616-45-5
Radium	7440-14-4
Radium-223	15623-45-7
Radium-224	13233-32-4
Radium-226	13982-63-3
Radium-228	15262-20-1
Ratio of Chromium-53 to Chromium-52	DELTA-CR53
Reserpine	50-55-5
Resorcinol	108-46-3
Ricinoleic Acid	7431-95-0
Ruthenium-103	13968-53-1
Ruthenium-106	13967-48-1
Safrol	94-59-7
Scandium	7440-20-2
Sebacic acid	111-20-6
sec-Butylbenzene	135-98-8
Selenium	7782-49-2
Selenium-79	15758-45-9

chemical	chemical_id
Silica	7631-86-9
Silicon	7440-21-3
Silver	7440-22-4
Silver-108 metastable	14391-65-2
Silver-110 metastable	378784-24-8
Sodium	7440-23-5
Sodium acetate	127-09-3
Sodium citrate	68-04-2
Sodium dithionite	7775-14-6
Sodium formate	141-53-7
Sodium nitrite	7632-00-0
Sodium-22	13966-32-0
Specific Conductance	CONDUCT
Strontium	7440-24-6
Strontium-89	14158-27-1
Strontium-90	10098-97-2
Strychnine	57-24-9
Styrene	100-42-5
Sulfate	14808-79-8
Sulfide	18496-25-8
Sulfur	7704-34-9
sym-Trinitrobenzene	99-35-4
Technetium-99	14133-76-7
Temperature	TEMPERATURE
tert-Butylbenzene	98-06-6
Tetrachlorodibenzofurans	55722-27-5
Tetrachlorodibenzo-p-dioxins	41903-57-5
Tetrachloroethene	127-18-4
Tetrachlorophenol	25167-83-3
Tetracyanonickelate(II)	NI(CN)4
Tetradecane	629-59-4
Tetradecanoic acid	544-63-8
Tetraethyl dithiopyrophosphate (Sulfotepp)	3689-24-5
Tetraethylpyrophosphate	107-49-3
Tetrahydrofuran	109-99-9
Thallium	7440-28-0
Thioacetamide	62-55-5
Thiofanox	39196-18-4
Thiourea	62-56-6
Thiuram	137-26-8
Thorium	7440-29-1
Thorium-228	14274-82-9
Thorium-230	14269-63-7
Thorium-232	TH-232

chemical	chemical_id
Thorium-234	15065-10-8
Tin	7440-31-5
Tin-113	13966-06-8
Tin-125	14683-08-0
Tin-126	15832-50-5
Titanium	7440-32-6
Toluene	108-88-3
Toluenediamine	25376-45-8
Total alpha energy emitted from Radium	ALPHA-RA
Total beta radiostrontium	SR-RAD
Total carbon	TC
Total cresols	1319-77-3
Total dissolved solids	TDS
Total halogens (all)	TOTHALOGEN
Total Inorganic Carbon	TIC
Total iron cyanide	FE(CN)6
Total organic carbon	TOC
Total organic halides	59473-04-0
Total petroleum hydrocarbons	TPH
Total petroleum hydrocarbons - diesel range	TPHDIESEL
Total petroleum hydrocarbons - gasoline range	TPHGASOLINE
Total petroleum hydrocarbons - kerosene range	TPHKEROSENE
Total petroleum hydrocarbons - motor oil (high boiling)	TPH/OILH
Total solids	TS
Total solids - volatile	TSV
Total suspended solids	TSS
Total suspended solids - volatile	TSSV
Total Trihalomethanes	THM
Total volatile organic compounds	TVOC
Toxaphene	8001-35-2
trans-1,2-Dichloroethylene	156-60-5
trans-1,3-Dichloropropene	10061-02-6
trans-1,4-Dichloro-2-butene	110-57-6
trans-Chlordane	5103-74-2
Tributyl phosphate	126-73-8
Trichloroacetyl chloride	76-02-8
Trichloroethene	79-01-6
Trichloromethanethiol	75-70-7
Trichloromonofluoromethane	75-69-4
Trichlorophenol	25167-82-2
Trichloropropane	25735-29-9
Tricosane	638-67-5
Tricyanocuprate(I)	CU(CN)3
Tridecane	629-50-5

chemical	chemical_id
Triethylene glycol	112-27-6
Trimethylsilanol	1066-40-6
Tris(2,3-dibromopropyl) phosphate	126-72-7
Tris-2-chloroethyl phosphate	115-96-8
Tritetracontane	7098-21-7
Tritium	10028-17-8
Turbidity	TURBIDITY
Undecane	1120-21-4
Undecane, 3-methyl-	1002-43-3
Undecanoic acid	112-37-8
Unknown	I99
Unknown aliphatic alcohol	UNKALIALCO
Unknown aliphatic hydrocarbon	I98
Unknown aliphatic substituted cyclohexane	UNKALSUBCY
Unknown amide	UNKAMIDE
Unknown aromatic hydrocarbon	I97
Unknown composite	M05
Unknown halogenated hydrocarbon	UNKHALHYDC
Unknown polycyclic aromatic hydrocarbon	UNKPCARHYC
Uranium	7440-61-1
Uranium-233/234	U-233/234
Uranium-234	13966-29-5
Uranium-234/Uranium-238 ratio	U234/238RT
Uranium-235	15117-96-1
Uranium-235/236	U-235/236
Uranium-235/Uranium-238 ratio	U235/238RT
Uranium-236	13982-70-2
Uranium-238	U-238
Vanadium	7440-62-2
Vinyl acetate	108-05-4
Vinyl chloride	75-01-4
Warfarin	81-81-2
Xylenes (total)	1330-20-7
Yttrium	7440-65-5
Zinc	7440-66-6
Zinc-65	13982-39-3
Zirconium	7440-67-7
Zirconium/Niobium-95	ZR/NB-95
Zirconium-95	13967-71-0

Pacific Northwest National Laboratory

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99354
1-888-375-PNNL (7665)

www.pnnl.gov