

Aquifer Injection Modeling (AIM) Toolbox User Guide

March 2021

Christian D. Johnson
Tycko Franklin
Valentin Molina
Joshua Q. Wassing
Paul K. Tran
Matthew S. Kump
Inci Demirkanli
Catherine M. Yonkofski
Fred Zhang

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Pacific Northwest National Laboratory
Richland, Washington 99354

Abstract

The Aquifer Injection Modeling Toolbox (“AIM Toolbox”) software was developed by the Pacific Northwest National Laboratory (PNNL) for the U.S. Environmental Protection Agency (EPA) to provide a collection of analytical solutions suitable for evaluating the potential extent of the area impacted by subsurface injection operations. Subsurface injection operations are regulated under the EPA’s Underground Injection Control (UIC) program and are typically related to oil/gas development, waste disposal, or subsurface mining or storage. The analytical algorithms provided in the AIM Toolbox each have different approaches/assumptions/focus with respect to the nature and processes in subsurface and the nature of the injection operations. Collectively the set of analysis algorithms provides a broader evaluation of the area that can potentially be impacted by an injection operation. By providing estimates for the injectate plume extent, the software supports technical aspects of planning, evaluation, and overseeing injection activities. That is, the results help assess when further regulatory controls (e.g., monitoring, reporting) may be required and, in the case of proposed disposal activities into an underground source of drinking water, the extent of the impacted area that would require exemption from protection under the Safe Drinking Water Act. The AIM Toolbox software is available as a single-page web application, providing an interface for necessary inputs and visualization of results in both chart and map panes. This User Guide describes the AIM Toolbox software, information required, user interactions, and the underlying basis of the calculations.

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This work has not been subject to the USEPA review and therefore does not necessarily reflect the views of the Agency, and no official endorsement should be inferred.

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Acronyms and Abbreviations

2D	Two dimensional
AE	Aquifer Exemption
AIM	Aquifer Injection Modeling
BGS	Below ground surface
EPA	U.S. Environmental Protection Agency
CRS	Coordinate reference system
EPSG	European Petroleum Survey Group
EOR	Enhanced oil recovery
GW	Groundwater
ID	Identifier
IDE	Integrated development environment
IT	Information technology
IW	Injected water
JSON	JavaScript Object Notation
Lat	Latitude
Lon	Longitude
MD	Measured depth
PNNL	Pacific Northwest National Laboratory
QA	Quality assurance
QAPP	Quality Assurance Project Plan
REST	Representational State Transfer
SDWA	Safe Drinking Water Act
SQAP	Software Quality Assurance Plan
STOMP	Subsurface Transport Over Multiple Phases
TDS	Total dissolved solids
TVD	True vertical depth
UIC	Underground Injection Control
USDW	Underground Source of Drinking Water
UTM	Universal Transverse Mercator
SPCS	State plane coordinate system

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1.0 Introduction

The purpose of the Aquifer Injection Modeling Toolbox (“AIM Toolbox”) software is to provide a user-friendly package of scientific, data-driven methods to estimate the extent of the subsurface area impacted by underground injection operations. Subsurface injection operations are regulated under the U.S. Environmental Protection Agency (EPA) Underground Injection Control (UIC) program, with well classification generally based on the type(s) of injection operations (i.e., what is being injected and the location of the injection zone relative to underground sources of drinking water¹ [USDWs]). These injection operations are typically related to oil/gas development, waste disposal, or subsurface mining or storage. Boundary delineation of the impacted area related to proposed subsurface injection operations provides an estimate for the extent within a targeted formation where further regulatory controls may be required (e.g., monitoring, reporting). In the case of disposal into an USDW, the extent of the impacted area would require exemption from protection under the Safe Drinking Water Act (SDWA). Relevant web pages describing EPA’s UIC program and aquifer exemptions (AE) include the following:

- <https://www.epa.gov/uic/general-information-about-injection-wells>
- <https://www.epa.gov/uic/aquifer-exemptions-underground-injection-control-program>
 - <https://www.epa.gov/uic/aquifer-exemptions-map> (with a link to an [interactive map](#))
- <https://www.epa.gov/uic/class-ii-oil-and-gas-related-injection-wells>

Current practices for delineating the extent of the impacted subsurface area often rely on simplistic methods, such as interpretations based on a fixed radius and basic structural assumptions. Because key physical and chemical subsurface processes are not fully represented in these approaches, new tools are needed to provide a more subsurface process-oriented, scientific, and data-driven methodology for delineating the area of impact (e.g., aquifer exemption boundaries).

The AIM Toolbox was developed by the Pacific Northwest National Laboratory (PNNL) for the EPA to provide a collection of analytical solutions suitable for evaluating the potential extent of the area impacted by subsurface injection operations. Although, individually, these analytical solutions generally will focus on certain subsurface processes/aspects, collectively they provide a broader evaluation of the area that can potentially be impacted by an injection operation. The estimated results can account for variations in geology (e.g., aquifer thickness), hydraulic flow parameters (e.g., hydraulic gradient, porosity, hydraulic conductivity), in situ fluid properties (e.g., specific gravity or density), and injection operation parameters (e.g., injectate specific gravity or density, flow rate, injection duration). By providing estimates for the injectate plume extent, the software supports technical aspects of planning, evaluation, and overseeing injection activities.

The intended use of the AIM Toolbox is to evaluate disposal operations for brine disposal (e.g., produced water from oil and gas operations that would be disposed into UIC Class IID wells). Figure 1 depicts the general concept of subsurface injection and evaluation of associated impacts. Given that the injectate (brine) would be heavier than the aquifer formation water,

¹ A USDW resource is an aquifer or part of an aquifer that either supplies a public water system or contains a sufficient quantity of groundwater to supply a public water system, and either currently supplies drinking water for human consumption or contains fewer than 10,000 mg/L of total dissolved solids (TDS), and which is not an exempted aquifer [40 CFR 144.3].

some density effects could be expected, where there is more spread in the injectate at lower depths. Where an aquifer has non-negligible groundwater flow (due to natural gradients and hydraulic conductivity), the distribution of injectate would be expected to be asymmetric, with more spread in the downgradient direction.

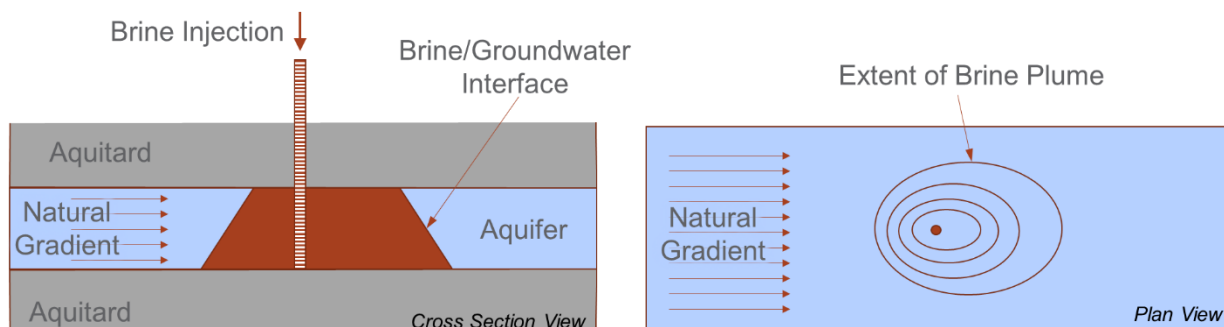


Figure 1. Generic representation of the subsurface injection process and evaluation of the impacts of injection.

This User Guide describes how to use the AIM Toolbox software (Section 2.0), provides some usage examples (Section 3.0), describes the underlying equations/calculations (Section 4.0), discusses software testing (Section 5.0), provides information on the software development context (6.0), and reflects on features that could be included in future versions. Some of the information related to these topics was captured in the Quality Assurance (QA) document package (which is comprised of the software quality assurance plan [SQAP] and associated documents). Select elements of the QA document package are excerpted for presentation in this User Guide.

2.0 Software Use

Based on early design discussions, it was determined that a single-page web application would best serve the needs of EPA and their users (versus a traditional compiled/executable desktop application or a Microsoft® Excel®-based spreadsheet application). The web application approach has the advantage of being readily accessible, providing a responsive experience, and readily tying into mapping resources, at the expense of increased complexity in developing the software, potential for network interruptions, and ongoing hosting costs.

The AIM Toolbox software was designed for use in the Google Chrome™ web browser on a Microsoft® Windows® machine. Being a web-based software application, the AIM Toolbox may function properly on other operating systems (e.g., Apple® Macintosh®, Android™, Linux®) and other web browsers (e.g., Mozilla® Firefox®, Microsoft Edge®, Apple® Safari®), however those configurations have not been tested and are unsupported.

During development by PNNL, the AIM Toolbox software was implemented through Amazon Web Services™ (AWS), though deployment in a cloud computing context is not required (the website could also be deployed via an on-premise server). The final long-term deployment approach and URL for the software is not yet determined. Visit the Aquifer Injection Modeling Toolbox project website at <https://www.pnnl.gov/projects/aim-toolbox> to access the software.

2.1 Data Sources

The data for the AIM Toolbox software are of limited quantity and thus can be contained in JSON files or hard-coded lists; no databases or network data services are required. JSON (JavaScript Object Notation) is a lightweight data-interchange format that is human readable and easy to programmatically ingest and manipulate. The data types used in AIM Toolbox software, along with their sources and references, are listed in Table 1.

Table 1. AIM Toolbox data types, sources, and references.

Data Type	Data Source	See ...
List of coordinate reference systems (CRS) and their associated EPSG identifier codes	https://spatialreference.org/ (accessed on Aug. 24, 2020) and http://epsg.io/ (accessed on Dec. 19, 2020)	Table 8
Aquifer property information for different types of geological materials	Multiple references (see Section 2.2.4)	Table 7
Standard density of water	CRC Handbook of Chemistry and Physics (HBCP, 2015)	Figure 6
Existing aquifer exemptions (from the publicly available EPA database and converted to JSON-formatted text)	Aquifer Exemption Geospatial Data at https://www.epa.gov/uic/aquifer-exemption-data (accessed on July 28, 2020)	the indicated database website or https://epa.maps.arcgis.com/apps/MapSeries/index.html?appid=426ef9d346f9487e96ee5899ab67a2e4

Existing aquifer exemption data was extracted from the EPA “Aquifer Exemption Geospatial Data” database. The data was processed to exclude certain fields, alter field names, convert coordinates to Web Mercator values in meters, and convert the date/time format prior to storing in JSON-formatted files. Table 2 compares the fields of the EPA AE database with the fields used in the AIM Toolbox software. The quality codes (Qual) used in the AIM Toolbox JSON data are mapped to descriptive text as shown in Table 3; the descriptive text is what is displayed to the user. An example of the JSON-formatted data that is used in the AIM Toolbox software is shown in Figure 2. As additional aquifer exemptions are added to EPA’s database/list, they will need to be manually added to the AIM Toolbox software (as described in Section 2.4.13), with such updates envisioned to occur annually (or more frequently, if desired). If EPA were to provide the AE data as a service (e.g., a REST endpoint) in the future, then the AIM Toolbox software could be modified to retrieve the data directly from that data service.

Table 2. Crosswalk of data fields between the EPA AE database and the AIM Toolbox.

EPA AE Database Field	AIM Toolbox JSON Field ^a	Example Data from the EPA AE Database
wkt_geom ^b	geometry ^b	MultiPolygonZ (((-104.12391042318148493 41.29845162032728467 0.0, -104.1239033957156721 41.30208201883993979 0.0, ...)))
OBJECTID	—	2530
ID	AEID	8_4657
Region	—	8
Number	—	4657
CentroidX	—	-104.1191373
CentroidY	—	41.30579217
Injection_Well_ID	WellID	Docket 1071-2014
Well_Class	WellClass	IIR
Injection_Activity	InjType	EOR
State	State	WY
County	County	Laramie
Tribe	Tribe	Wind River Joint
State_or_Tribe	—	Wind River Joint (WY)
AE_Area	Area	0.52
AE_Area_Units	AreaUnits	square miles
Depth	Depth	7532
Depth_Units	DepthUnits	feet below ground (BGS, TVD, or MD)
Injection_Zone	InjZone	Lower Cretaceous J Sandstone Formation
Formation_Thickness	FormationThick	88
Lithology	Lithology	sandstone
Injectate_Characteristics	—	Water produced with oil
Decision_Date ^c	AEDate ^c	2017-03-10T00:00:00.000
Data_Quality_Category	Qual ^d	Precise location
Shape_Length	—	0.076057558
Shape_Area	—	0.000240963

^a Fields marked with — are not included in the existing aquifer exemption JSON data in the AIM Toolbox.

^b AE shape geometry is converted from the EPA AE database format (shown in the truncated example here) to the JSON format shown below, with coordinates converted from Lat/Lon to Web Mercator (meters).

^c In the EPA AE database, the time is represented in a format of "2017-03-10T00:00:00.000", which is converted to a format of "2017/03/10 00:00:00" for the AIM Toolbox JSON data.

^d In the EPA AE database, the data quality consists of standard descriptive text, whereas the AIM Toolbox JSON data stores a quality code that maps to the descriptive text, as shown in Table 3.

Table 3. Data quality codes and the associated meaning.

Qual	Quality Definition
1	Precise Location
2	Less precise location and some attributes missing
3	Imprecise location or several attributes missing
4	County location available only

```

{
  "type": "FeatureCollection",
  "name": "Aquifer Exemptions",
  "crs": "urn:ogc:def:crs:EPSG::3857",
  "features": [
    {
      "type": "Feature",
      "AEID": "8_4657",
      "WellID": "Docket 1071-2014",
      "WellClass": "IIR",
      "InjType": "EOR",
      "State": "WY",
      "County": "Laramie",
      "Tribe": "Wind River Joint",
      "Area": 0.52,
      "AreaUnits": "square miles",
      "Depth": 7532,
      "DepthUnits": "feet below ground (BGS, TVD, or MD)",
      "InjZone": "Lower Cretaceous J Sandstone Formation",
      "FormationThick": 88,
      "Lithology": "sandstone",
      "AEDate": "2017/03/10 00:00:00",
      "Qual": "1",
      "geometry": {
        "type": "MultiPolygon",
        "coordinates": [
          [
            [-11591020.7, 5056463.4], [-11591019.9, 5057001.3], [-11591553.1, 5057001.4],
            [-11591551.7, 5057536.9], [-11591550.3, 5058072.4], [-11591548.9, 5058608.1],
            [-11591015.3, 5058608.2], [-11590481.8, 5058605.6], [-11589950.2, 5058605.3],
            [-11589455.9, 5058602.3], [-11589461.2, 5058066.7], [-11589951.6, 5058069.6],
            [-11589953, 5057533.9], [-11589421.1, 5057530.9], [-11589422.3, 5056995.3],
            [-11589423.5, 5056459.2], [-11589955.2, 5056461], [-11590486.9, 5056462.8],
            [-11591020.7, 5056463.4]
          ]
        ]
      }
    },
    ...
  ]
}

```

Figure 2. JSON format for AE data, with the example data corresponding to the example in Table 2.

2.2 Interface and Inputs

The AIM Toolbox software interface and input parameters, with associated options are described in this section.

2.2.1 Application Interface

The AIM Toolbox software interface consists of two pages, an initial login page, and the application itself. The login page shown in Figure 3 is the initial view that is displayed to the user when accessing the website.

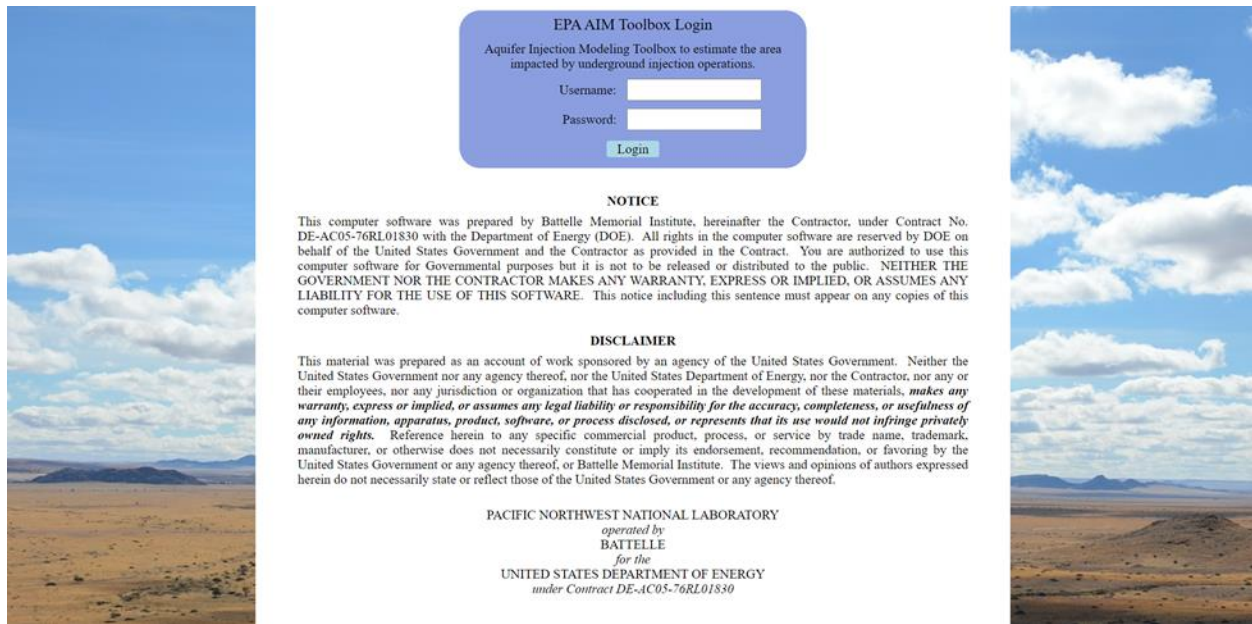


Figure 3. Login page for the AIM Toolbox software.

After logging in, the user is presented with the application interface. Figure 4 shows the AIM Toolbox software interface along with quick reference annotations that describe the interface elements and functionality. The interface consists of three main panes: the left side analysis configuration pane, the top right map pane, and the lower right chart/results pane. The user must first define their scenario in the analysis configuration pane by specifying input parameters. Once defined, clicking the “Calculate” button will produce results in the form of time series plots, a two-dimensional XY plot, or tabulated results in the chart pane and contours in the map pane. The analysis configuration lists two possible analysis modes, injectate extent and pressure distribution. The pressure distribution analysis mode is intended for future expansion of software capabilities and thus has no selectable analysis algorithm options.

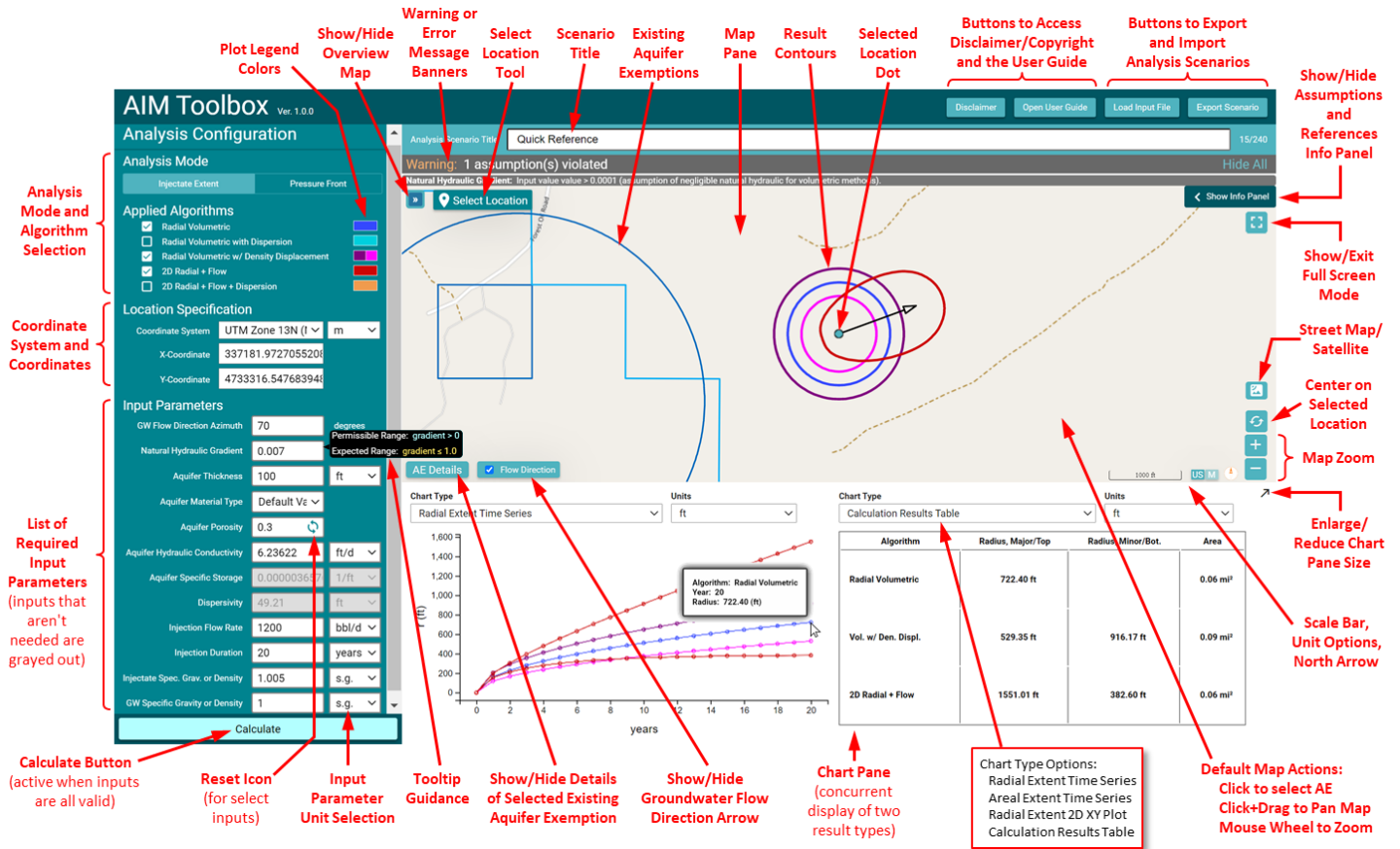


Figure 4. Interface for the AIM Toolbox software, with quick reference annotations describing software elements and functionality.

2.2.2 Injectate Extent Analysis Algorithm Options

The injectate extent analysis mode offers the five analysis algorithm options listed in Table 4.

Table 4. Analysis algorithm options and associated shorthand identifier.

Method ID	Analysis Algorithm (Method)
A	Radial Volumetric
B	Radial Volumetric with Dispersion
C	Radial Volumetric with Density Displacement
D	2D Radial + Flow
E	2D Radial + Flow + Dispersion

The injectate extent analysis algorithms represent different approaches and assumptions. This set of injectate extent analysis algorithms should be used collectively to provide an overall assessment of the extent of potential impacts of injection operations, rather than focusing on a single method. The algorithms are summarized in the following list, with details of the calculations and assumptions given in Section 4.0.

- The **Radial Volumetric** method represents volumetric displacement of formation (aquifer) groundwater by injectate fluid.
- The **Radial Volumetric with Dispersion** method adds an estimate of injectate spread due to dispersion to the volumetric displacement.
- The **Radial Volumetric with Density Displacement** method represents displacement without dispersion, but accounting for differences in formation groundwater and injectate fluid densities (or, equivalently, specific gravities). The injectate fluid is assumed to be heavier than the formation groundwater, resulting in a conical frustum that is narrower at the top and wider at the bottom of the aquifer.
- The **2D Radial + Flow** method represents displacement of formation groundwater by injectate fluid, but accounts for groundwater flow, leading to an asymmetric distribution of the injectate.
- The **2D Radial + Flow + Dispersion** method adds an estimate of injectate spread due to dispersion to the displacement with groundwater flow.

2.2.3 Input Parameters

A limited set of input parameters is required for calculation of analysis algorithm results. Table 5 lists the parameters that are required for each analysis algorithm (by the method IDs listed in Table 4). Some parameters are not required for calculating the results for an analysis algorithm, but are instead used for assessing assumption violations or for displaying results in the map pane. Input parameters in the Analysis Configuration pane are only accessible to the user when appropriate analysis algorithm options are selected. For example, the user cannot enter a value for the Dispersivity unless one of the dispersion-related analysis algorithms are selected. While the AIM Toolbox interface (Figure 4) includes an entry for aquifer specific storage, that parameter is always inaccessible (and not included in Table 5) because it is intended for future functionality.

The input parameters are generally self-descriptive, relating to the aquifer or the injection. The parameters describe natural groundwater flow (azimuth and hydraulic gradient), aquifer characteristics (thickness, porosity, hydraulic conductivity, and groundwater density), degree of plume dispersivity in the aquifer, and injection operations (location, flow rate, duration, and injectate density). Additionally, the user can specify an aquifer material type to reflect the geology/lithology of the aquifer. Material types are discussed in detail in Section 2.2.4.

Table 5. Mapping of input parameters to analysis methods.¹

Input Parameter	Method ID				
	A	B	C	D	E
Location / Map Coordinates	m	m	m	m	m
Groundwater Flow Direction Azimuth				m	m
Aquifer Hydraulic Gradient (in direction of flow)	a	a	a	X	X
Injection Rate	X	X	X	X	X
Duration of Injection	X	X	X	X	X
Aquifer Thickness	X	X	X	X	X
Aquifer Material Type	X	X	X	X	X
Aquifer Porosity	X	X	X	X	X
Aquifer Hydraulic Conductivity			X	X	X
Dispersivity		X			X
Groundwater Density (specific gravity)	a	a	X	a	a
Injectate Density (specific gravity)	a	a	X	a	a

- ¹ X = used as an input for the algorithm calculations
m = used for displaying results on the Map
a = used for assessing whether an assumption has been met or not

Table 6 provides additional information on the input parameters. Specifically, the default units and the options for additional units are listed for each parameter, though some input parameters are unitless and there is only one unit used for the groundwater flow direction azimuth. Bounds for input parameter values are described in Table 6, with the permissible range representing hard limits and an “expected range” representing a typical range for the input parameter. If the user enters a value outside of the permissible range for an input parameter, the software will indicate that there is an error and will not allow calculation of results. If the user enters a value within the permissible range, but outside the expected range of typical values, the software will allow calculation of results, but will warn the user. Finally, Table 6 lists the initial values for each input parameter. The initial values are arbitrary, but allow the user to simply select one or more analysis algorithm options, click the “Calculate” button, and see example results. The user is expected to adjust the input parameter values to reflect a particular site or scenario of interest.

Table 6. Input parameters, associated units, bounds, and initial values.

Parameter	Sym.	Standard Units	Unit Options	Permissible Range	Warning When... ^a	Default (Initial) Value and Units ^b
Location (coordinate reference system [CRS] and XY coordinates)	—	Web Mercator, m	m, ft, U.S. survey ft	Lat/Lon, UTM, or SPCS must be nominally within CRS bounds	significantly outside CRS bounds	Lat/Lon 42.922415, -106.290012 (in Web Mercator, X = -11832150, Y = 5300170)
GW Flow Direction Azimuth	α	degrees (°)	°	$0 \leq \alpha \leq 360^\circ$ ($360^\circ = 0^\circ$)	—	70 °
Natural Hydraulic Gradient	i	—	—	$i > 0$	$i > 1$	0.007
Aquifer Thickness	H	m	m, ft	$H \geq 0.3048$ m	—	100 ft
Aquifer Material Type	—	—	—	selection list (see Table 7)	—	None selected (Default Values)
Aquifer Porosity	n	—	—	$0 < n < 1$	$n < 0.045$ or $n > 0.7$	0.2
Aquifer Hydraulic Conductivity	K	m/y	cm/s, m/d, m/y, ft/s, ft/d, ft/y	$K > 0$	$K < 3.0 \text{ E-}14$ or $K > 0.1$ m/s	6.23622 ft/d
Dispersivity	D	m	m, ft	$D > 0$	—	49.21 ft
Injection Flow Rate	Qi	m ³ /y	bbl/d, ft ³ /d, m ³ /d, m ³ /y, L/min, gpd, gpm	$Q_i > 0$	—	1200 bbl/d
Injection Duration	t _{total}	y	y, d	t _{total} > 0	—	20 y
Injectate Spec. Grav. or Density	ρ_i	kg/m ³	s.g., kg/m ³ , g/mL, mg/L, °API, °Bé	$800 \leq \rho_i \leq 2500$ kg/m ³ and $\rho_i > \rho_w$	$\rho_i < 1000$ or $\rho_i > 1400$ kg/m ³	1.005 s.g.
Groundwater Spec. Grav. or Density	ρ_w	kg/m ³	s.g., kg/m ³ , g/mL, mg/L, °API, °Bé	$800 \leq \rho_w \leq 2500$ kg/m ³ and $\rho_i > \rho_w$	$\rho_w < 900$ or $\rho_w > 1050$ kg/m ³	1.0 s.g.

^a These bounds represent the “expected ranges.” Outside of these bounds, a warning is displayed.

^b These are the initial parameter values when the application starts and are not tied to any specific material type (so the material type is initially listed as “Default Values”). These initial values are internally specified in metric units to two significant digits, but are displayed here with more significant digits to have equivalent values after unit conversions.

2.2.4 Material Types

The user may select a material type from a selection list corresponding to Table 7. Multiple references (Domenico and Mifflin, 1965; Morris and Johnson, 1967; Bear, 1972; Freeze and Cherry, 1979; Wolff, 1982; Batu, 1988; Domenico and Schwartz, 1990; Gelhar et al., 1992; Macfarlane, 1996; Heath, 2004; Fitts, 2012; Heywood et al., 2016; Sterckx et al., 2017; Duffield, 2019) were used to compile porosity and hydraulic conductivity data, and the minimum, maximum, and mean values are shown in the table. When the user selects a material type, the aquifer porosity and aquifer hydraulic conductivity values (and dispersivity, which is discussed in

Section 2.2.5) are automatically changed to the default values for the material type, with the defaults being the mean values in Table 7. These default values are intended to be a rough approximation for each material type. However, it is always better to use site-specific information, when available, because a given material type can have property values that range widely from location to location. Thus, the user is encouraged to alter the porosity and hydraulic conductivity input parameter values, though the default values are representative if the user doesn't have any site-specific information. A sensitivity analysis could be performed to address uncertainty in aquifer property values.

Table 7. Material types, associated default values (mean), and the minimum/maximum of values from the references.

Material Type	Porosity (%) ^a			Hydraulic Conductivity (m/s) ^a		
	Min.	Max.	Mean	Min.	Max.	Mean
Basalt	0.10	35	7.3	9.3 E-14	1.8 E-01	1.8 E-02
Clay	8.7	58	45	3.0 E-13	1.0 E-06	7.4 E-08
Dolomite	0.41	33	6.2			1.1 E-05
Gravel	19	44	31	1.0 E-05	1.0 E+00	6.9 E-02
Igneous and Metamorphic Rock	0.0	57	4.5	3.0 E-14	1.0 E+00	4.5 E-02
Limestone	0.0	56	8.1	1.3 E-08	2.0 E-02	1.8 E-03
Limestone/Dolomite	0.07	67	8.3	1.0 E-10	1.0 E-02	1.7 E-03
Outwash	18	39	30			7.5 E-04
Sand	3.0	61	38	1.0 E-08	1.0 E-02	7.5 E-04
Sandstone	0.0	54	20	1.0 E-10	3.5 E-04	1.9 E-05
Shale	0.80	42	12	1.0 E-16	2.3 E-09	2.1 E-09
Silt	31	61	45	1.0 E-09	3.5 E-05	9.3 E-06
Siltstone	1.1	48	32	1.0 E-11	1.4 E-08	7.0 E-09
Till	12	41	27	5.0 E-13	3.5 E-06	9.2 E-07

^a The mean values (in bold) were used as the material-specific default values in the AIM Toolbox. Empty minimum/maximum entries indicate that multiple data values were not available, so the single available value was used as the mean.

2.2.5 Dispersivity

In environmental analyses, dispersivity is generally approached as a function of scale of the groundwater plume of interest, not as a material type property. Dispersivity is also frequently treated as a fitting parameter to match observed data. So, estimates of dispersivity have a broad range. Gelhar et al. (1992) compiled a large list of dispersivity values for a wide range of site types, materials, and plume scales. This compiled dispersivity data as a function of plume scale exhibits a lot of scatter, indicating the wide variation and uncertainty in this parameter. Although dispersivity is not a material property, the Gelhar et al. (1992) data nominally for consolidated rock material types (basalt, igneous rock, sandstone, dolomite, limestone, chalk) was used to determine a default value for all material types in the AIM Toolbox.

Several equations were used to provide a correlation between plume scale (s) and dispersivity (D), including Equation 1309 from the TableCurve2D (Systat Software, San Jose, California)

software (but without the $s^{2.5}$ term), a logarithmic increase equation, and the equation 12b correlation from Xu and Eckstein (1995), which is a commonly cited source for a dispersivity correlation. In all but one case a least-squares “best fit” was used to determine equation coefficients. The equations for the curve fits are given below using Microsoft Excel function notation with the plume scale (s) and dispersivity (D) in units of meters and including truncation at a minimum dispersivity of 0.01 m. The other case (also shown in the equations below) was a “visual fit” through the consolidated rock dispersivity data that was plotted on a log-log plot (Figure 5). Though visually pleasing, the visual fit is somewhat arbitrary due to the nature of the log-log plot. Note that the Xu and Eckstein (1995) correlation was determined using all of the Gelhar et al. (1992) dispersivity data, not just consolidated rock data. Given the scatter in data over the range of plume scales, any of the least squares correlations (which are presented below in Figure 5) could be used. For the AIM Toolbox software, every material type (excluding the “Default Values”) is assigned a dispersivity of 34 m (111.5 ft), determined with the TableCurve2D Equation 1309 least-squares fit at a plume scale of 400 m. As with other input parameter values, the user is encouraged to change the default value to reflect site-specific information, if it is available, and to assess uncertainty with a sensitivity analysis.

- Logarithmic Least Squares: $D = \text{MAX}(\text{IFERROR}(10^{(1.25641*\text{LN}(\text{LOG}(s)) + 0.277989)}, 0.01), 0.01)$ (1)
- Eqn. 1309 Least Squares: $D = \text{MAX}(\text{EXP}(4.05240 - 10.4625/\text{SQRT}(s)), 0.01)$ (2)
- Eqn. 1309 Visual Fit: $D = \text{MAX}(\text{EXP}(4.6 - 12.5/\text{SQRT}(s)), 0.01)$ (3)
- Xu and Eckstein, 1995, Eq. 12b $D = 1.2*(\text{LOG}(s))^{2.958}$ (4)

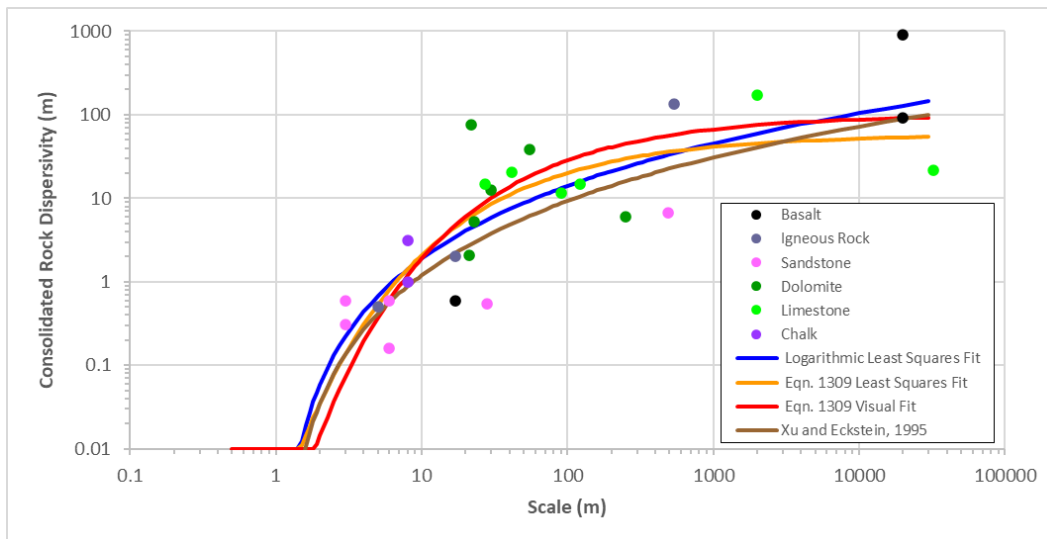


Figure 5. Dispersivity data from Gelhar et al. (1992) for consolidated rock materials, along with “best fit” curve fits to describe the correlation to the scale of interest.

2.2.6 Density and Specific Gravity

The injectate and groundwater specific gravity or density are required in the AIM Toolbox software either for calculating results or for checking assumptions. Multiple approaches can be used to quantify the amount of a liquid in a given volume. The standard approach in chemistry

is to specify the liquid density. Specific gravity (s.g.) is the ratio of the density of a liquid (ρ_{liquid}) to the standard density of water (ρ_w).

$$\text{s.g.} = \rho_{\text{liquid}} / \rho_w \tag{5}$$

Thus, the density of water is required in the AIM Toolbox for the purpose of unit conversions. To be more generic and provide options for future functionality, data for the standard density of water as a function of temperature (from 5°C to 99.974°C) was taken from the CRC Handbook of Chemistry and Physics (HBCP, 2015) and a sixth-order polynomial was fit to the data, as shown Figure 6. The equation for this sixth-order polynomial correlation between groundwater temperature (T_w , °C) and density of water (ρ_w , kg/m³) is given in Equation (6).

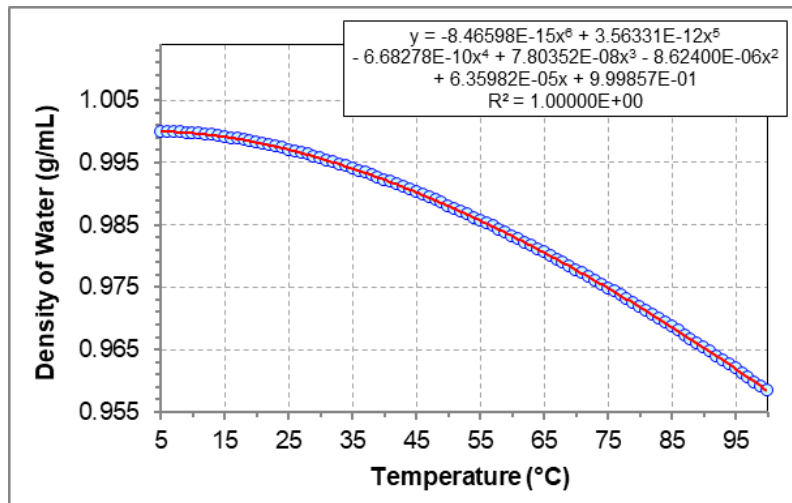


Figure 6. Data and curve fit for standard density of water.

$$\rho_w = (-8.46597983347259E-15 \times T_w^6 + 3.56330987510766E-12 \times T_w^5 - 6.68278049698719E-10 \times T_w^4 + 7.80352447210771E-08 \times T_w^3 - 8.62399682192574E-06 \times T_w^2 + 0.000063598117986193 \times T_w + 0.999856592456876) \times 1000 \tag{6}$$

The relative density of liquids can be measured with a hydrometer, which is based on the concept of buoyancy. Several hydrometer scales may be relevant to specifying injectate liquid density, including API gravity (°API) and the Baumé scale (°Bé). The former is often used to compare densities of petroleum liquids, while the latter typically finds use in industrial chemistry settings. The Baumé scale has two formulations, one for density of liquids heavier than water and the other for liquids lighter than water; only the former is relevant to the AIM Toolbox software. Conversions for API and Baumé scales (Considine and Considine, 1995; Hughes, 1954) are shown in Equations 7 and 8 as follows, including reference temperature information.

$$^{\circ}\text{API} = \frac{141.5}{\text{s.g. (at } 60^{\circ}\text{F)}} - 131.5 \tag{7}$$

$$^{\circ}\text{Bé} = 145 - \frac{145}{\text{s.g. (at } 60^{\circ}\text{F)}} \text{ (for liquids heavier than water)} \tag{8}$$

2.2.7 Location Specification and Coordinates

The location of interest is an input that is not used in analysis algorithm calculations, but is used for presentation of results. The location can be specified in two ways, as a set of coordinates in a defined coordinate system or by selecting a location on the map. In the left pane, the user can choose from standard coordinate systems (Lat/Lon, UTM, or State Plane) and then enter coordinate values. A list of coordinate systems available in the AIM Toolbox and their associated EPSG identifier codes are given in Table 8. Latitude and longitude values are entered as decimal values in degrees. UTM and SPCS (State Plane) X and Y (Easting and Northing) coordinates can be entered in units of m, ft, or US survey ft (0.3048 m = 1 ft and 1200/3937 m = 1 US survey ft). When coordinates are entered, the map view centers on the new location, identified by the location dot. Alternately, the user can pan/zoom to the location of interest, click the “Select Location” button on the map pane to enter location selection mode, then click on the location of interest in the map. Selection of a location in the map results in the map centering on that location and the coordinates in the left pane being updated to reflect the selected location. Note that in location selection mode, the action of a pointer “click” to specify/select the location of interest, but the user can still pan and zoom the map. To return to standard selection mode (where existing AE shapes can be selected), toggle the “Select Location” button. While coordinates are displayed in the selected coordinate system, behind the scenes the AIM Toolbox software tracks coordinates in the web standard Web Mercator coordinate system (EPSG 3857).

For additional information on coordinate systems, a few representative/example online resources include the following:

Coordinate Reference System Information

https://en.wikipedia.org/wiki/Spatial_reference_system

https://docs.qgis.org/testing/en/docs/gentle_gis_introduction/coordinate_reference_systems.html

<https://www.esri.com/arcgis-blog/products/arcgis-pro/mapping/coordinate-systems-difference/>

Lists of Coordinate Reference System IDs/Info

<https://spatialreference.org/ref/epsg/?page=1>

Performing Coordinate Transformations

<https://epsg.io/>

<https://geodesy.noaa.gov/NCAT/index.xhtml>

UTM

https://www.xmswiki.com/wiki/UTM_Coordinate_System

https://en.wikipedia.org/wiki/Universal_Transverse_Mercator_coordinate_system

State Plane Coordinate System

https://www.xmswiki.com/wiki/State_Plane_Coordinate_System

https://en.wikipedia.org/wiki/State_Plane_Coordinate_System

Table 8. Coordinate reference systems (CRS) and their EPSG codes.

EPSG	CRS Name and Datum
3857	Web Mercator
4326	Lat/Long
26929	Alabama East (NAD83)
26930	Alabama West (NAD83)
26931	Alaska Zone 1 (NAD83)
26932	Alaska Zone 2 (NAD83)
26933	Alaska Zone 3 (NAD83)
26934	Alaska Zone 4 (NAD83)
26935	Alaska Zone 5 (NAD83)
26936	Alaska Zone 6 (NAD83)
26937	Alaska Zone 7 (NAD83)
26938	Alaska Zone 8 (NAD83)
26939	Alaska Zone 9 (NAD83)
26940	Alaska Zone 10 (NAD83)
26949	Arizona Central (NAD83)
26948	Arizona East (NAD83)
26950	Arizona West (NAD83)
26951	Arkansas North (NAD83)
26952	Arkansas South (NAD83)
26941	California Zone 1 (NAD83)
26942	California Zone 2 (NAD83)
26943	California Zone 3 (NAD83)
26944	California Zone 4 (NAD83)
26945	California Zone 5 (NAD83)
26946	California Zone 6 (NAD83)
26954	Colorado Central (NAD83)
26953	Colorado North (NAD83)
26955	Colorado South (NAD83)
26956	Connecticut (NAD83)
26957	Delaware (NAD83)
26958	Florida East (NAD83)
26960	Florida North (NAD83)
26959	Florida West (NAD83)
26966	Georgia East (NAD83)
26967	Georgia West (NAD83)
26961	Hawaii Zone 1 (NAD83)
26962	Hawaii Zone 2 (NAD83)
26963	Hawaii Zone 3 (NAD83)
26964	Hawaii Zone 4 (NAD83)
26965	Hawaii Zone 5 (NAD83)
26969	Idaho Central (NAD83)
26968	Idaho East (NAD83)
26970	Idaho West (NAD83)
26971	Illinois East (NAD83)
26972	Illinois West (NAD83)
26973	Indiana East (NAD83)
26974	Indiana West (NAD83)
26975	Iowa North (NAD83)
26976	Iowa South (NAD83)
26977	Kansas North (NAD83)

EPSG	CRS Name and Datum
26978	Kansas South (NAD83)
2205	Kentucky North (NAD83)
26979	Kentucky North (NAD83)
3088	Kentucky Single Zone (NAD83)
26980	Kentucky South (NAD83)
26981	Louisiana North (NAD83)
32199	Louisiana Offshore (NAD83)
26982	Louisiana South (NAD83)
26983	Maine East (NAD83)
26984	Maine West (NAD83)
26985	Maryland (NAD83)
26987	Massachusetts Island (NAD83)
26986	Massachusetts Mainland (NAD83)
26989	Michigan Central (NAD83)
26988	Michigan North (NAD83)
26990	Michigan South (NAD83)
26992	Minnesota Central (NAD83)
26991	Minnesota North (NAD83)
26993	Minnesota South (NAD83)
26994	Mississippi East (NAD83)
26995	Mississippi West (NAD83)
26997	Missouri Central (NAD83)
26996	Missouri East (NAD83)
26998	Missouri West (NAD83)
32100	Montana (NAD83)
32104	Nebraska (NAD83)
32108	Nevada Central (NAD83)
32107	Nevada East (NAD83)
32109	Nevada West (NAD83)
32110	New Hampshire (NAD83)
32111	New Jersey (NAD83)
32113	New Mexico Central (NAD83)
32112	New Mexico East (NAD83)
32114	New Mexico West (NAD83)
32116	New York Central (NAD83)
32115	New York East (NAD83)
32118	New York Long Island (NAD83)
32117	New York West (NAD83)
32119	North Carolina (NAD83)
32120	North Dakota North (NAD83)
32121	North Dakota South (NAD83)
32122	Ohio North (NAD83)
32123	Ohio South (NAD83)
32124	Oklahoma North (NAD83)
32125	Oklahoma South (NAD83)
32126	Oregon North (NAD83)
32127	Oregon South (NAD83)

EPSG	CRS Name and Datum
32128	Pennsylvania North (NAD83)
32129	Pennsylvania South (NAD83)
32130	Rhode Island (NAD83)
32133	South Carolina (NAD83)
32134	South Dakota North (NAD83)
32135	South Dakota South (NAD83)
32136	Tennessee (NAD83)
32139	Texas Central (NAD83)
32137	Texas North (NAD83)
32138	Texas North Central (NAD83)
32141	Texas South (NAD83)
32140	Texas South Central (NAD83)
32143	Utah Central (NAD83)
32142	Utah North (NAD83)
32144	Utah South (NAD83)
32145	Vermont (NAD83)
32146	Virginia North (NAD83)
32147	Virginia South (NAD83)
32148	Washington North (NAD83)
32149	Washington South (NAD83)
32150	West Virginia North (NAD83)
32151	West Virginia South (NAD83)
32153	Wisconsin Central (NAD83)
32152	Wisconsin North (NAD83)
32154	Wisconsin South (NAD83)
32155	Wyoming East (NAD83)
32156	Wyoming East Central (NAD83)
32158	Wyoming West (NAD83)
32157	Wyoming West Central (NAD83)
26901	UTM Zone 1N (NAD83)
26902	UTM Zone 2N (NAD83)
26903	UTM Zone 3N (NAD83)
26904	UTM Zone 4N (NAD83)
26905	UTM Zone 5N (NAD83)
26906	UTM Zone 6N (NAD83)
26907	UTM Zone 7N (NAD83)
26908	UTM Zone 8N (NAD83)
26909	UTM Zone 9N (NAD83)
26910	UTM Zone 10N (NAD83)
26911	UTM Zone 11N (NAD83)
26912	UTM Zone 12N (NAD83)
26913	UTM Zone 13N (NAD83)
26914	UTM Zone 14N (NAD83)
26915	UTM Zone 15N (NAD83)
26916	UTM Zone 16N (NAD83)
26917	UTM Zone 17N (NAD83)
26918	UTM Zone 18N (NAD83)
26919	UTM Zone 19N (NAD83)

2.3 Result Outputs

When the user clicks the “Calculate” button, the AIM Toolbox software conducts the calculations for each selected analysis algorithm option. For each analysis algorithm option that successfully returns results, several types of results are presented in the map and chart panes (Figure 7). Contours are displayed on the map to represent the injectate extent at the end of the injection duration time period. If either of the 2D Radial + Flow analysis algorithm options are selected, then the groundwater flow direction azimuth is used to orient the direction of the asymmetric contours on the map. Note that the Radial Volumetric with Density Displacement results include two contours, one for the radius at the top of the aquifer and one for the radius at the bottom of the aquifer. In the chart pane, the user can select from three chart types and one table for display in two side-by-side slots. The chart types include a radial extent time series, an areal extent time series, and a 2D XY plot of contours (aligned with the X axis). Radius and area results at the injection duration time are tabulated in the table for each selected analysis algorithm option.

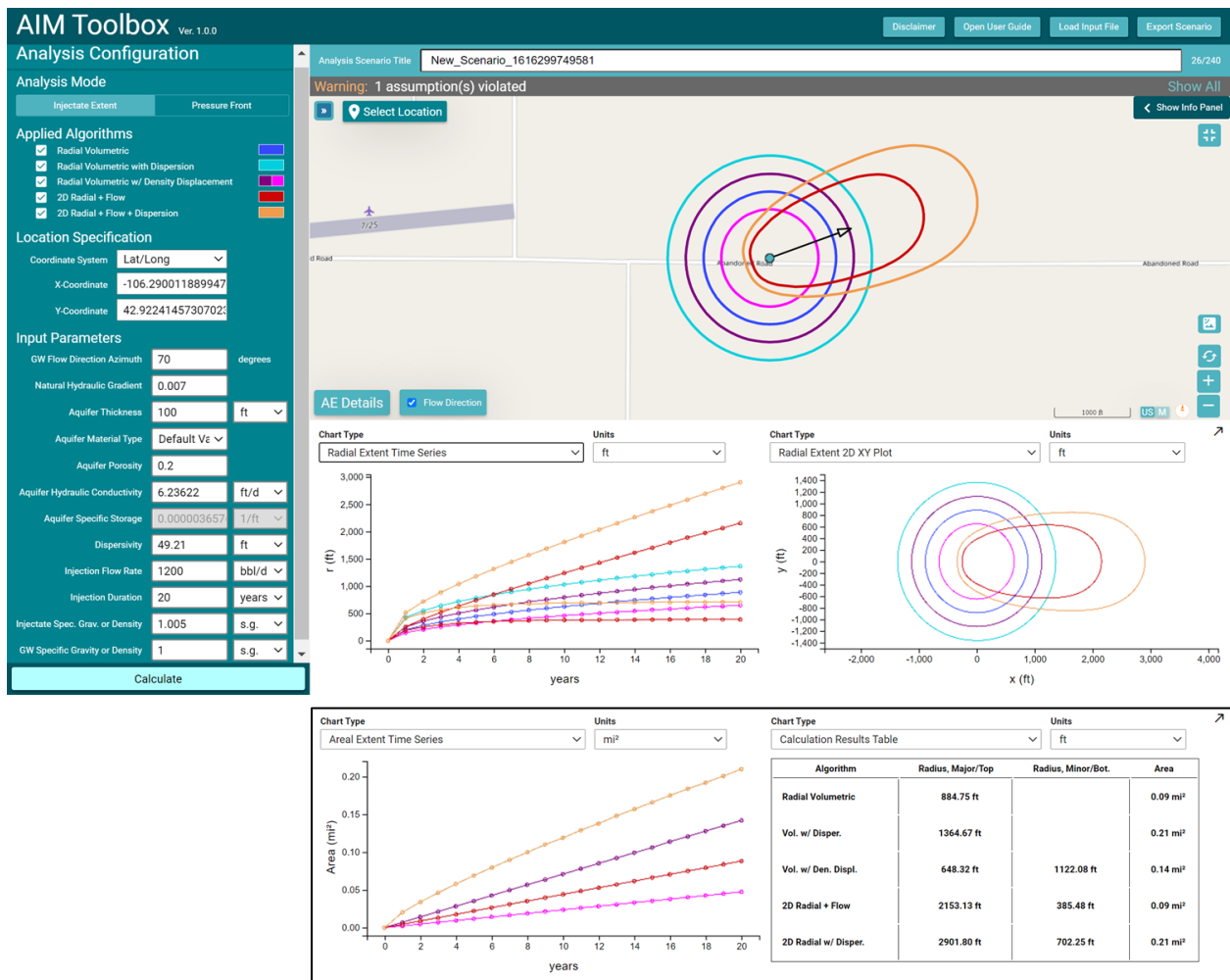


Figure 7. Example output from the AIM Toolbox software, including contours on the map, radial extent time series, areal extent time series, 2D XY plot of contours, and table of values at the injection duration (final) time.

2.4 Interactions

The user interactions within the AIM Toolbox software interface are described in this section.

2.4.1 Selecting a Location

The process of selecting a location of interest is described in Section 2.2.7, including how to enter coordinates or select a location on the map and the interaction between those two approaches.

2.4.2 Selecting Analysis Algorithm Options

The primary user interactions in the left side analysis configuration pane are to define the analysis scenario and input parameter values (Section 2.2). Selection of specific analysis algorithm options has several consequences. First, the input parameters relevant to that analysis algorithm are made available for editing (if they were previously unavailable). Second, the “Calculate” button is made active (as long as the input parameters are all valid). Third, the assumptions and references relevant to that analysis algorithm are displayed in the information panel accessed from the “Show Info Panel” button at the top right corner of the map pane (Figure 8). By selecting a single analysis algorithm, the user can see which assumptions and reference(s) apply to that particular algorithm.

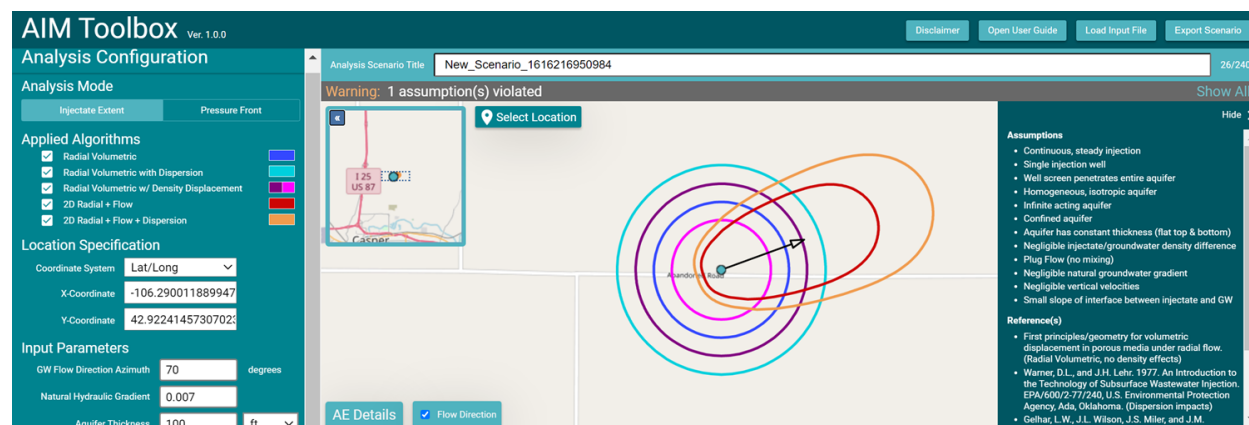


Figure 8. Assumptions and references relevant to the selected analysis algorithm options can be reviewed by clicking on the “Show Info Panel” button at the top right of the map pane.

2.4.3 Entering Input Parameter Values

Input parameter values can be entered/alterd by selecting the input text box, changing the value, and hitting the “Enter” key (or clicking a location outside of the input text box. If a non-numeric value is entered, the value reverts to the prior value. When the user enters/clicks inside a text input box for one of the input parameters, a tooltip is displayed (e.g., Figure 9) to indicate the permissible and expected ranges (Section 2.2.3), as appropriate, for the parameter value. The initial units for input parameters are Imperial units but the user can select different units (Table 6). The input parameter value is left unchanged when the user changes the units for an input parameter. Thus, the user will need to enter the appropriate value for the selected units, but see also the discussion of resetting default values below in Section 2.4.4.

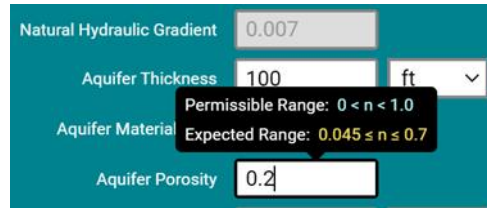


Figure 9. Example tooltip showing, in this instance, both permissible and expected ranges for the parameter value.

2.4.4 Selection of Material Type

Selection of a specific material type is not required to calculate results, but can be done for completeness or to use the associated default parameter values for aquifer porosity, aquifer hydraulic conductivity, and dispersivity. Selection of material types is described in Section 2.2 and Table 7. If the user selects a material type, then changes the input parameter value for aquifer porosity, aquifer hydraulic conductivity, and dispersivity, a reset icon will appear in the input text box (Figure 10). Similarly, a reset icon appears if the user changes the units of the input parameter. The user can proceed with the calculations or click on the reset icon to return to the default value. If the units were changed, then the return to the default value via the reset icon honors the new units and changes the value to be equivalent to the default in the current units. Other than through this reset icon action, no values are altered when the input parameter units change (as discussed in Section 2.4.3).

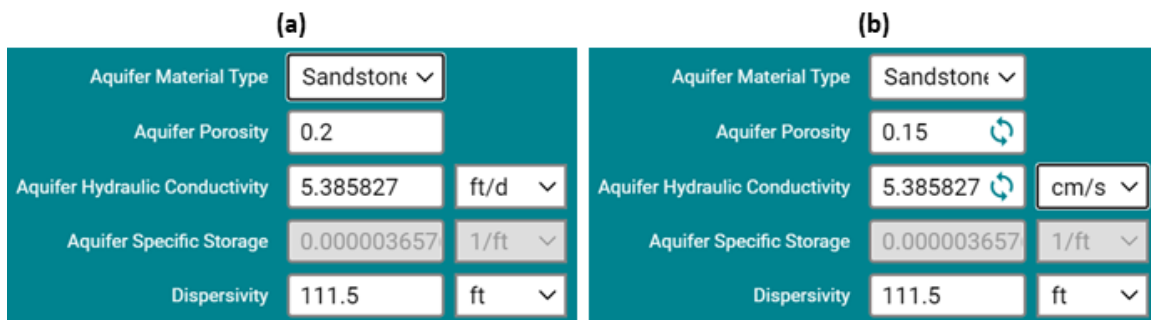


Figure 10. When the initial or default values of aquifer porosity, aquifer hydraulic conductivity, or dispersivity are altered by the user, a reset icon/button is displayed. Here the (a) default aquifer porosity value for sandstone has been (b) altered and the units for aquifer hydraulic conductivity have been changed.

2.4.5 Errors and Warnings

The AIM Toolbox software provides several types of error or warning indicators and messages to inform and guide the user (Figure 11). If an input parameter value is outside the expected range of values (described in Section 2.2.3 and Table 6), then the input text box for that parameter is highlighted in orange and a warning banner/message is displayed at the top of the map pane. The warning banner can be opened to show a message about which input parameter(s) have an issue. If the user enters an input parameter value that is outside the permissible range (Section 2.2.3 and Table 6), then the input text box is highlighted in red, an error banner is displayed at the top of the map pane, and the “Calculate” button is disabled. If the values of the natural hydraulic gradient or injectate/groundwater density inputs violate the

assumptions for the currently selected algorithm options, a warning banner/message is displayed at the top of the map pane. The assumption warning can be opened to display more detail on which assumption triggered the warning. In some cases, all of the input parameters are within the permissible ranges, but an algorithm (Radial Volumetric with Density Displacement or either of the 2D Radial + Flow analysis algorithm options) may fail to calculate results due to the value of a combination of parameters. When an analysis algorithm cannot calculate results, a warning banner/message is displayed at the top of the map pane and no results are displayed for those analysis algorithms. The algorithm failure banner can be opened to see details of which algorithm failed.

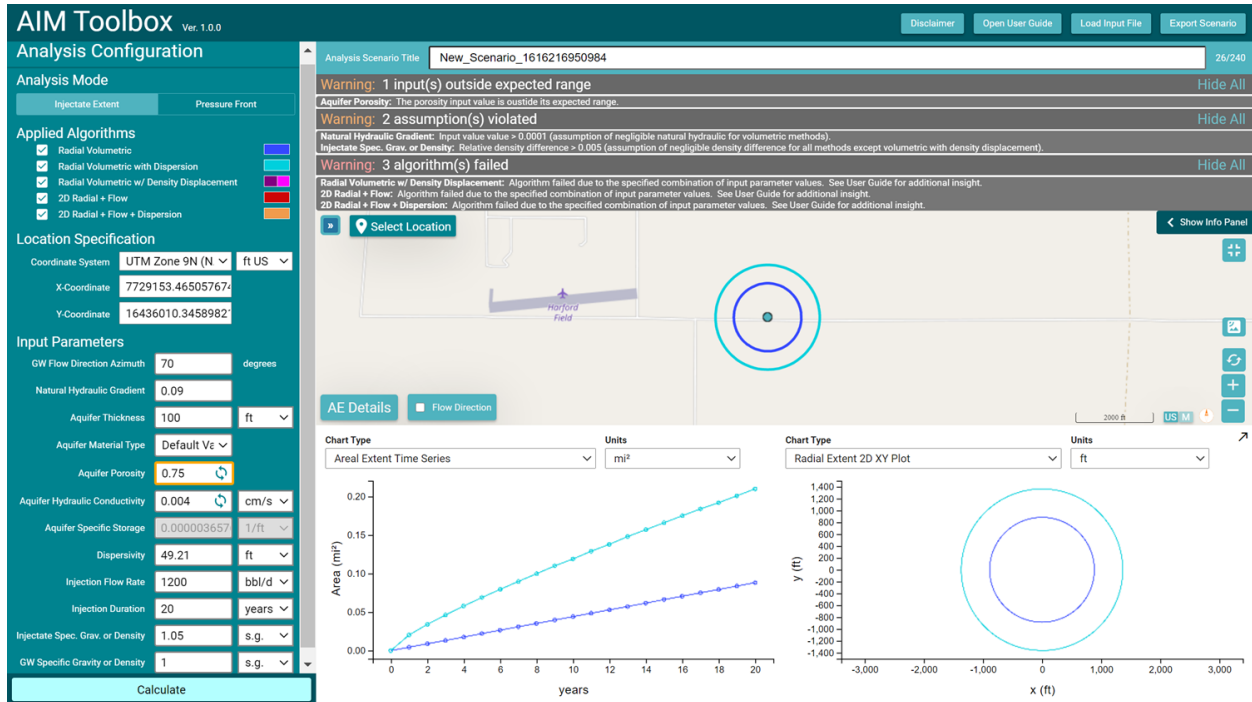


Figure 11. Examples of warning/error indicators and messages in the AIM Toolbox software.

2.4.6 Map Pane Interactions

The user can interact with the map pane in a variety of ways. The map pane allows standard actions of pan (click and drag), zoom (by mouse wheel or the zoom buttons), and recenter on the selected location dot. The map also includes standard elements of a scale bar, a choice of scale bar units (metric or US), and a north arrow. The button at the top left of the map pane can be clicked to provide an overview map (Figure 8) that gives a broader context view for the main map view. The basemap for the map pane can be switched between the street view and satellite view (Figure 12) using the button above the recenter and zoom buttons at bottom right in the map pane. Finally, though not map-specific, the button at top right in the map pane can be used to put the whole AIM Toolbox window into full screen mode (and to revert back to the windowed mode).

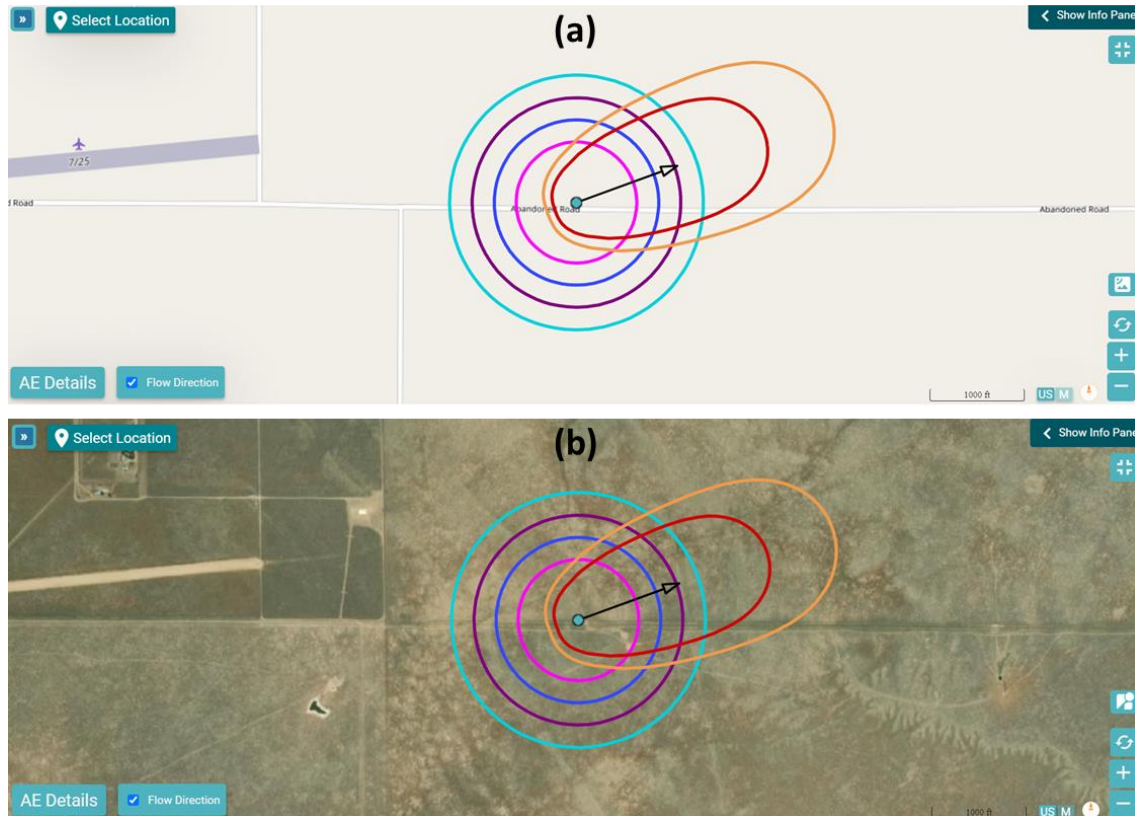


Figure 12. The map can display (a) a street view or (b) satellite basemap using the toggle button above the map reset button.

2.4.7 Existing Aquifer Exemption Information

As described in Section 2.2.7, the default cursor mode allows click-to-select an existing aquifer exemption (versus the “select location” mode to define the location of interest). When an existing AE is selected, it is highlighted in the map and the user can click on the “AE Details” button to display information about that AE. Figure 13 shows an example of the AE details information (which is also discussed in Table 2 and Figure 2 in Section 2.1). If there are overlapping existing AEs, then the “next” button at the bottom right of the AE Details panel will be available and the user can cycle through the overlapping AEs.

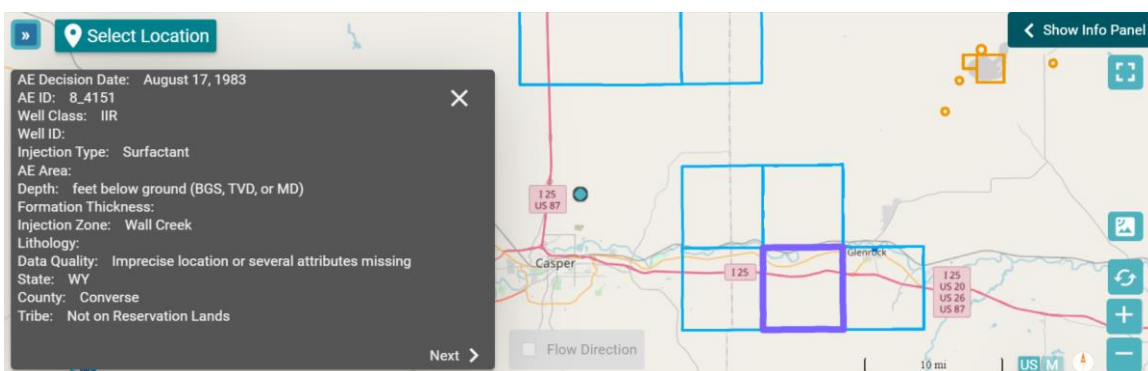


Figure 13. Example of AE Details information for the selected existing aquifer exemption.

2.4.8 Flow Direction Arrow

If the user has selected either 2D Radial + Flow analysis algorithm option, then the “Flow Direction” toggle button at the bottom left in the map pane is available. Selection of this button will place an arrow starting at the selected location dot on the map and pointing in the groundwater flow direction azimuth direction (e.g., Figure 8).

2.4.9 Chart Pane Size

One of the interactions with the chart pane is the ability to enlarge the chart pane to encompass the entire right side of the application window by clicking on the arrow at the top right of the chart pane. The same button is used to reduce the chart pane to the default size. Figure 14 shows an example with the chart pane enlarged.

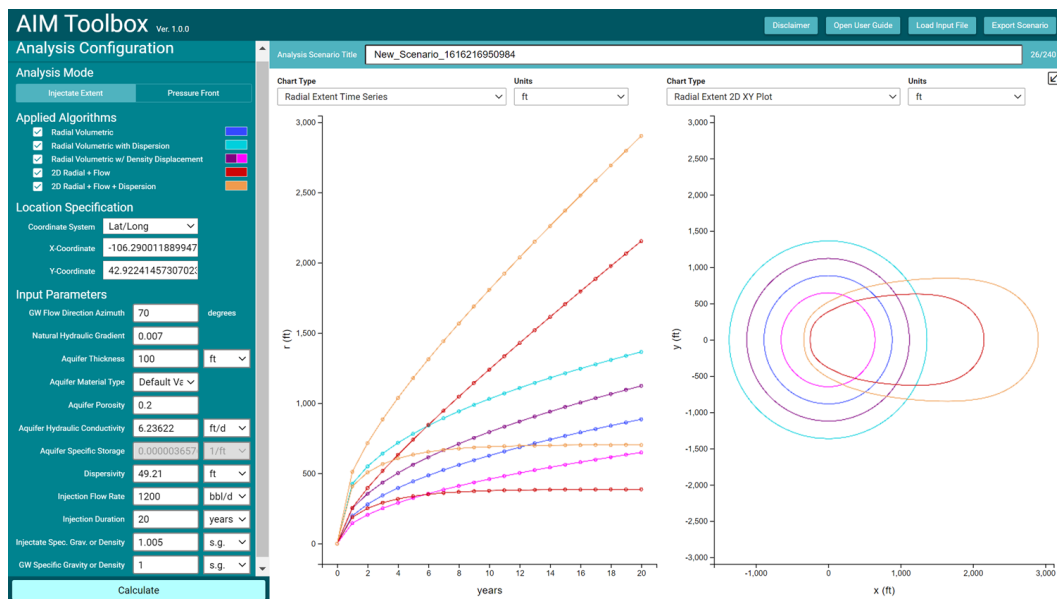


Figure 14. Example of an enlarged chart pane.

2.4.10 Chart Pane Result Options

As discussed in Section 2.3, the user can select from three chart types and a table for the output to display in the two side-by-side result slots. The chart types include a radial extent time series, an areal extent time series, and a 2D XY plot of contours (aligned with the X axis). Radius and area results at the injection duration time are tabulated in the table for each selected analysis algorithm option. The user can also choose to display results in metric or Imperial units. When the user hovers the mouse pointer over a point in a time series plot or a contour line in a 2D XY plot, information for that point is shown in a pop-up tool-tip (Figure 15).

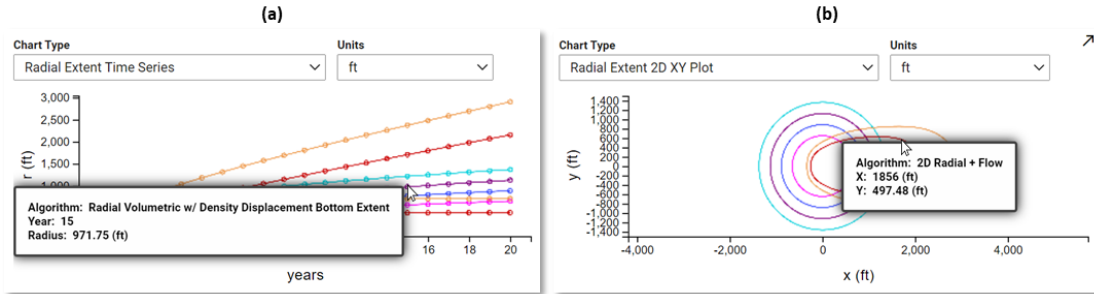


Figure 15. A tool-tip is displayed when the mouse pointer is hovered over (a) a time series point or (b) a contour in the 2D XY plot.

2.4.11 Exporting, Saving, and Sharing

There are several features to help the user with documenting, saving, and sharing an AIM Toolbox analysis scenario (Figure 16). The user can enter a scenario title of up to 240 characters long in the input text box above the map. Several items can be exported by clicking on the “Export Scenario” button in the application header. The user can export the currently visible plots in the chart pane and the current map view as images (Figure 17). The user can also export the analysis scenario to a JSON text file. Each of these exported files uses the scenario title in the file name (with spaces converted to underscores), along with prefixes of “AIM_Chart-L__”, “AIM_Chart-R__”, “AIM_Map__”, or “AIM_Scenario__”, as appropriate. The “Load Input File” button brings up a dialog window (Figure 17) to select and load a previously saved AIM_Scenario__*.json file for an AIM Toolbox analysis scenario. Thus, a saved analysis scenario file provide both a record of the analysis and can also be shared with others. Another way to document the analysis is to use the web browser print functionality with a “Save as PDF” destination. When printing, the user will likely want to adjust the print settings to obtain a single page document on their system (e.g., set the output format to use a landscape orientation with a custom scale of 80%). Printing with background graphics is optional.

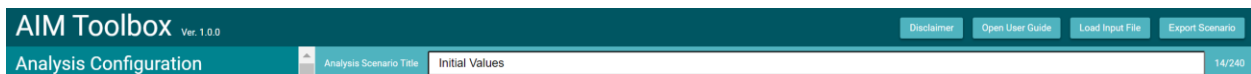


Figure 16. The scenario title input box, export/import buttons, and information buttons in the AIM Toolbox software.

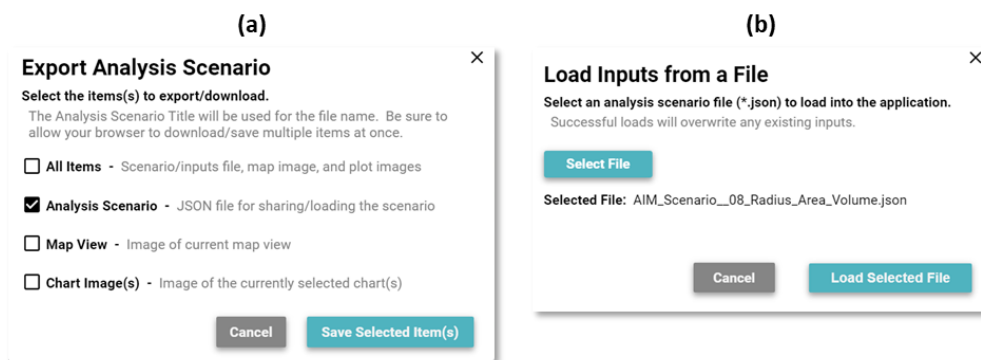


Figure 17. Dialog windows for (a) exporting AIM Toolbox elements and (b) for importing a scenario.

2.4.12 In-Application Guidance

As has been discussed, a variety of features are intended to provide in-application help, including labels and tool-tips. In addition to those features, the AIM Toolbox provides a “User Guide” button in the application header (Figure 16) so that the user can view the User Guide, which is a PDF file. Also, in the application header, the “Disclaimer” button can be used to display the software Disclaimer and copyright notice.

2.4.13 Updating the Existing Aquifer Exemptions

On the server where the AIM Toolbox website is deployed, existing aquifer exemption (AE) data is contained in the \public\geojson directory in files titled AEbounds2cj2_#.json and AEmountains2cj2_#.json, where # is 0, 1, 2, or 3. To manually add new aquifer exemptions in the future, data will be added to one of the *.json files in this directory. There is no restriction on which file(s) are selected for addition of new AE data other than that the files should be maintained at less than 10 MB in size. To add new AE data, it needs to be extracted from the EPA database (Section 2.1), have fields culled and mapped per Table 2, and then stored in the JSON format listed in Figure 2. This JSON data chunk can then be inserted into one of the *.json files before the very last square bracket (“]”) as a comma-separated item. Figure 18 shows the tail end of the AEbounds2cj2_1.json file as an example, indicating the last chunk of data for an AE and the point of insertion for a new chunk of JSON data. Note that the user should load the *.json file into a text editor that can handle files without line breaks, such as the VSCode editor by Microsoft.

```

{"type":"MultiPolygon","coordinates":[[[-11636626.3,5896695.3],[-11636626.9,5896988.6],[-11636627.6,5897281.9],
[-11636039.1,5897284.9],[-11636039,5896697.4],[-11636626.3,5896695.3]]]},{
"wellID":null,"wellClass":"IIR","injType":"EOR","State":"MT","County":"Wibaux","Tribe":null,"Area":0.19635,
"AreaUnits":"square miles","Depth":null,"DepthUnits":"feet below ground (BGS, TVD, or MD)","InjZone":"Silurian
Undifferentiated","FormationThick":null,"Lithology":null,"AEDate":"1984/06/25 00:00:00","Qual":"1","geometry":
{"type":"MultiPolygon","coordinates":[[[-11636624.7,5894337.4],[-11636624.1,5894926.6],[-11636036.7,5894928.6],
[-11636037,5894339.6],[-11636624.7,5894337.4]]]}}
    
```

Last AE data chunk currently in this file

↑ Insert "{JSON for new AE}" here between the "}" and the "]"

Figure 18. Tail end of the AEbounds2cj2_1.json file as an example of the existing AE data files, with annotations indicating where to insert new chunks of JSON data for additional AEs.

2.4.14 Reporting Issues or Making Feature Requests

As discussed in Section 5.0 below, the AIM Toolbox has been extensively tested. However, if a user were to find an issue with the software, or if a user would like to submit a new feature request, they may contact the developers by e-mail with details of the issue/request. Contact information is available on the Aquifer Injection Modeling Toolbox project website at <https://www.pnnl.gov/projects/aim-toolbox>.

3.0 Examples and Applying the Software

Inputs and results for several scenarios are presented here as examples of applying the AIM Toolbox software. Table 9 lists input parameter values for five scenarios, including the initial values (Table 6). Results for the initial values scenario are shown in Figure 7. Figures 19 through 22 show results for the remaining four Table 9 scenarios.

Table 9. Input values for a few example cases, with all analysis algorithm options selected.

Scenario Title	CRS EPSG	Longitude or X Coord.	Latitude or Y Coord.	GW Flow Azimuth	Hydraulic Gradient	Aquifer Thickness	Aquifer Material Type
Initial Values	4326	-106.290012	42.922415	70°	0.007	100 ft	Default Values
Radius Area Volume	4326	-106.312439	42.848703	90°	0.0132	55 m	Default Values
Contour Size Check	4326	-106.302760	42.922369	90°	4.635	10 m	Default Values
Dakota Low Gradient	26913	406982.19	4765784.68	70°	0.00038	10 m	Sandstone
Dakota High Gradient	26913	406982.19	4765784.68	70°	0.0079	10 m	Sandstone

Scenario Title	Aquifer Porosity	Aquifer Hydraulic Conductivity	Dispersivity	Injection Flow Rate	Injection Duration	Injectate Spec. Grav. or Density	GW Specific Gravity or Density
Initial Values	0.2	6.23622 ft/d	49.21 ft	1200 bbl/d	20 years	1.005 s.g.	1 s.g.
Radius Area Volume	0.2	0.0022 cm/s	49.21 ft	1200 bbl/d	20 years	1.00591 s.g.	1 s.g.
Contour Size Check	0.1	3.17098e-6 cm/s	15 m	967 bbl/d	14 years	1.005 s.g.	1 s.g.
Dakota Low Gradient	0.2	0.0022 cm/s	1 m	1200 bbl/d	20 years	1205 kg/m ³	1000 kg/m ³
Dakota High Gradient	0.2	0.0022 cm/s	1 m	1200 bbl/d	20 years	1205 kg/m ³	1000 kg/m ³

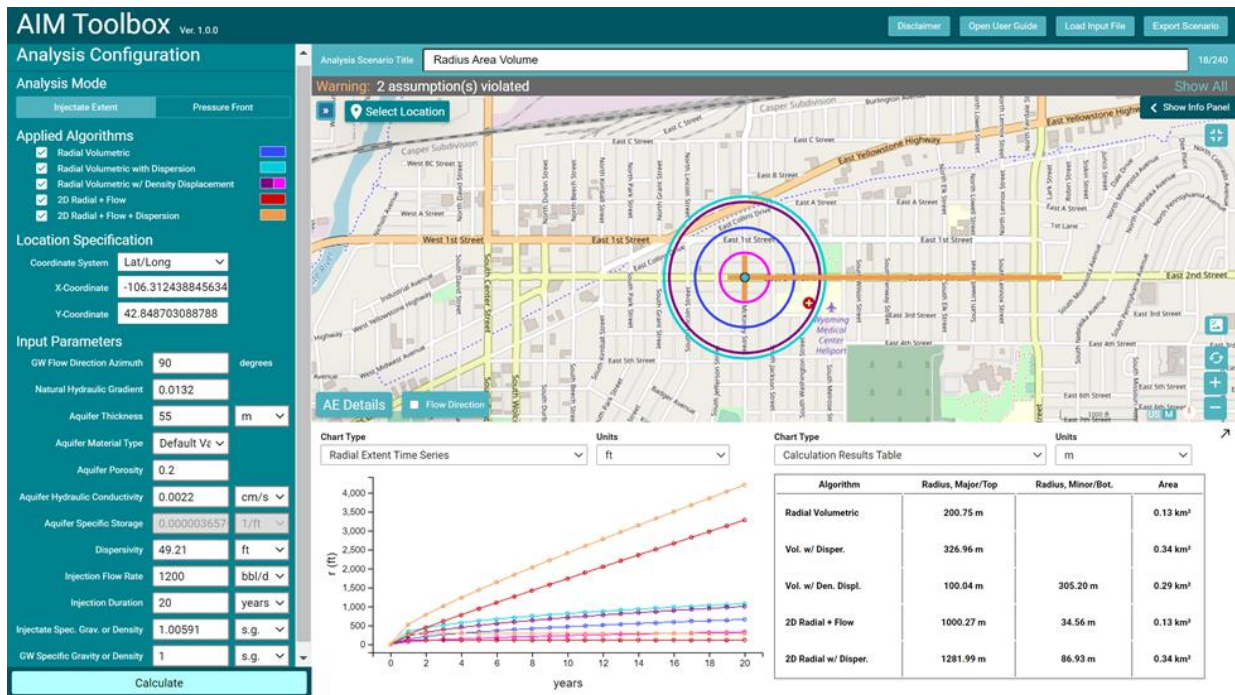


Figure 19. Inputs and results for the “Radius Area Volume” scenario used as a test case for quality assessment. The location is within a city only to provide reference features for assessing the calculation results. The 2D Radial + Flow methods are depicted as cross bars because of the elongated nature of the result, as discussed in Section 4.2.4.

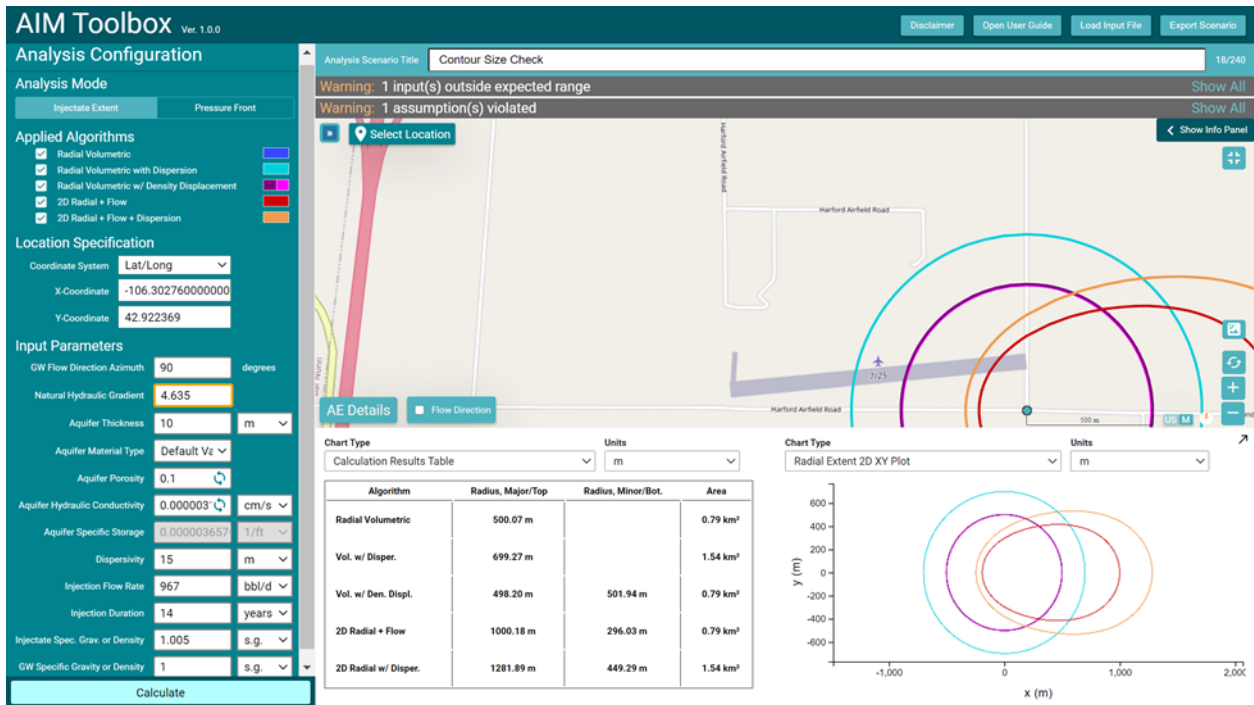


Figure 20. Inputs and results for the “Contour Size Check” scenario used as a test case for quality assessment. The input parameter values were selected to obtain specific radius values and do not represent any site-specific conditions. The radii for the three Radial Volumetric methods are nearly overlapping in the displayed inner circle contour.

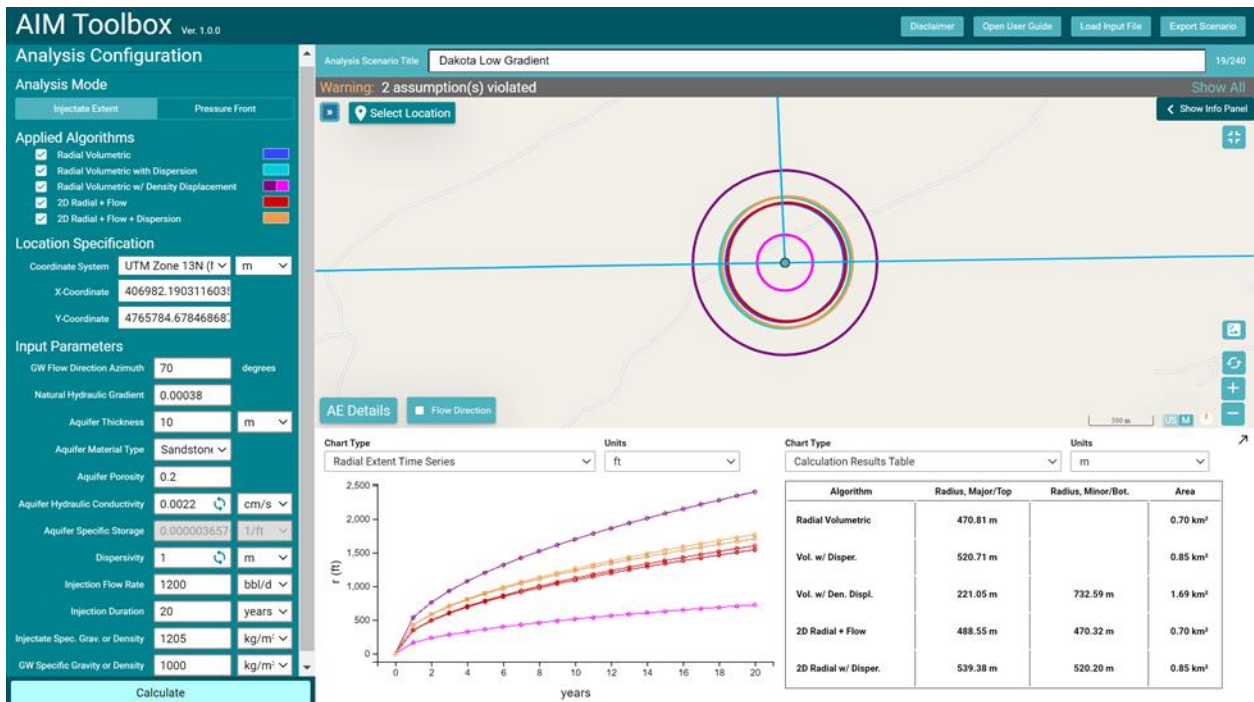


Figure 21. Inputs and results for the “Dakota Low Gradient” scenario.

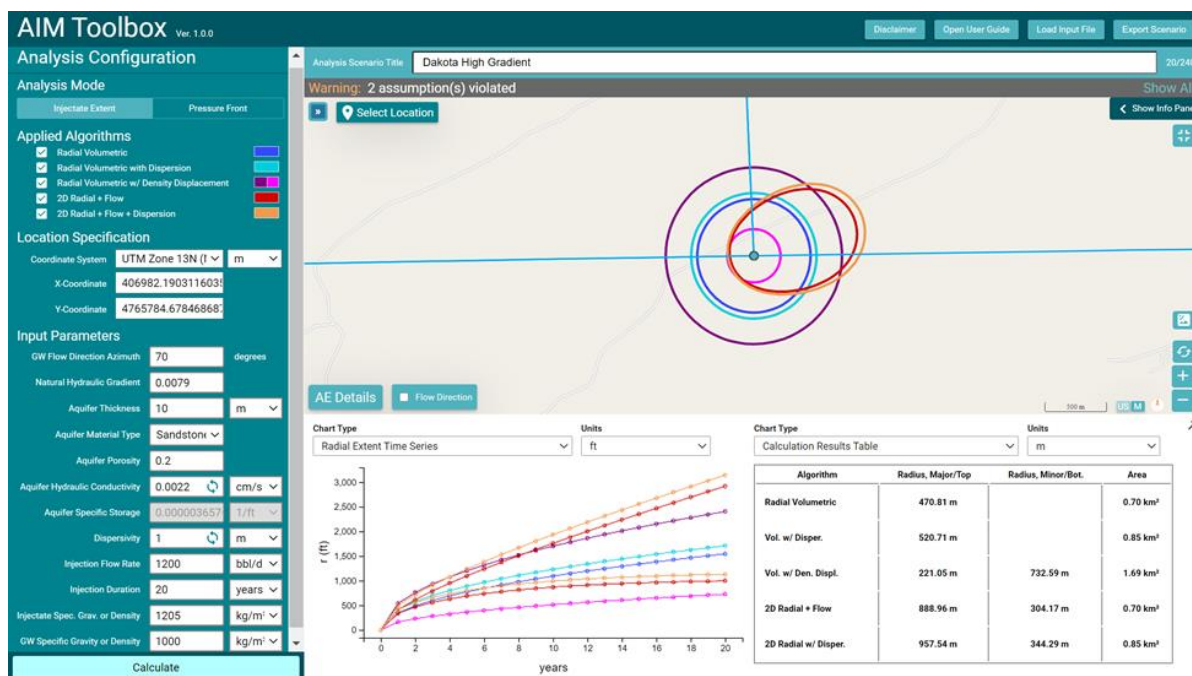


Figure 22. Inputs and results for the “Dakota High Gradient” scenario.

As discussed in Section 2.2, the intent of this software is that the multiple analysis algorithms are used collectively to provide an overall assessment of the extent of potential impacts of injection operations. The AIM Toolbox software provides quantitative estimates of the area impacted by injection operations, but the analysis algorithms are still simplified analytical approaches that don’t account for some real-world complexities such as formation heterogeneity, partially penetrating wells, or post-injection drift (i.e., movement of the injectate plume with natural groundwater flow after injection has ceased). The algorithm assumptions and calculations, described in the next section, should be assessed in the context of site-specific information. If a site significantly deviates from what these algorithms can represent, then site-specific numerical modeling should be considered (e.g., using STOMP [White and Ostrom, 2006]).

4.0 Calculations

The five analysis algorithms used in the AIM Toolbox software for estimating injectate extent are listed in Table 4. The assumptions and calculations associated with these methods are discussed in this section.

4.1 Design Basis

When aqueous solution is injected into a confined aquifer, the injected water tends to flow in a radial manner, displacing the existing groundwater and forming an interface between injected water (injectate) and aquifer formation water (groundwater). The location of the injectate/groundwater interface expands outwards with time as more fluid is injected. When the groundwater velocity is relatively small relative to the injection flow rate and the injection is through a fully penetrated well, the injected water has a cylindrical shape whose height is the

same as the aquifer thickness. If the groundwater velocity is not negligible relative to the injection flow rate, then the shape of the injectate plume becomes asymmetric in an sort of elliptical shape, with the bulk of the injectate migrating in the downgradient direction. When the injectate contains considerable salt or total dissolved solids, it will have a density (specific gravity) greater than the groundwater. This density difference between injectate and groundwater results in a larger fraction of injectate moving to the lower part of the aquifer, thus giving more of a frustum-shaped injectate plume (instead of cylindrically shaped). When there is mixing between the injectate and the groundwater, due primarily to dispersion, the interface between the two fluids is no longer a sharp front (like would be seen for immiscible fluids). That is, a plot of injectate concentration with radial distance would be a step function for immiscible fluids (sharp front) versus a sigmoidal function where mixing occurs, and the concentration gradually changes with distance. The mixing due to dispersion results in an increased radius of influence. These concepts underly the five injectate extent analysis algorithms. The radial extent of injectate can be estimated for these analysis algorithms based on the references listed in Table 10. The subsequent sections elucidate further on the calculations for each method.

Table 10. Basis for the AIM Toolbox injectate extent analysis algorithm options.

Reference	Method ID	A	B	C	D	E
Volumetric radial displacement (first principles); e.g., Warner and Lehr, 1977, Eqn. 3-10		X	X			
Gelhar et al., 1972, Section 3.1 (Immiscible Displacement and Recharge Cycle), with $0 < \epsilon_r \leq (4 \sqrt{406} - 56) / 15$				X		
Bear and Jacobs, 1965, Section 2, Eqn. 11 (for y at x = 0 and for y values to describe the shape of the injectate front) and Eqn. 14 (for the maximum X extents, positive and negative), with the constraint that groundwater velocity (i.e., gradient times hydraulic conductivity > 0.001 m/y (below this point the solution collapses to algorithm A)					X	X
Warner and Lehr, 1977, Eqn. 3-11 for impact of dispersion			X			X

These analysis algorithms involve simplifications that allow the algorithms to be calculated analytically (versus calculated by numerical methods). The assumptions for the injectate extent analysis algorithms are listed in Table 11, denoting which assumptions apply to which methods.

Table 11. Crosswalk between assumptions and analysis algorithm options.

Assumption	Method ID	A	B	C	D	E
Continuous, steady injection		X	X	X	X	X
Single injection well		X	X	X	X	X
Fully penetrating well screen across aquifer thickness		X	X	X	X	X
Homogeneous, isotropic aquifer		X	X	X	X	X
Infinite-acting aquifer (no boundary effects)		X	X	X	X	X
Confined aquifer (impermeable top & bottom)		X	X	X	X	X
Aquifer has constant thickness with flat top & bottom		X	X	X	X	X
Negligible injectate/groundwater density difference		X	X		X	X
Plug Flow (no mixing)		X	X		X	X
Negligible natural groundwater gradient		X	X	X		
Negligible vertical velocities (only horizontal GW flow)				X ¹		
Small slope of interface between injectate and GW				X ¹		

¹ Gelhar et al. (1972) note that their analysis “is strictly correct only when the interface slope is small and hence the vertical velocities are small,” before continuing to assess a range of situations, thus highlighting that their approach is an approximation.

As discussed in Section 2.2, input parameter information is requested to evaluate two assumptions. The calculations to check whether an assumption is violated are shown in Table 12.

Table 12. Assumption check calculations.

Assumption	Assumption Check Calculation (provide a warning when the check is True)	Applicable Methods
Negligible natural groundwater gradient	Aquifer Hydraulic Gradient > 0.0001	A, B, C
Negligible injectate/ groundwater density difference	$\frac{ \text{Groundwater Density} - \text{Injectate Density} }{\text{Groundwater Density}} > 0.005$	A, B, D, E

4.2 Algorithms

The injectate extent analysis algorithm calculations are described in the following sections.

4.2.1 Radial Volumetric

A mass balance/first principles approach (e.g., equation 3-10 of Warner and Lehr [1977]) can be used to determine injectate displacement of groundwater. Given the assumption of negligible groundwater flow, the result is a cylindrical injectate plume.

For continuous injection of fluid at a constant rate Q_i over a total time t , the total volume of water injected is:

$$V = Q_i t \tag{9}$$

Accounting for the porosity of the aquifer, n , the cylindrical zone of injectate will have a radius, r , calculated by

$$r = \sqrt{\frac{V}{\pi H n}} \tag{10}$$

4.2.2 Radial Volumetric with Dispersion

Warner and Lehr (1977) solved equation 10.6.65 of Bear (1972) to determine an equation for the radial distance at which the injection front has a chemical concentration of 0.2 percent of the injected fluid due to dispersion.

Warner and Lehr’s equation 3-11 for the influence of dispersion on radial distance is:

$$r_{dispersion} = r + 2.3\sqrt{D \cdot r} \tag{11}$$

where D is the dispersivity of the groundwater aquifer. Note that Warner and Lehr (1977) incorrectly referred to D as the dispersion coefficient instead of dispersivity.

4.2.3 Radial Volumetric with Density Displacement

The difference in density between the injectate and the groundwater is expected to impact the vertical distribution of injectate in the aquifer. For equal densities and negligible groundwater flow, a cylindrical injectate plume (e.g., Figure 23a) is expected, just the same as in Section 4.2.1. At the other extreme of an injectate with a density significantly different from the groundwater, the injectate plume could be conceptualized as essentially a cone, with a minimal radius at the top and large radius at the bottom of the aquifer (Figure 23c). For density differences in between, the injectate plume could be conceptualized as a frustum of a cone (Figure 23b).

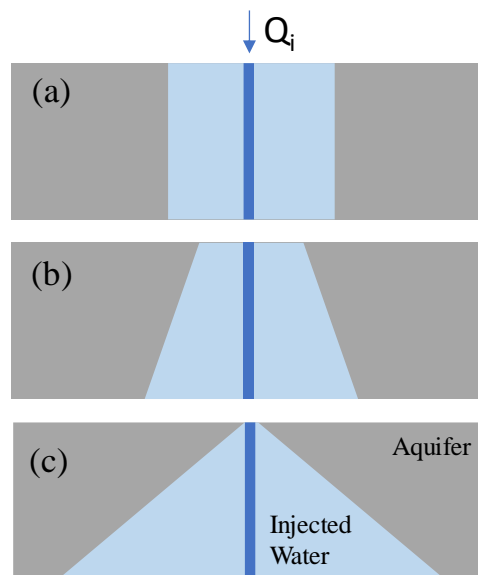


Figure 23. Conceptual cross-section of injectate in an aquifer when the density difference between the injectate and the groundwater is (a) negligible, (b) small/intermediate, or (c) significant, conceptually resulting in injectate plumes in the shape of a cylinder, frustum of a cone, and a cone, respectively.

In their section on Immiscible Displacement and Recharge Cycle, Gelhar et al. (1972) developed approximate expressions to describe the impact of density of the injectate on the injectate/groundwater interface. Gelhar et al. (1972) defined the following quantities:

$$D = \frac{HK(\rho_i - \rho_w)}{n\rho_w}; \quad A = \frac{Q_i}{2\pi nH}; \quad \varepsilon_r = \sqrt{\frac{D}{A}} \quad (12)$$

and the similarity variable at the interface endpoints (where z_1 is for the bottom and z_0 is for the top in our brine injection scenario):

$$\begin{aligned} z_0 &= -1 + \frac{\varepsilon_r}{4} + \frac{5\varepsilon_r^2}{224} \\ z_1 &= 1 + \frac{\varepsilon_r}{4} - \frac{5\varepsilon_r^2}{224} \end{aligned} \quad (13)$$

Then, Gelhar et al. (1972) describe equations for the radii of the injected water at the top and bottom of the aquifer, r_{top} and r_{bot} :

$$\begin{aligned} r_{top} &= \sqrt{\frac{(1 + \varepsilon_r z_0)Q_i t}{\pi nH}} \\ r_{bot} &= \sqrt{\frac{(1 + \varepsilon_r z_1)Q_i t}{\pi nH}} \end{aligned} \quad (14)$$

The solution for Equation 14 is bounded by $0 < \varepsilon_r \leq (4\sqrt{406} - 56) / 15$, which is based on the minimum possible radius at the top of the aquifer.

4.2.4 2D Radial + Flow

In Section 2 of their work, Bear and Jacobs (1965) describe equations to determine the shape of an injectate plume in an aquifer for a constant injection flow rate into a fully penetrating well in an aquifer (assuming negligible density difference between the injected water and groundwater) with groundwater flowing at a given Darcy velocity, $q = K \cdot i$. They relate a dimensionless travel time, \bar{t} , to dimensionless coordinates \bar{x} and \bar{y} , which describes the injectate front, in the following implicit equation:

$$\exp(\bar{x} - \bar{t}) = \cos(\bar{x}) + \frac{\bar{x}}{\bar{y}} \sin(\bar{y}) \quad (15)$$

The dimensionless variables are calculated by:

$$\bar{t} = \frac{2\pi q^2 H t}{nQ_i}; \quad \bar{x} = \frac{2\pi q H x}{Q_i}; \quad \bar{y} = \frac{2\pi q H y}{Q_i} \quad (16)$$

When \bar{y} approaches zero, Equation 15 becomes:

$$\bar{t} = \bar{x} + \ln(1 + \bar{x}) \quad (17)$$

For a given time t , the front of the injected water at $y = 0$ can be estimated by Equation 17, and the front location at $x = 0$ can be estimated by Equation 15.

When the groundwater Darcy velocity (i.e., gradient times hydraulic conductivity) is 0.001 m/y or less, the solution collapses to the cylindrical Radial Volumetric solution (Section 4.2.1). Regardless of the regime, the area covered by the injectate plume front is equal to that of the Radial Volumetric solution due to mass balance considerations.

Because these equations for the location of the front are implicit equations, they must be solved iteratively. In the AIM Toolbox software a secant solver (e.g., Gerald and Wheatley, 1994) is used to find the solution of the implicit equations to define the radius of the injectate plume at a given time along the X axis (in both the positive and negative directions, and to find a set of (X, Y) values to define the injectate front in 2D space. As the injectate plume becomes more elongated, the secant solver behaves poorly (likely due to proximity to an asymptote and/or as a result of the limits of floating-point numbers), giving erratic results. Hence, when the ratio of the positive X radius to the negative X radius exceeds 10, only the radii and area are returned and the shape contour of the injectate plume front is not displayed.

4.2.5 2D Radial + Flow + Dispersion

The same approach as described in section 4.2.2 with Equation 1 (from Warner and Lehr, 1977) is applied on the asymmetric 2D Radial + Flow results to give the dispersion impacts when groundwater flow is not negligible.

5.0 Testing

The AIM Toolbox software was developed under a software quality assurance plan (SQAP), with content equivalent to an EPA Quality Assurance Project Plan (QAPP). Document PNNL-AIM-SQAP, Rev. 0 and the associated attachments specify the approach to the software quality, including a software design description (PNNL-AIM-SDD, Rev. 0), the software requirements specification (PNNL-AIM-SRS, Rev. 0), and the software test plan (PNNL-AIM-STP, Rev. 0). Additionally, the SQAP document package described the software used in the development of the AIM Toolbox (e.g., see Section 6.0) and the programming standards and conventions. The software design description provides information on the layout, look, and interactions of the software. The software requirements specification describes 10 general hardware/software requirements, 19 data input requirements, 23 requirements related to interactions and intermediate calculations, and 12 output requirements. The software test plan details 21 multi-element test cases based on 11 sets of base case input parameter scenarios. The testing was a comprehensive assessment of software operation, user interactions, and quantitative results. Quantitative results were independently checked by hand and spreadsheet calculations. The testing per the software test plan was conducted, with all tests passing. The software test plan and testing were independently reviewed for concurrence. The SQAP document package was reviewed and approved by the PNNL software quality practitioner. The final documentation of the SQAP document package (including the testing) was provided to EPA as a separate signed document.

5.1 Validation of the Analytical Approach

The analytical solutions were verified in previous work with STOMP (White and Oostrom, 2006) simulations of an injection into the Dakota aquifer. This prior work is discussed in Yonkofski et al. (2017, 2019). Select results from this prior work are included here to demonstrate that the analytical solutions are suitable in certain cases and have shortcomings in other cases.

In this earlier work, the Dakota aquifer was conceptualized as either a stratified homogeneous or a heterogeneous system (Figure 24). For each aquifer system variant, three levels (i.e., zero, low, and high) of groundwater gradient were considered to represent three magnitudes of groundwater flow. For each gradient, three injectate salt concentrations (low, mid, and high TDS) were investigated to represent three situations for the density difference between injectate fluid and the groundwater. The simulation cases are summarized in Table 13.

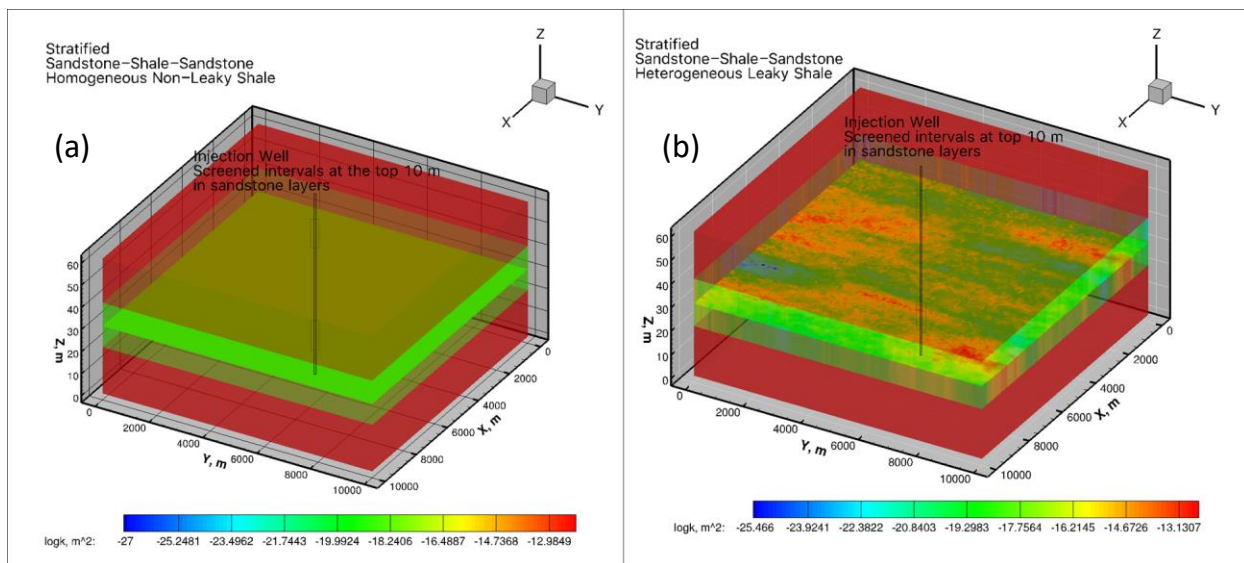


Figure 24. Two conceptualizations of the Dakota aquifer geology that were used in assessing the suitability of analytical solutions: (a) stratified homogeneous aquifer and (b) heterogeneous aquifer.

Table 13. Dakota aquifer simulation cases assessed in previous work.

Heterogeneity	Case No.	Groundwater Gradient ^a	Density ^b
Homogeneous (Figure 24a)	s1	Zero	Low
	s2		Mid
	s3		High
	s4	Low	Low
	s5		Mid
	s6		High
	s7	High	Low
	s8		Mid
	s9		High
Heterogeneous (Figure 24b)	s10	Zero	Low
	s11		Mid
	s12		High
	s13	Low	Low
	s14		Mid
	s15		High
	s16	High	Low
	s17		Mid
	s18		High

^a For the gradient, low = 0.00038 and high = 0.0079.

^b Differing densities were represented by TDS at levels ranging from 5,000 to 270,000 mg/L and a midpoint value.

Figure 25 compares the extent of the injected solution of low TDS and high TDS injectate fluids without groundwater flow. The area of influence increases with increasing TDS concentration in injectate. The analytical solution reasonably corresponds to these results. Figure 26 shows the injectate plume in a vertical cross-section for the same two low TDS and high TDS simulation cases. For the low TDS case, the injectate plume is distributed nearly uniformly across the entire aquifer thickness, representing a cylindrical plume. For the high TDS case, more injectate went to the bottom of the aquifer due to the higher injectate density versus the groundwater density.

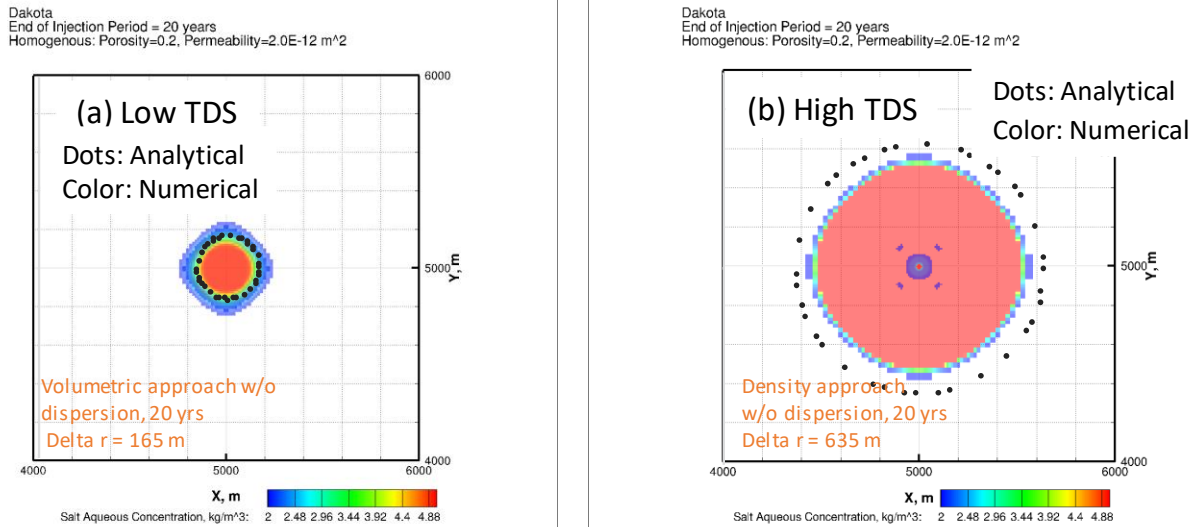


Figure 25. Comparison of the injectate plume extent at 20 years for (a) zero gradient (groundwater flow) and no dispersion in the homogenous aquifer with low density (TDS) using the radial volumetric approach and (b) the same conditions except that high density (TDS) and the volumetric with density displacement approach are used. The analytical solution for (b) represents the radius at the bottom of the aquifer.

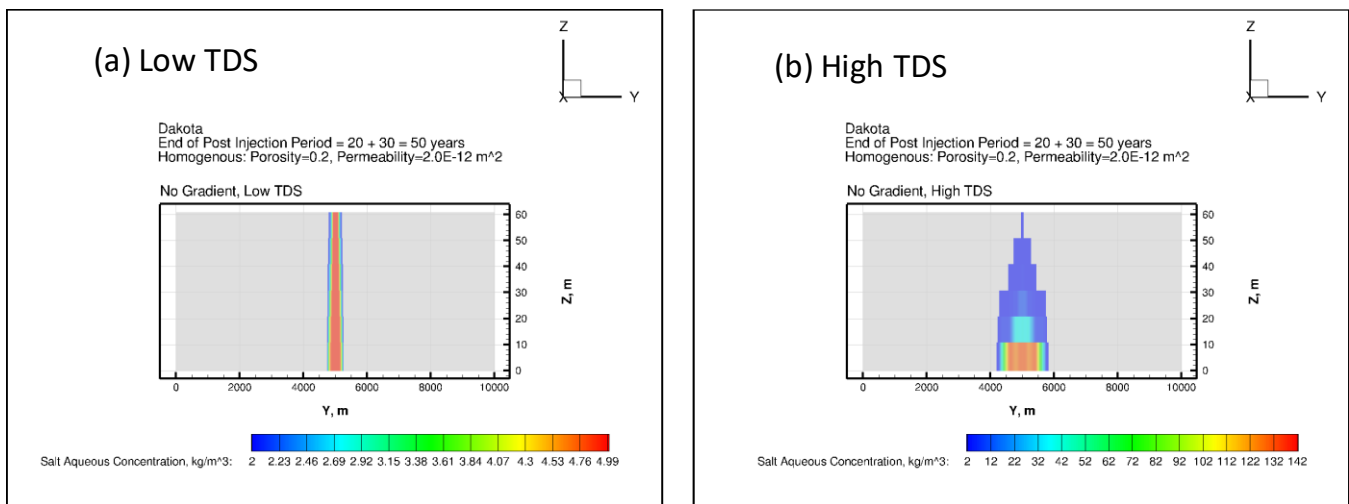


Figure 26. Cross section showing injectate plume distribution at 50 years for the volumetric with density displacement approach with zero gradient (groundwater flow) and no dispersion in the homogenous aquifer where injectate has (a) with low density (TDS) or (b) high density (TDS). Note the differing color scales for the two images.

Figure 27 compares the extent and shape of the injectate plume with no, low, and high hydraulic gradients (groundwater flow). The groundwater flow clearly impacts the shape of the injectate plume, with higher groundwater flow causing more asymmetry. For injectate fluids with low TDS, the 2D Radial + Flow method captures overall injectate plume behavior, but underestimated the area in the case of the high hydraulic gradient.

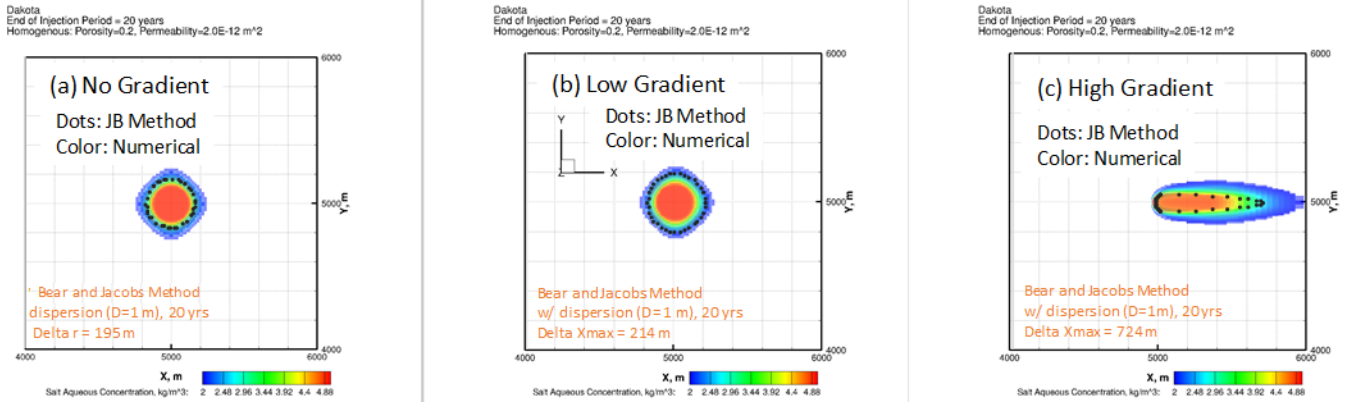


Figure 27. Comparison of the extent of the injectate plume at 20 years using the 2D Radial + Flow + Dispersion approach (the “JB method”) with (a) no gradient, (b) low gradient, and (c) high hydraulic gradients, reflecting the degree of groundwater flow.

Figure 28 compares the extent and shape of the injectate plume in a heterogeneous aquifer with a low groundwater hydraulic gradient and low TDS injectate fluid. The analytical solution significantly underestimated the plume size because, as expected, heterogeneity effects are not captured by the simpler analytical solution.

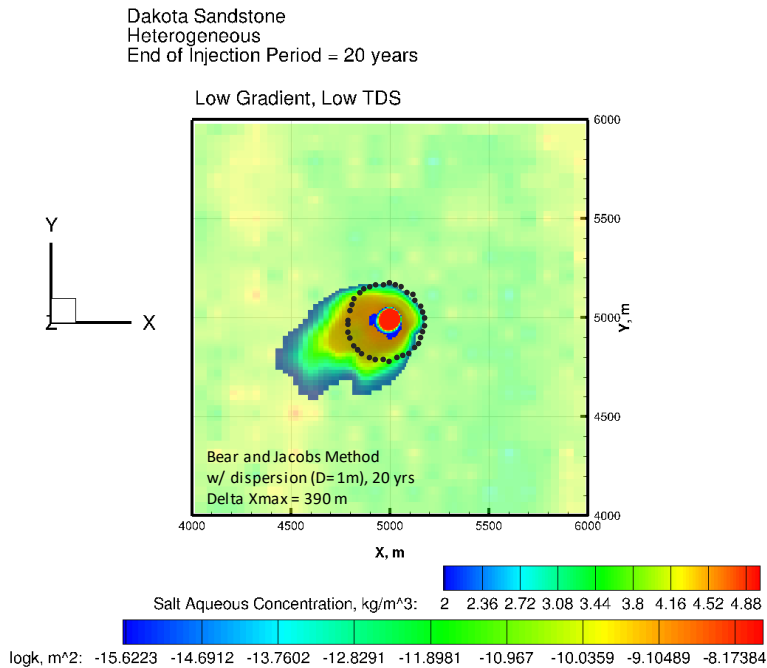


Figure 28. Comparison of the extent of injectate in a heterogeneous aquifer with low groundwater gradient and low TDS (simulation case s13). As expected, the heterogeneity effects are not captured by the simpler analytical solution.

6.0 Development Info

The AIM Toolbox software was developed as a web application in the React framework with the Redux state management library, incorporating the OpenLayers library for displaying map data and the D3.js library for data visualization. The software project uses ECMAScript version 6 (ECMAScript 2015, <http://www.ecma-international.org/ecma-262/6.0/>) for the JavaScript coding. Table 14 gives the list of third-party software used in development of the AIM Toolbox software. The support software listed in Table 15 provided the development and management tools for editing and managing code, building and debugging the application, tracking issues, and documenting the software and its development.

Table 14. List of third-party software used for development of the AIM Toolbox.

Support Software Name	Version or Date	Developer / Company
Create-React-App	2	Facebook, https://reactjs.org/docs/create-a-new-react-app.html
D3.js	5.15.0	Mike Bostock, https://d3js.org/
OpenLayers	5.3.3	https://openlayers.org/
React	16.12.0	Facebook, https://reactjs.org/
React-dom	16.12.0	Facebook, https://reactjs.org/docs/react-dom.html
React-redux	7.0.3	Dan Abramov, https://react-redux.js.org/
React-scripts	3.4.0	https://www.npmjs.com/package/react-scripts
redux	4.0.1	Dan Abramov, https://redux.js.org/
redux-logger	3.0.6	https://www.npmjs.com/package/redux-logger
redux-saga	0.16.0	https://redux-saga.js.org/
husky	1.3.1	https://www.npmjs.com/package/husky
prettier	1.17.0	https://prettier.io/
pretty-quick	1.10.0	https://www.npmjs.com/package/pretty-quick

Table 15. List of support software used for development of the AIM Toolbox.

Support Software Name	Version or Date	Developer / Company
JIRA	managed by PNNL IT Dept.	Atlassian
Confluence	managed by PNNL IT Dept.	Atlassian
Stash/Bitbucket	managed by PNNL IT Dept.	Atlassian
Git	2.27.0.windows.1	Git
Jenkins	managed by PNNL IT Dept.	Open Source community project
Visual Studio Code (IDE)	1.47.0 (version auto updates)	Microsoft
Chrome Browser	managed by PNNL IT Dept.	Google
Node.js	13.5.0	Node.JS
Node Package Manager	6.13.4	NPM

7.0 Future Work

Several ideas based on prior work or proposed during project discussions are captured in this section as features that could be implemented in future work on the AIM Toolbox software.

- Add an injectate extent algorithm option that includes dispersion/mixing effects along with the radial volumetric density displacement effects.
- Add functionality for estimating the pressure front (e.g., the Theis method) for an injection well.
- Add algorithms/functionality to address multiple injection wells in the same vicinity. The concept is that an injection well may be proposed in a location near existing injection wells, thus it would be useful to be able to estimate the effects of interactions between wells.
- Add algorithms/functionality to allow estimation of radial injectate extent and/or pressure front distribution for a horizontal well.
- Consider whether post-injection drift based on the groundwater flow could be added for longer-term assessments.
- Expand the requirements, with associated code updates and testing to allow the software to be used on other web browsers (e.g., Edge, Firefox).
- Provide a two-point distance measuring tool, whereby the user can click on one point, then click on a second point on the map, and the numeric distance between the points will be displayed, as well the points and a line connecting those points.
- Provide a method for exporting a geo-referenced shapefile (vector data) or geoTIFF image of the calculated contours (i.e., those shown on the map).
- Allow the user to upload a georeferenced image (e.g., geoTIFF, geoJPEG) for display in the Map pane.
- Include methods for adding annotations (text, lines, boxes) to plots or the map.

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Pacific Northwest National Laboratory

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

www.pnnl.gov