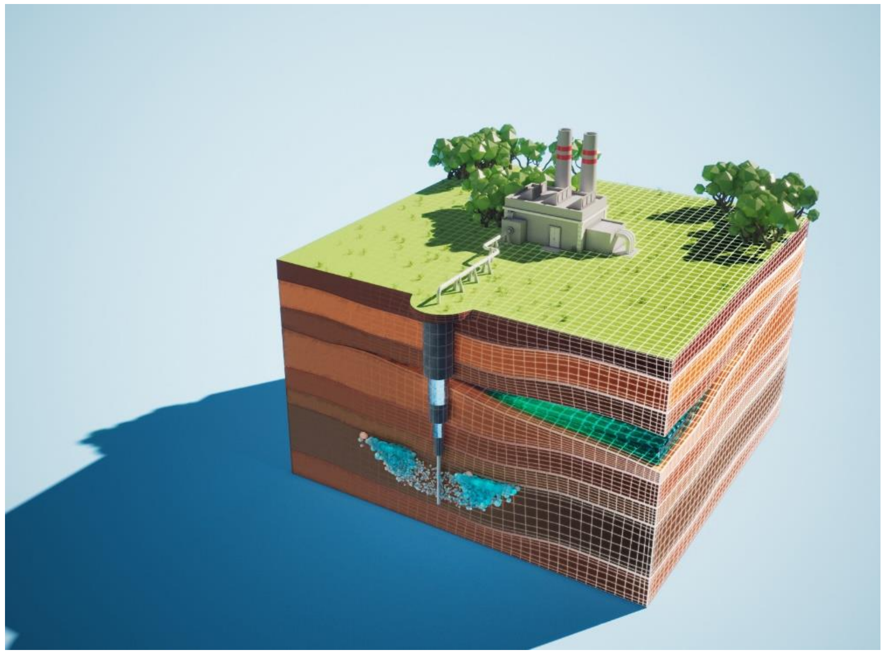

Rules and Tools Crosswalk: A Compendium of Computational Tools to Support Geologic Carbon Storage Environmentally Protective UIC Class VI Permitting

31 May 2022

Office of Fossil Energy and Carbon Management

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Cover Illustration: Simplified cross section of a geologic carbon storage computational model.

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Rules and Tools Crosswalk: A Compendium of Computational Tools to Support Geologic Carbon Storage Environmentally Protective UIC Class VI Permitting

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Acronyms and Abbreviations

Term	Description
AIM	Aquifer Injection Modeling
AoR	Area of review
CMG	Computer Modeling Group
CCS	Carbon Capture and Storage
CO_2	Carbon dioxide
CO2BRA	CO_2 Brine Relative Permeability Accessible Database
CO2-SCREEN	CO_2 Storage prospeCtive Resource Estimation Excel aNalysis
CUSP	Carbon Utilization and Storage Partnership of the Western United States
CSIL	Cumulative Spatial Impact Layers
DOE	U.S. Department of Energy
DREAM	Designs for Risk Evaluation and Management
E4D	4D Geophysical Modeling and Inversion Code
EASiTool	Enhanced Analytical Simulation Tool
EDX	Energy Data eXchange
EM	Electromagnetic
EMGeo	Electromagnetic-data Geologic Mapper
EPA	U.S. Environmental Protection Agency
ERT	Electrical resistivity tomography
FECM	Fossil Energy and Carbon Management
FEHM	Finite Element Heat & Mass Transfer Code
FEMA	Federal Emergency Management Agency
HAST	Heat and Salinity Transport
GWB	Geochemist's Workbench
GCS	Geologic carbon storage
GSDT	Geologic Sequestration Data Tool
IMI	Infrastructure Model and Inversion Module
IP	Induced polarization
IP	Interactive Petrophysics
IPCC	Intergovernmental Panel on Climate Change
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory

Acronyms and Abbreviations (cont.)

Term	Description
LLNL	Lawrence Livermore National Laboratory
MATLAB	MATrix LABoratory
MODFLOW	Modular Three-Dimensional Finite-Difference Groundwater Flow Model
MRCI	Midwest Regional Carbon Initiative
MRST	Matrix Laboratory (MATLAB) Reservoir Simulation Tool
MVA	Monitoring, Verification, and Accounting
NETL	National Energy Technology Laboratory
NRAP	National Risk Assessment Partnership
NUFT	Nonisothermal, Unsaturated Flow and Transport
Open-IAM	Open-source Integrated Assessment Model
PCOR Partnership	Plains CO_2 Reduction Partnership Initiative to Accelerate Carbon Capture, Utilization, and Storage Deployment
pGEMINI	parallel Geophysical Electromagnetic Modeling and Inversion of Natural and Induced sources
PHREEQC	PH Redox Equilibrium (in C language)
PISC	Post-injection site care
PNNL	Pacific Northwest National Laboratory
RCSP	Regional Carbon Sequestration Partnerships
SALSA	Semi-Analytical Leakage Solutions for Aquifers
SGeMs	Stanford Geostatistical Modeling Software
SECARB-USA	Southeast Regional Carbon Utilization and Storage Partnership
SIMPA	Spatially Integrated Multivariate Probabilistic Assessment
SOSAT	State of Stress Analysis Tool
STOMP	Subsurface Transport Over Multiple Phases
STSF	Short-term Seismic Forecasting Tool
TESLA	The Evidence Support Logic Application
TOUGH	Transport Of Unsaturated Groundwater and Heat
TPFLOW	Two-Phase Flow Model
UIC	Underground injection control
U.S.	United States
USDW	Underground source of drinking water
USGS	United States Geological Survey

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EXECUTIVE SUMMARY

This report identifies computational tools useful for addressing aspects of the dedicated carbon storage (Class VI) well permit application under the U. S. Environmental Protection Agency's (EPA) Underground Injection Control (UIC) Program.

The survey was conducted by researchers of the National Energy Technology Laboratory's (NETL) Research and Innovation Center in collaboration with representatives of the U.S. EPA, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Pacific Northwest National Laboratory (PNNL), and the four Regional Initiatives to Accelerate Carbon Capture, Utilization, and Storage: Carbon Utilization and Storage Partnership of the Western United States (CUSP), Plains CO_2 Reduction Partnership Initiative to Accelerate Carbon Capture, Utilization, and Storage Deployment (PCOR Partnership), Midwest Regional Carbon Initiative (MRCI), and the Southeast Regional Carbon Utilization and Storage Partnership (SECARB-USA).

Experts from each of these institutions used their knowledge of, and experience with, the UIC Class VI permit application to identify valuable computational tools. Information was collected by compiling individual fact sheets for each tool completed by the various contributing organizations. A total of 59 tools were identified through the elicitation for this report. The fact sheets for each tool are included in the Appendix. The body of this report provides a brief summary of UIC Class VI permit application elements and tables that cross-reference the computational tools with their general application (Table 2) and their relevance to elements of the Class VI permit application (Table 3). The report concludes by identifying gaps and possible areas for future investigation.

This report is intended to serve as a reference that can be used by geologic carbon storage stakeholders to identify computational tools that may be used to develop Class VI permit applications. The list of computational tools compiled herein is not intended to be exhaustive. References to any computational tool, service, and/or company are not intended to be endorsements of those tools, services, and/or companies. Furthermore, failure to reference a computational tool, service, and/or company is not intended as a repudiation of that computational tool, service, or company. In addition to this report, information contained herein will also be made available online through NETL's Energy Data Exchange (EDX) and updated periodically as new information on relevant computational tools becomes available.

1. INTRODUCTION

Carbon capture and storage (CCS) technology is capable of substantially reducing atmospheric emissions of carbon dioxide (CO_2) from power plants and other large point-source emitters (IPCC, 2005). Deployment of CCS at a scale that will impact global carbon budgets will require numerous commercial-scale geologic carbon storage (GCS) operations. Some of these operations are expected to store on the order of one hundred million metric tons of CO_2 (National Academies of Sciences, Engineering, and Medicine, 2021). GCS operations rely on one or more injection wells to safely deliver large volumes of CO_2 into deep underground formations (e.g., saline aquifers) (IPCC, 2005). Recognizing the unique conditions under which dedicated GCS wells operate, the U. S. Environmental Protection Agency (EPA) defined a new classification of injection wells (Class VI) under its Underground Injection Control (UIC) Program for GCS injection, with Federal Requirements found at 75 FR 77230, December 10, 2010, and codified in the U.S. Code of Federal Regulations (40 § CFR 146.81 *et seq.*). The Class VI well standard is intended to facilitate implementation of GCS while protecting underground sources of drinking water. U.S. EPA regulations define specific requirements for siting, construction, operation, testing, monitoring, and closure of Class VI wells. A summary of the Federal Class VI Rule Requirements is shown in Table 1.

The U.S. Department of Energy's (DOE) Office of Fossil Energy and Carbon Management (FECM) Carbon Storage Program has funded efforts to understand the risks associated with GCS. The U.S. DOE FECM released a set of Best Management Practices for GCS (NETL, 2017), which shared insights from research and their Regional Carbon Sequestration Partnerships (RCSP) field laboratory initiative. These documents outline essential activities common to the success of all GCS projects, including:

- Monitoring, Verification, and Accounting (MVA) for Geologic Storage Projects
- Public Outreach and Education for Geologic Storage Projects
- Site Screening, Site Selection, and Site Characterization for Geologic Storage Projects
- Risk Management and Simulation for Geologic Storage Projects
- Operations for Geologic Storage Projects
- Geologic Formation Storage Classification

GCS projects are inherently complex. Class VI permit applications are multifaceted and require input from experts with diverse expertise in geology, geochemistry, petroleum engineering, risk assessment, finance, and law. Several activities in the permitting process require the use of advanced computational tools to characterize the reservoir, assess risks, and forecast behavior in the subsurface throughout the injection and post-injection time periods and beyond. Some of the computational tools available for Class VI permitting are widely used by GCS stakeholders and experts in other related industries (e.g., oil and gas exploration and production) and are supported by commercial enterprises. Other tools have been developed by smaller research and development communities for specific applications and may be less known and used in practice. Consequently, prospective GCS site operators can choose from a panoply of available computational tools to engage in the Class VI permitting process.

The purpose of this report is to provide information on available computational tools that may be applied to various aspects of the Class VI permit application. This effort was led by the National Energy Technology Laboratory (NETL) in collaboration with: the U.S. EPA; the five U.S. DOE

National Laboratory members of the National Risk Assessment Partnership (NRAP): Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Pacific Northwest National Laboratory (PNNL); and the four Regional Initiatives to Accelerate Carbon Capture, Utilization, and Storage: Carbon Utilization and Storage Partnership of the Western United States (CUSP), Plains CO_2 Reduction Partnership Initiative to Accelerate Carbon Capture, Utilization, and Storage Deployment (PCOR Partnership), Midwest Regional Carbon Initiative (MRCI), and the Southeast Regional Carbon Utilization and Storage Partnership (SECARB-USA). Each participating organization was asked to provide a list of computational tools they use to address aspects of the Class VI well permitting process. NETL removed redundancies from the submitted tool lists and asked each organization to complete a fact sheet for each tool. Each fact sheet was designed to provide general information for a particular tool and describes how the tool may be used to address specific requirements for a Class VI well permit. Fifty-nine individual tools are described in this report. The Appendix contains the completed fact sheets from the contributing organizations. This compilation of computational tools is intended as an informational resource for practitioners seeking to understand or develop a Class VI permit application and is not intended to be exhaustive. Reference to any computational tool should not be seen as an endorsement of that tool by the coauthors or their organizations. Similarly, a lack of reference to any tool should not be seen as a repudiation of that tool by the coauthors or their organizations.

Table 1: Summary of Class VI Rule Requirements (modified from EPA, 2018)

Class VI Rule Requirement	Reference
Class VI permit information	**40 CFR 146.82**
Provide the information that owners or operators must submit to obtain a Class VI permit.	
Site screening and characterization (minimum criteria for siting)	**40 CFR 146.82(a)(2),(3),(5),(6); 146.83(a)(1)**
Establish that the proposed Class VI wells will be located in an area with a suitable geologic system, including an injection zone of sufficient areal extent, thickness, porosity, and permeability to receive the total anticipated volume of the carbon dioxide stream and confining zone(s) free of transmissive faults or fractures and of sufficient areal extent and integrity to contain the injected carbon dioxide stream and displaced formation fluids and allow injection at proposed maximum pressures and volumes without initiating or propagating fractures in the confining zone(s).	
Area of review (AoR) and corrective action plan	**40 CFR 146.82(a)(4),(13); 146.84**
Delineate the AoR - the region where injection operations may endanger an underground source of drinking water (USDW). Computational modeling that is based on available site characterization, monitoring, and operational data must be used to account for the physical and chemical properties of all phases of the injected carbon dioxide stream. Prepare an AoR and Corrective Action Plan for delineating the AoR, identifying all artificial penetrations that may require corrective action, performing all necessary corrective action, and periodically reevaluating the AoR and amending the plan if needed.	
Financial assurance demonstration (Financial responsibility)	**40 CFR 146.82(a)(14); 146.85**
Develop cost estimates for—and identify and provide financial assurance instruments sufficient to fund third-party implementation of—corrective action on improperly abandoned wells in the AoR, injection well plugging, post-injection site care (PISC) and site closure activities, and emergency and remedial response.	
Proposed well construction	**40 CFR 146.82(a)(11)(12); 146.86**
Specify the design materials and construction procedures for Class VI wells using materials that are compatible with the carbon dioxide stream and subsurface geochemistry over the duration of the Class VI project and sufficient to prevent interformational fluid movement and the endangerment of USDWs.	
Requirements for logging, sampling, and testing prior to operation	**40 CFR 146.82(a)(8); 146.87**
Specify activities, including logs, surveys, and tests of the injection well and formations, to be performed before injection of carbon dioxide commence.	
Injection well operating	**40 CFR 146.88**
Specify measures for Class VI well operation to ensure that the injection of carbon dioxide does not endanger USDWs, along with limitations on injection pressure and provisions for automatic shut-off devices.	
Mechanical integrity	**40 CFR 146.89**
Specify procedures for continuous monitoring to demonstrate internal mechanical integrity and annual external mechanical integrity tests.	
Testing and monitoring plan	**40 CFR 146.82(a)(15); 146.89; 146.90**
Prepare a testing and monitoring plan to verify that the geologic sequestration project is operating as permitted and is not endangering USDWs, to demonstrate the safe operation of the injection well, and to monitor changes withing the geologic system (e.g., carbon dioxide plume, pressure front, groundwater quality).	

Table 1 (cont.): Summary of Class VI Rule Requirements (modified from EPA, 2018)

Class VI Rule Requirement	Reference
Reporting	**40 CFR 146.91**
Design a program for the timely electronic reporting of Class VI well testing, monitoring, and operating results and meeting requirements for keeping records.	
Injection well plugging plan	**40 CFR 146.82(a)(16); 146.92(b)**
Specify materials and procedures whereby a Class VI injection well will be properly plugged to ensure that the well does not become a conduit for fluid movement into USDWs following cessation of injection.	
Post-injection site care (PISC) and site closure plan	**40 CFR 146.82(a)(17)(18); 146.93**
Specify activities for testing and monitoring following cessation of injection. The plan must provide for monitoring the site for 50 years following the cessation of injection, or for an approved alternative timeframe, or until it can be demonstrated that no additional monitoring is needed to ensure that the project does not pose an endangerment to USDWs; and for plugging the injection and monitoring wells and closing the site following that demonstration.	
Emergency and remedial response plan	**40 CFR 146.82(a)(19); 146.94**
Describe the actions to be taken to address events that may cause endangerment to a USDW or other resource during the construction, operation, and post-injection phases of the project.	
Class VI injection depth waiver	**40 CFR 146.95**
Demonstrate that injection zones and confining zones above and below the injection zones sufficiently protective of USDWs to qualify for waiver of the injection zone depth limitation requiring injection zones to be beneath the lowermost USDW. Such demonstrations will use computational modeling to show that USDWs above and below the injection zone will not be endangered as a result of fluid movement. This modeling should be conducted in conjunction with the area of review delineation.	
Stimulation program	**40 CFR 146.82(a)(9)**
Describe the stimulation fluids and procedures to be used and a provide evidence that stimulation will not interfere with containment (EPA, 2014).	

2. CROSSWALK

The 59 computational tools in this report are categorized by their primary type in Table 2. A detailed fact sheet describing each tool is available in the Appendix. Thirteen distinct tool types were identified: 1) geochemical modeling, 2) geologic model development, 3) geophysical data interpretation, 4) geospatial analysis, 5) geostatistical analysis, 6) project planning, 7) release, transport, and receptor response, 8) reservoir simulation, 9) resource estimation, 10) risk assessment, 11) seismic and geomechanical risk, 12) well test and log interpretation, and 13) well and pipeline design. Descriptions of these tool types are included in the Appendix.

Many of the tools have a diverse array of capabilities characteristic of multiple tool types. While the capabilities of each tool are described in their respective fact sheets, they are categorized only by their primary application to simplify the presentation of this report. Reservoir simulation tools were the most frequently referenced tool type, with 16 separate responses provided. Other common tool types addressed seismic and geomechanical risks (7 responses provided) and geologic model development (7 responses provided).

Class VI permit applications have twelve elements that include: 1) site characterization, 2) Area of Review and Corrective Action Plan, 3) financial assurance demonstration, 4) well construction details, 5) Pre-Operational Testing Plan, 6) proposed operating conditions, 7) Testing and Monitoring Plan, 8) the Injection Well Plugging Plan, 9) Post-Injection Site Care and Site Closure Plan, 10) Emergency and Remedial Response Plan, 11) Injection Depth Waiver Application, and 12) Aquifer Exemption Expansion (EPA, 2021). Table 3 provides a crosswalk between the 59 tools and the elements of the Class VI permit application.

Because owners and operators should also demonstrate that an adequate screening-level analysis was performed to determine that the project site is suitable, site screening was included in Table 3. The Pre-Operational Testing Plan was omitted from Table 3 because it pertains primarily to data collection and quality control. Both the Injection Depth Waiver Application and Aquifer Exemption Expansion involve demonstration of USDW non-endangerment and have been combined in Table 3 for simplicity of presentation.

Site Screening (46 responses provided) and Site Characterization (44 responses provided) were addressed by the largest number of tools in this report. A large number of tools were also valuable for developing the Area of Review and Corrective Action Plan (40 responses provided), Post-Injection Site Care and Site Closure Plan (31 responses provided), Testing and Monitoring Plan (30 responses provided), Emergency Remedial Response Plan (24 responses provided), proposed operating conditions (22 responses provided), and Injection Depth Waiver/Aquifer Exemption (17 responses provided). Fewer tools were applicable to the Injection Well Plugging Plan (8 responses provided), Well Construction Details (6 responses provided), and Financial Assurance Demonstration (5 responses provided).

Table 2: List of Considered Computational Tools Useful for Class VI Permitting Categorized by Type

Tool Name	Abbreviation	Website/Contact
Geochemical Modeling		
Geochemist's Workbench	GWB	https://www.gwb.com/index.php
PH REdox EQuilibrium (in C language)	PHREEQC	https://www.usgs.gov/software/phreeqc-version-3
Geologic Model Development		
CO_2 Brine Relative Permeability Accessible Database	CO2BRA	https://edx.netl.doe.gov/hosting/co2bra/
Decision Space 365		https://www.landmark.solutions/ds365
EarthVision		https://www.dgi.com/earthvision-software-for-3d-modeling-and-visualization/
GeoGraphix		https://www.gverse.com/home/GVERSEGeoGraphix20194
Petra		https://ihsmarkit.com/products/petra-geological-analysis.html
Petrel		https://www.software.slb.com/products/petrel
Voxler		https://www.goldensoftware.com/products/voxler
Geophysical Data Interpretation		
4D Geophysical Modeling and Inversion Code	E4D	https://www.pnnl.gov/projects/e4d
Electromagenetic-Data Geological Mapper	EMGeo	https://ipo.lbl.gov/lbnl2265/
HampsonRussell		https://www.geosoftware.tech/hampsonrussell
Kingdom		https://ihsmarkit.com/products/kingdom-seismic-geological-interpretation-software.html
parallel Geophysical Electromagnetic Modeling and Inversion of Natural and Induced sources	pGEMINI	https://energyenvironment.pnnl.gov/staff/staff_info.asp?staff_num=3506)
RokDoc		https://www.ikonscience.com/products/rokdoc/
Geospatial Analysis		
Cumulative Spatial Impact Layers	CSIL	https://edx.netl.doe.gov/dataset/cumulative-spatial-impact-layers

Table 2: List of Considered Computational Tools Useful for Class VI Permitting Categorized by Type (cont.)

Tool Name	Abbreviation	Website/Contact
Geostatistical Analysis		
Stanford Geostatistical Modeling Software	SGeMs	http://sgems.sourceforge.net/
Surfer		https://www.goldensoftware.com/products/surfer
Project Planning		
Designs for Risk Evaluation and Management	DREAM	https://github.com/pnnl/DREAM_V2
FE/NETL CO2 Saline Storage Cost Model		https://www.netl.doe.gov/energy-analysis/details?id=2403
SimCCS		https://www.carbonsolutionsllc.com/software/simccs/
Release, Transport, and Receptor Response		
Modular Three-Dimensional Finite-Difference Groundwater Flow Model (MODFLOW) with Mass Transport in 3-Dimensions (MT3DMS) or Reactive Transport in 3-Dimensions (RT3D)	MODFLOW	https://www.usgs.gov/mission-areas/water-resources/science/modflow-and-related-programs?qt-science_center_objects=0#qt-science_center_objects
Semi-Analytical Leakage Solutions for Aquifers	SALSA	https://eesa.lbl.gov/profiles/abdullah-cihan/
Tfrack		https://eesa.lbl.gov/profiles/quanlin-zhou/
Reservoir Simulation		
Aquifer Injection Modeling Toolbox	AIM Toolbox	https://www.pnnl.gov/projects/aim-toolbox
Computer Modeling Group GEM	CMG GEM	https://www.cmgl.ca/gem
ECLIPSE		https://www.software.slb.com/products/eclipse#sectionFullWidthTable
Enhanced Analytical Simulation Tool	EASiTool	https://www.jsg.utexas.edu/researcher/seyyed_hosseini
Finite Element Heat and Mass Transfer Code	FEHM	https://github.com/lanl/FEHM
GEOSX		http://www.geosx.org/
Heat and Salinity Transport	HAST	https://eesa.lbl.gov/profiles/abdullah-cihan/
MATLAB Reservoir Simulation Tool	MRST	https://www.sintef.no/projectweb/mrst/download/
Nexus		https://www.landmark.solutions/Nexus-Reservoir-Simulation

Table 2: List of Considered Computational Tools Useful for Class VI Permitting Categorized by Type (cont.)

Tool Name	Abbreviation	Website/Contact
Reservoir Simulation (cont.)		
Nonisothermal, Unsaturated-Saturated Flow and Transport	NUFT	https://ipo.llnl.gov/technologies/software/nuft
PFLOTRAN		https://bitbucket.org/pflotran/pflotran/wiki/Home
Subsurface Transport Over Multiple Phases – CO_2	STOMP-CO2	https://www.pnnl.gov/get-stomp
Transport Of Unsaturated Groundwater and Heat (TOUGH) 3– ECO2N/M or iTOUGH2-ECO2N/M	TOUGH3-ECO2N/M or iTOUGH2-ECO2N/M	https://marketplace.lbl.gov/
Transport of Unsaturated Groundwater and Heat – Fast Lagrangian Analysis of Continua	TOUGH-FLAC	https://tough.lbl.gov/; http://www.itascacg.com/software/FLAC3D
Transport of Unsaturated Groundwater and Heat REACT	TOUGHREACT	https://tough.lbl.gov/software/toughreact/
Two-Phase Flow Model	TPFLOW	https://eesa.lbl.gov/profiles/abdullah-cihan/
Resource Estimation		
CO_2 Storage prospeCtive Resource Estimation Excel aNalysis	CO2-SCREEN	https://edx.netl.doe.gov/dataset/co2-screen
Offshore CO_2 Saline Storage Calculator		https://edx.netl.doe.gov/dataset/offshore-co2-saline-storage-calculator
Risk Assessment		
Federal Emergency Management Agency (FEMA) Hazus	FEMA Hazus	https://www.fema.gov/flood-maps/products-tools/hazus
NRAP Open-Source Integrated Assessment Model	NRAP Open-IAM	https://edx.netl.doe.gov/nrap/nrap-open-iam/; https://gitlab.com/NRAP/OpenIAM
Spatially Integrated Multivariate Probabilistic Assessment	SIMPA	https://edx.netl.doe.gov/dataset/simpa-tool
The Evidence Support Logic Application	TESLA	https://www.quintessa.org/software/downloads-and-demos/tesla-2.1.1

Table 2: List of Considered Computational Tools Useful for Class VI Permitting Categorized by Type (cont.)

Tool Name	Abbreviation	Website/Contact
Seismic and Geomechanical Risk		
Athena Data Management System		https://www.nanometrics.ca/services/passive-seismic-monitoring/athena-data-management-system
Fault Slip Potential		https://scits.stanford.edu/software
RiskCat		https://gitlab.com/NRAP/RiskCat
RSQsim		https://profiles.ucr.edu/james.dieterich; https://profiles.ucr.edu/app/home/profile/keithrd
Seismogenic Index Model		https://github.com/RyanJamesSchultz/SeismogenicIndex; https://github.com/amignan/rseismTLS
Short-Term Seismic Forecasting Tool	STSF	https://edx.netl.doe.gov/nrap/short-term-seismic-forecasting-stsf/
State of Stress Analysis Tool	SOSAT	https://github.com/pnnl/SOSAT; https://edx.netl.doe.gov/nrap/state-of-stress-analysis-tool-sosat/
Well Test and Log Interpretation		
IHS WellTest		https://ihsmarkit.com/products/welltest-reserve-pta-software.html
Interactive Petrophysics	IP	https://www.lr.org/en-us/ip-well-analysis-software/
Neuralog		https://www.neuralog.com/well-log-digitizing-software-neuralog/
Strater		https://www.goldensoftware.com/products/strater
Techlog		https://www.software.slb.com/products/techlog
Well and Pipeline Design		
PIPESIM		https://www.software.slb.com/products/pipesim

Table 3: Crosswalk Between Class VI Permit Elements and Considered Computational Tools

Tool Name	Site Screening	Site Characterization	Area of Review and Corrective Action Plan	Financial Assurance Demonstration	Well Construction Details	Testing and Monitoring	Injection Well Plugging Plan	Post-Injection Site Care and Site Closure Plan	Emergency and Remedial Response Plan	Proposed Operating Conditions	Injection Depth Waiver/Aquifer Exemption
Geochemical Modeling											
GWB	X	X				X				X	
PHREEQC	X	X				X				X	
Geologic Model Development											
CO2BRA	X	X	X			X		X			
Decision Space 365	X	X	X		X						
EarthVision	X	X									
GeoGraphix	X	X	X	X	X	X	X	X			
Petra	X	X	X			X					
Petrel	X	X	X			X		X			
Voxler	X	X	X								
Geophysical Data Interpretation											
E4D		X				X		X			
EMGeo						X					
HampsonRussell		X	X								
Kingdom		X	X								
pGEMINI		X				X					
RokDoc		X				X					
Geospatial Analysis											
CSIL	X		X					X			

Table 3: Crosswalk Between Class VI Permit Elements and Considered Computational Tools (cont.)

Tool Name	Site Screening	Site Characterization	Area of Review and Corrective Action Plan	Financial Assurance Demonstration	Well Construction Details	Testing and Monitoring	Injection Well Plugging Plan	Post-Injection Site Care and Site Closure Plan	Emergency and Remedial Response Plan	Proposed Operating Conditions	Injection Depth Waiver/Aquifer Exemption
Geostatistical Analysis											
SGeMs	X	X	X								
Surfer	X	X	X								
Project Planning											
DREAM		X				X		X			
FE/NETL CO2 Saline Storage Cost Model	X			X	X						
SimCCS	X	X	X					X			
Release, Transport, and Receptor Response											
MODFLOW with MT3DMs or RT3D		X				X			X		
SALSA	X		X					X	X		
Tfrack			X					X	X		
Reservoir Simulation											
AIM Toolbox	X	X	X								X
CMG GEM	X	X	X			X	X	X	X	X	X
ECLIPSE	X	X	X			X	X	X	X	X	X
EASiTool	X		X			X		X	X		X
FEHM	X	X	X			X		X	X	X	X
GEOSX	X	X	X					X	X	X	X
HAST	X		X					X	X		X

Table 3: Crosswalk Between Class VI Permit Elements and Considered Computational Tools (cont.)

Tool Name	Site Screening	Site Characterization	Area of Review and Corrective Action Plan	Financial Assurance Demonstration	Well Construction Details	Testing and Monitoring	Injection Well Plugging Plan	Post-Injection Site Care and Site Closure Plan	Emergency and Remedial Response Plan	Proposed Operating Conditions	Injection Depth Waiver/Aquifer Exemption
Reservoir Simulation											
MRST	X	X	X			X		X	X		X
Nexus	X	X	X			X	X	X	X		X
NUFT	X	X	X			X		X	X		X
PFLOTRAN	X	X	X			X		X	X	X	X
STOMP-CO2	X	X	X			X		X	X	X	X
TOUGH3-ECO2N/M or iTOUGH2-ECO2N/M	X		X					X	X	X	X
TOUGH-FLAC	X	X	X			X		X	X	X	X
TOUGHREACT	X	X	X			X		X	X		X
TPFLOW	X	X	X			X		X	X		X
Resource Estimation											
CO_2-SCREEN	X	X	X								
Offshore CO_2 Saline Storage Calculator	X		X								
Risk Assessment											
FEMA Hazus	X	X	X	X		X	X	X			
NRAP Open-IAM	X	X	X			X		X	X		X
SIMPA	X	X	X			X		X			
TESLA	X	X	X	X					X		

Table 3: Crosswalk Between Class VI Permit Elements and Considered Computational Tools (cont.)

Tool Name	Site Screening	Site Characterization	Area of Review and Corrective Action Plan	Financial Assurance Demonstration	Well Construction Details	Testing and Monitoring	Injection Well Plugging Plan	Post-Injection Site Care and Site Closure	Emergency and Remedial Response Plan	Proposed Operating Conditions	Injection Depth Waiver/Aquifer Exemption
Seismic and Geomechanical Risk											
Athena Data Management System						X			X	X	
Fault Slip Potential	X	X				X				X	
RiskCat	X							X	X		
RSQsim	X							X	X	X	
Seismogenic Index Model	X							X	X	X	
STFS						X				X	
SOSAT		X								X	
Well Test and Log Interpretation											
IHS WellTest		X	X	X	X	X	X	X		X	
IP	X	X	X							X	
Neuralog	X	X	X							X	
Strater	X	X	X		X		X	X		X	
Techlog	X	X								X	
Well and Pipeline Design											
PIPESIM	X				X		X			X	

3. FUTURE WORK

The information collected in this report is derived from a survey administered to members of the CCS research and development community knowledgeable in GCS site selection, permitting, development, operation, and closure. Relatively few tools were identified for some elements of the Class VI permit application (e.g., well design, well plugging, and well stimulation). Input from the broader GCS community is needed to compile a more complete list of computational tools that informs these additional aspects of the Class VI permit application. Furthermore, a detailed analysis of tools used by applicants for specific Class VI permit application data (including those required to be submitted to the UIC program through the Geologic Sequestration Data Tool (GSDT)) may be beneficial. This effort could show how data and information from analyses conducted in support of each element of the permit can be integrated to effectively and efficiently communicate information on forecasted GCS site performance, and related uncertainty. Future work may also consider developing an interactive website on NETL's EDX platform based on the findings of this report. Periodic updates to such a website with additional submissions of tool descriptions from the GCS community would provide the most up-to-date resource for Class VI permit applicants. Disseminating information about available computational tools and their application to the Class VI permitting process will be critical to the widespread deployment of GCS in the U.S. and will complement the strategic investments of the U.S. DOE FECM Carbon Storage Program into research and development for CCS deployment (NETL, 2017).

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4. REFERENCES

EPA. Class VI Permit Application Outline. U.S. Environmental Protection Agency (EPA), 2021. https://www.epa.gov/uic/class-vi-permit-application-outline (last accessed April 2022).

EPA. Geologic Sequestration of Carbon Dioxide: Underground Injection Control (UIC) Program Class VI Primacy Manual for State Directors; U.S. Environmental Protection Agency, 2014.

EPA. Underground Injection Control (UIC) Program Class VI Implementation Manual for UIC Program Directors; EPA 816-R-18-001; U.S. Environmental Protection Agency (EPA), 2018. https://www.epa.gov/sites/default/files/2018-01/documents/implementation_manual_508_010318.pdf.

Federal Requirements Under the Underground Injection Control (UIC) Program for Carbon Dioxide Geologic Sequestration (GS) Wells. *U.S. Code of Federal Regulations*, 75 FR 77230, December 10, 2010.

IPCC. *Carbon Dioxide Capture and Storage*; Mertz, B., Davidson, O., de Coninck, H., Loos, M., Meyer, L., Eds.; Intergovernmental Panel on Climate Change; Cambrige University Press: Cambridge, United Kingdom and New York, NY, 2005.

National Academies of Sciences, Engineering, and Medicine. Accelerating Decarbonization of the U.S. Energy System. The National Academies Press: Washington, DC, 2021. https://doi.org/10.17226/25932

NETL. Best Practices Manuals for Geologic Carbon Storage. U.S. Department of Energy, National Energy Technology Laboratory, 2017. https://www.netl.doe.gov/coal/carbon-storage/strategic-program-support/best-practices-manuals

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APPENDIX

A.1 GEOCHEMICAL MODELING

CO_2 injection alters the chemistry of the target formation and may trigger precipitation or dissolution reactions. Tools in this category are primarily used for aqueous geochemical modeling, which is necessary to evaluating the impact that CO_2 may have on a formation.

A.1.1 Geochemist's Workbench

Tool Name	Geochemist's Workbench (GWB)
Developer/Owner	Aqueous Solutions LLC
Tool Type	Geochemical Modeling
Description	An integrated geochemical modeling package used for balancing chemical reactions, calculating stability diagrams and the equilibrium states of natural waters, tracing reaction processes, modeling reactive transport, plotting the results of these calculations, and storing the related data. GWB can couple chemical reaction with hydrologic transport to produce simulations known as reactive transport models. GWB can calculate flow fields dynamically or import flow fields as numeric data or calculated directly from the USGS hydrologic flow code MODFLOW.
Tool Licensing and Access	Licensed as a subscription with 3 versions available: professional ($2,599/year), standard ($1,299/year), and essential ($699/year). An additional chemistry plugin is available ($2,599/year). https://www.gwb.com/index.php
Model Input	Groundwater geochemical analyses
Model Output	One-dimensional (1D) and two-dimensional (2D) simulations of reactive transport in single and dual-porosity media, including bioreaction, stable isotopes, and migrating colloids. Results can be graphed and animated. Calculates Eh-pH and activity diagrams and creates a spectrum of specialty plots. Balance reactions, calculate equilibrium constants, and create geochemical spreadsheets.
Risks Behavior Considered	Risk of mobilization of metals in groundwater and the impacts to groundwater of CO_2 or brine leakage
Relevant Permitting Phase	Characterization, risk assessment, and monitoring
Class VI Permit Element Addressed	Site Screening, Site Characterization, Testing and Monitoring Plan
How the Tool is Used	Used to assess risk to groundwater or surface water in the event of a release of brine or CO_2 into a USDW. Would be used in risk assessment and to design the monitoring program.
Last Updated	Subscription to the GWB provides improvements and new capabilities continuously.
Ongoing Development	The tool is highly supported and up to date. https://www.gwb.com/support.php
Ease of Use	The GWB is designed for personal computers running Microsoft Windows. It is highly supported with online tutorials and community interaction. There is a graphical user interface.
Computational Speed	Computational speeds are not limiting. The model runs in minutes

Tool Verification	https://www.nrc.gov/docs/ML0804/ML080430497.pdf
Related References	https://www.gwb.com/ https://www.gwb.com/documentation.php

A.1.2 PHREEQC

Tool Name	PHREEQC Version 3
Developer/Owner	David L. Parkhurst. This software is a product of the U.S. Geological Survey (USGS).
Tool Type	Geochemical Modeling
Description	PHREEQC is a software written in the C++ programming language, which is designed to perform a wide variety of aqueous geochemical calculations. PHREEQC has capabilities for batch reactions, which include aqueous, mineral, and gas phase, and one-dimensional (1D) transport calculations. The solubility of gases in gas mixtures at (very) high pressures and temperatures can be calculated with the Peng–Robinson equation of state (Peng and Robinson, 1976).
Tool Licensing and Access	Users do not need a license or permission from USGS to use this software. https://www.usgs.gov/software/phreeqc-version-3
Model Input	Formation water chemistry Formation mineralogical composition Gas phase (CO_2 at formation temperature and pressure)
Model Output	Change in pH over simulation period Mineral dissolution/precipitation due to CO_2 reactivity Change in aqueous and mineralogical compositions
Risks Behavior Considered	Model potential dissolution/reprecipitation of minerals in the confining layers to evaluate the geochemical behavior and compatibility of the injected CO_2 stream with the rocks and fluids in the confining zones
Relevant Permitting Phase	Site characterization/evaluation
Class VI Permit Element Addressed	Site Screening, Site Characterization, Testing and Monitoring Plan
How the Tool is Used	A vertically oriented 1D transport simulation model is created using a stack of multiple cells; typically each cell is 1 meter in thickness. The confining intervals are exposed to CO_2 at the top and bottom boundaries of the injection zone, and CO_2 is allowed to enter the PHREEQC confining zone model by diffusion and/or advection/dispersion processes. For cap rocks at the top of the CO_2 storage reservoir, the simulation considers molecular diffusion in a single aqueous phase as the dominant mass transport process. No advection is assumed in the modeled system (no net flow of formation water/brine). For confining rocks at the bottom of the CO_2 storage reservoir, the simulation considers an advection–dispersion transport mechanism in an aqueous phase as the dominant mass transport process (dissolved CO_2 through the water-saturated pore space). Results are calculated at the center of each cell starting from the confining layer–CO_2 exposure boundary. The simulations are based on mass balance laws that include all the species present in the specific CO_2 storage sites and their corresponding equilibrium constants. Each cell is defined by the specific mineralogical composition of the confining rocks obtained from the X-ray diffraction (XRD) analysis of core samples.
Last Updated	August 2021
Ongoing Development	Ongoing minor development (for instance: existing database/basic functions development) Active user community
Ease of Use	PHREEQC has a graphical user interface that is easy to follow.

Computational Speed	Fast computational speed (not more than a couple of minutes)
Tool Verification	Tool verified by multiple authors and published research articles (see below).
Related References	Gaus, I.; Azaroual, M.; Czernichowski-Lauriol, I. Reactive transport modelling of the impact of CO_2 injection on the clayey cap rock at Sleipner (North Sea). *Chemical Geology* **2005,** *217*, 319–337. Hemme, C.; Van Berk, W. Change in cap rock porosity triggered by pressure and temperature dependent CO_2–water–rock interactions in CO_2 storage systems. *Petroleum* **2017,** *3*, 96–108. Parkhurst, D. L.; Appelo, C. A. J. *Description of input for PHREEQC version 3 – a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations*; U.S. Geological Survey: Denver, CO, 2013. Peng, D. Y.; Robinson, D. B. A new two-constant equation of state. *Industrial & Engineering Chemistry Fundamentals* **1976,** *15*, 59–64. Talman, S.; Perkins, E.; Wigston, A.; Ryan, D.; Bachu, S. 2013, Geochemical effects of storing CO_2 in the Basal Aquifer that underlies the Prairie Region in Canada. *Energy Procedia* **2013,** *37*, 5570–5579.

A.2 GEOLOGIC MODEL DEVELOPMENT

Geologic modeling is a necessary aspect of the Class VI well permitting process that requires diverse input from multiple data sources. Tools in this category synthesize a diverse array of information for the building and visualization of three-dimensional (3D) geologic models.

A.2.1 CO_2BRA

Tool Name	CO_2 Brine Relative Permeability Accessible (CO_2BRA) Database
Developer/Owner	NETL Research and Innovation Center
Tool Type	Geologic Model Development
Description	Relative permeability data is poorly described in the literature yet is critical to describe multiphase subsurface transport. This database provides core and experimental details of unsteady relative permeability measurements of super-critical CO_2 and brine through rock cores from a wide variety of depositional environments.
Tool Licensing and Access	Open datasets are available on: https://edx.netl.doe.gov/hosting/co2bra/
Model Input	Depositional environment and/or reservoir properties (porosity, permeability, etc.) of desired properties
Model Output	Relative permeability curves for model incorporation
Risks Behavior Considered	Multiphase transport
Relevant Permitting Phase	Site characterization and screening
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	Identify most relevant core data to apply to site, download. and utilize relative permeability curves in reservoir models
Last Updated	Summer 2021
Ongoing Development	Ongoing additions of new core flow data as available
Ease of Use	Data is downloadable in spreadsheet or accessible right from a web browser
Tool Verification	Documentation on website describes processing methods
Related References	Moore, J.; Crandall, D.; Holcomb, P. Relative Permeability in Reactive Carbonate Rock. International Society of Porous Media (InterPore) 13th Annual Meeting, May 31–June 4. Moore, J.; Crandall, D.; Holcomb, P.; Workman, S. Unsteady-state CO_2-Brine relative permeability measurements of reactive cores. 2020 Fall American Geophysical Union Meeting, San Francisco, CA, Dec 7–11, 2020. Moore, J.; Holcomb, P.; Crandall, D.; King, S.; Choi, J.-H.; Brown, S.; Workman, S. Rapid determination of relative permeability curves for brine and supercritical CO_2 systems using CT and unsteady state flow methods. *Advances in Water Resources* **2021**.

A.2.2 Decision Space 365

Tool Name	Decision Space 365
Developer/Owner	Halliburton/Landmark Graphics Corporation
Tool Type	Geologic Model Development
Description	The tool has functionality for data loading, seismic and well based interpretation, kinematic modeling, petrophysics, seismic processing, and static/geologic modeling
Tool Licensing and Access	Commercial licensing: https://www.landmark.solutions/ds365
Model Input	Geologic data types, not limited to but including seismic, well log and interpretation, contour and structure information, and conceptual model inputs
Model Output	A facies and petrophysical geologic model exported as input to flow model
Risks Behavior Considered	Geologic lithotypes and reservoir heterogeneity
Relevant Permitting Phase	Site characterization, site screening
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Well Construction Details
How the Tool is Used	Screening of site and reservoir characterization by multi-disciplinary team with Realtime interpretation updates across team
Last Updated	September 2021
Ongoing Development	Yes
Ease of Use	Integrated user environment with client/server configurations. Includes visual workflow assistant and training.
Computational Speed	The performance scales to the workload based on size of problem. The software is designed to handle both small and large problems.
Tool Verification	Industry certified subsurface tool used to measure and record reservoir capacities
Related References	www.landmark-solutions.com

A.2.3 EarthVision

Tool Name	EarthVision
Developer/Owner	Dynamic Graphics Inc.
Tool Type	Geologic Model Development
Description	EarthVision is a software for 3D model building, analysis, and visualization, with precise 3D models that can be quickly created and updated. Accurate maps and cross-sections, reservoir characterization, and volumetric analysis are made easy. EarthVision's advanced 3D/4D Viewer enables model examination and interrogation in the context of datasets from throughout the asset development team, which serves to improve and simplify quality control, well planning, and communication to management, investors, partners, and other team members.
Tool Licensing and Access	Commercial: Contact: https://www.dgi.com/contact-dynamic-graphics-inc/
Model Input	ASCII data, LAS files, shapefiles. The input is 3D geological information about the number of layers, their thickness, location of faults, wells, and other information required to create a model of the subsurface.
Model Output	ASCII data, shapefiles, DGI formatted files. The output is the 3D model itself. The software allows creation of cross-sections, 2D maps, contours, and calculation of volumes, etc.
Risks Behavior Considered	Not applicable
Relevant Permitting Phase	High-level regional models, site screening, site characterization, injection, post-injection, etc.
Class VI Permit Element Addressed	Site Screening, Site Characterization
How the Tool is Used	The tool is used to create a geological model for the site of interest
Last Updated	EarthVision 12
Ongoing Development	Yes
Ease of Use	The tool comes with a graphical user interface. Training courses are offered.
Tool Verification	Unable to locate
Related References	Wagoner, J. *3D Geologic Modeling of the Southern San Joaquin Basin for the Westcarb Kimberlina Demonstration Project- A Status Report*; 2009. doi:10.2172/948987. Several other references included at https://www.dgi.com/earthvision-software-for-3d-modeling-and-visualization/ under the articles and papers section.

A.2.4 GeoGraphix

Tool Name	GeoGraphix
Developer/Owner	Gverse
Tool Type	Geologic Model Development
Description	GeoGraphix is a complete geoscience platform offering leading-edge mapping, geological, geophysical, and petrophysical interpretation, structural modeling, well and field planning, and state-of-the-art 3D visualization.
Tool Licensing and Access	Commercial license: https://www.gverse.com/home/GVERSEGeoGraphix20194
Model Input	Well logs, seismic, core tests, LAS files, SEGY, SHP files, basemaps, well data
Model Output	Maps, cross sections
Risks Behavior Considered	Leakage, storage resource, faults, fractures, boundaries
Relevant Permitting Phase	Site Screening, Site Characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Financial Assurance Demonstration, Well Construction Details, Testing and Monitoring Plan, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan
Last Updated	2019
Ongoing Development	Commercial, regular updates
Related References	https://www.gverse.com/geographix https://www.lmkr.com/geographix/GVERSE-GeoGraphix-Brochure.pdf

A.2.5 Petra

Tool Name	Petra IHS
Developer/Owner	IHS (Information Handling Services) Markit
Tool Type	Geologic Model Development
Description	Petra is a cost-effective software solution for managing, manipulating, and visualizing integrated geological, geophysical, and engineering data
Tool Licensing and Access	PetraLicensing@ihs.com PETRAQuoteRequest@ihs.com
Model Input	Depth registered raster images and LAS (Log ASCII Standard) files - digital log curve data
Model Output	Maps of geologic structures within a consistent stratigraphic framework to increase knowledge of depositional environments
Risks Behavior Considered	No risks or behaviors
Relevant Permitting Phase	Site screening, Site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan
How the Tool is Used	Petra's direct connection to IHS enables the user to download multiple information (3 million U.S. wells, providing current, historical and production data). Mapping (display contour grids; create customizable maps to assist in reservoir analysis and well location) and Cross Section (display digital/raster log curves, pick formation tops across a basin or play; display fault gaps, cored and completed zones; interpolate the value of well logs between wells) Modules model and analyze the areas of interest.
Last Updated	2020
Ongoing Development	https://ihsmarkit.com/products/petra-geological-analysis.html CustomerCare@ihsmarkit.com
Ease of Use	Microsoft Windows Vista/Windows 7 64-bit dual monitor System. no need for computer programming skills to use the tool
Computational Speed	Computational speeds are not limiting in any way
Related References	https://petraftp.ihsenergy.com/Petraman.pdf

A.2.6 Petrel

Tool Name	Petrel
Developer/Owner	Schlumberger
Tool Type	Reservoir Simulation
Description	Petrel is a software platform that allows users to integrate geologic data from many disciplines to study and characterize reservoirs. Seismic data, geophysical well log data, and geostatistics can be used to perform well correlation, build detailed reservoir models, estimate petrophysical properties, calculate volumes, and visualize results.
Tool Licensing and Access	Commercial proprietary software. On-premise and cloud solutions available. Licensing options purchased via communication with Schlumberger. https://www.software.slb.com/products/petrel
Model Input	Geophysical well log data, core data, geologic formation tops, and wellhead data
Model Output	3D reservoir models, including geometric and petrophysical property distributions, 3D surfaces/maps, well correlations, and seismic interpretations
Risks Behavior Considered	Parameter uncertainty/sensitivity analysis, geologic uncertainty, and volumetric estimations
Relevant Permitting Phase	Site screening, site characterization, and application preparation
Class VI Permit Element Addressed	Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	Petrel can be used to evaluate and interpret many types of geologic information. It can be used to estimate geologic properties with nearby legacy data for site screening, creating a model for feasibility studies and creating a detailed model with site-specific data for reporting/permit application activities.
Last Updated	August 6, 2021 (latest major release)
Ongoing Development	Schlumberger develops, supports, and maintains the software. It is a standard tool in the oil and gas industry.
Ease of Use	The tool has an interactive graphical user interface. No programming skills are required, but VBA (Visual Basic for Applications) or SQL (Structured Query Language) experience can be utilized in Petrel workflows. Fundamental geologic knowledge is recommended before use. Geostatistics and/or data analysis experience is a plus.
Computational Speed	3D modeling can generate loads of varying sizes on computational resources. Generating models with large cell counts and uncertainty workflows could potentially lead to long computational times. Basic tasks (loading well logs, viewing well logs, generating 3D surfaces, and geometric properties) are generally not computationally intensive, but a workstation with a dedicated graphics processing unit (GPU) is recommended.
Tool Verification	The tool has been used for several years throughout the oil and gas industry.
Related References	https://www.software.slb.com/products/petrel https://www.software.slb.com/products/product-library-v2?product=Petrel&tab=Case%20Studies

A.2.7 Voxler

Tool Name	Voxler
Developer/Owner	Golden Software
Tool Type	Geologic Model Development
Description	3D visualization software with utility for subsurface geologic and geophysical data visualization and interpolation, and functionality to facilitate communication of data and interpretation to stakeholders
Tool Licensing and Access	Commercial license: https://www.goldensoftware.com/products/voxler
Model Input	GIS data, map surfaces, geotechnical data
Model Output	3D maps
Risks Behavior Considered	Leakage, storage resource, faults, fractures, boundaries
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization Plan, Area of Review and Corrective Action Plan
Last Updated	Version 4.6.913.
Ongoing Development	Commercial, regular updates
Related References	https://www.goldensoftware.com/products/voxler

A.3 GEOPHYSICAL DATA INTERPRETATION

Geophysical analyses are essential for subsurface characterization and monitoring at GCS sites. Tools in this category are primarily used to interpret geophysical information (e.g., well logs, seismic data).

A.3.1 E4D

Tool Name	4D Geophysical Modeling and Inversion Code (E4D)
Developer/Owner	Pacific Northwest National Laboratory (PNNL), Developers: Timothy Johnson, Piyoosh Jaysaval, Judy Robinson
Tool Type	Geophysical Data Interpretation
Description	Three-dimensional (3D) forward and inverse modeling of static and time-lapse electrical resistivity tomography (ERT), induced polarization (IP), and travel-time tomography for seismic and ground penetrating radar.
Tool Licensing and Access	Available for download at https://github.com/pnnl/E4D. The copyright agreement is contained within the source code. An Infrastructure Model and Inversion (IMI) Module is available for modeling of metallic infrastructure within the geoelectrical run modes. Licenses are available by contacting the PNNL Commercialization Manager.
Model Input	Geophysical datasets and a priori site information to be used as constraints.
Model Output	3D or four-dimensional (4D) distributions of conductivity and/or velocity.
Relevant Permitting Phase	Site characterization, injection, and post-injection
Class VI Permit Element Addressed	Site Characterization, Testing and Monitoring Plan
How the Tool is Used	This tool is used to interpret geophysical data to identify any local or regional faulting, faults, or fractures that could serve as fluid migration pathways, confirming lateral extent of the reservoir and upper and lower confining zones and generating products (depth horizons and inversion volumes) for use in geologic models to simulate the CO_2 plume to help establish the area of review. The tool can also be used to interpret time-lapse electrical resistivity data to image the CO_2 plume as part of the monitoring program.
Last Updated	Last updated: September 2021
Ongoing Development	E4D is updated with additional capabilities in response to sponsor needs.
Ease of Use	There is a learning curve to use E4D, mostly due to the flexibility built into the inputs that allow for its usage in a wide variety of environments. Users should have a general knowledge of the geophysical applications for which E4D is being used.
Computational Speed	E4D was designed to work in distributed-memory, high-performance computing systems. It is also highly parallelized. E4D can accommodate geophysical surveys with thousands of measurements and model domains with millions of parameters.
Tool Verification	E4D is NQA-1 qualified from ASME.

Related References	Website: https://www.pnnl.gov/projects/e4d An online user guide is available at: https://e4d-userguide.pnnl.gov/index.html Publications: Johnson, T. C.; Versteeg, R. J.; Ward, A.; Day-Lewis, F. D.; Revil, A. Improved hydrogeophysical characterization and monitoring through parallel modeling and inversion of time-domain resistivity and induced-polarization data. *Geophysics* **2010,** *75*. Johnson, T. *E4D: A distributed memory parallel electrical geophysical modeling and inversion code User Guide - Version 1.0*.; Pacific Northwest National Laboratory, Richland, WA, 2014

A.3.2 Electromagnetic-data Geological Mapper (EMGeo)

Tool Name	EMGeo Electromagnetic-data Geological Mapper
Developer/Owner	Lawrence Berkeley National Laboratory (LBNL), Developers: Gregory A. Newman, Michael Commer
Tool Type	Geophysical Data Interpretation
Description	Forward and inverse modeling of frequency-domain electromagnetic (EM) data. Supported data types are controlled-source EM, magnetotelluric, and electrical resistivity tomography (ERT).
Tool Licensing and Access	Licensed through Technology Transfer of LBNL. It can be purchased by contacting LBNL Technology Transfer. https://ipo.lbl.gov/lbnl2265/
Model Input	Model of electrical resistivity/conductivity of the subsurface
Model Output	The model produces EM data simulations based on the three-dimensional (3D) resistivity/conductivity distribution.
Risks Behavior Considered	It can simulate resistivity/conductivity anomalies due to leakage
Relevant Permitting Phase	It can be used during all phases of a Class VI permit (e.g., for pre-injection and post-injection characterization)
Class VI Permit Element Addressed	Testing and Monitoring Plan
How the Tool is Used	The tool can be used within an imaging procedure embedded into a Class VI permitting workflow. Imaging provides spatial maps of injected fluid flow.
Last Updated	Last updated: September 2021.
Ongoing Development	The tool is still under development. Some companies who have licensed are the current user community. Support is available.
Ease of Use	There exists a graphical user interface for model viewing and manipulation. Users do not need computer programming skills to use the tool. General knowledge of geophysical EM modeling and inversion is helpful.
Computational Speed	The tool is designed for computational efficiency because it is highly parallel. Simulation times depend on model size, but they can be scaled if computing resources are available.
Tool Verification	The tool has been verified. Comparative model studies and calibration data inversions are in journal publications by Commer and Newman.
Related References	Website: https://ipo.lbl.gov/lbnl2265/ Manual available through licensing or request Publications: Commer, M.; Newman G. A. New advances in three-dimensional controlled-source electromagnetic inversion. *Geophysical Journal International* ***2008***, *172*, 513–535. Commer, M.; Newman G. A. Three-dimensional controlled-source electromagnetic and magnetotelluric joint inversion. *Geophysical Journal International* ***2009***, *178*, 1305–1316. Commer, M.; Newman G. A.; Carazzone J. J.; Dickens T. A.; Green K. E.; Wahrmund L. A.; Willen, D. E.; Shiu J. Massively-parallel electrical-conductivity imaging of hydrocarbons using the Blue Gene/L supercomputer. *IBM Journal of Research and Development* **2008,** *52-1/2*, 93–103.

A.3.3 HampsonRussell

Tool Name	HampsonRussell
Developer/Owner	Topicus and Vela (previously CGG)
Tool Type	Geophysical Data Interpretation
Description	The software is a suite of reservoir characterization tools that integrates well logs, seismic data, and geophysical processes for advanced geophysical interpretation and analysis with applicability for field development and maximizing recovery in mature reservoirs.
Tool Licensing and Access	The tool is licensed through Flexlm tools on a license server. https://www.geosoftware.tech/hampsonrussell
Model Input	Seismic data (stacked or gather), well logs, and velocities
Model Output	The software generates conditioned seismic data that include attribute volumes, crossplotting, and interpretation functions for locating AVO (amplitude variation with offset) anomalies.
Relevant Permitting Phase	Site characterization, injection, and post-injection
Class VI Permit Element Addressed	Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	This tool is used to interpret seismic data to identify any local or regional faulting, faults, or fractures that could serve as fluid migration pathways, confirming lateral extent of the reservoir and upper and lower confining zones and generating products (depth horizons and inversion volumes) for use in geologic models to simulate the CO_2 plume to help establish the area of review. The tool can also be used to condition and interpret time-lapse seismic data to image the CO_2 plume as part of the monitoring program.
Last Updated	June 2021, Version 11.0
Ongoing Development	The software is still under development and offers support.
Ease of Use	The application has a graphical interface. Computer programming is not necessary to use the application. Advanced understanding of seismic data is required.
Computational Speed	The speed varies depending on the size of the project and whether the data are networked or on a local drive.
Tool Verification	Verification can be found at https://www.cgg.com/geosoftware/hampsonrussell
Related References	https://www.cgg.com/geosoftware/hampsonrussell https://www.cgg.com/sites/default/files/2020-12/HampsonRussell%20Overview.pdf

A.3.4 Kingdom

Tool Name	Kingdom
Developer/Owner	IHS Markit
Tool Type	Geophysical Data Interpretation
Description	Kingdom integrates geoscience, geophysics, and engineering subsurface data into a single software solution.
Tool Licensing and Access	Licensed through a proprietary IHS license manager on a license server. https://ihsmarkit.com/products/kingdom-seismic-geological-interpretation-software.html
Model Input	Seismic data, well data, and well log data
Model Output	A better understanding of the subsurface, with advanced interpretation and visualization of seismic data
Relevant Permitting Phase	Site characterization, injection, and post injection
Class VI Permit Element Addressed	Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	This tool is used to interpret seismic data to Identify any local or regional faulting, faults, or fractures that could serve as fluid migration pathways, confirming lateral extent of the reservoir and upper and lower confining zones and generating products (depth horizons) for use in geologic models to simulate the CO_2 plume to help establish the area of review. The tool can also be used to interpret time-lapse seismic data to image the CO_2 plume as part of the monitoring program.
Last Updated	July 2021, Version 2021
Ongoing Development	The application is still under development with support. There is an active user community.
Ease of Use	The application has a graphical interface, and the user does not need programing skills. The user will need advanced knowledge of subsurface geoscience data.
Computational Speed	The speed varies depending on the size of the project and whether the data are networked or on a local drive.
Tool Verification	Verification can be found at: https://ihsmarkit.com/products/kingdom-seismic-geological-interpretation-software.html
Related References	https://ihsmarkit.com/products/kingdom-seismic-geological-interpretation-software.html

A.3.5 pGEMINI

Tool Name	pGEMINI: parallel Geophysical Electromagnetic Modeling and Inversion of Natural and Induced sources
Developer/Owner	Piyoosh Jaysaval (PNNL)
Tool Type	Geophysical Data Interpretation
Description	Three-dimensional (3D) forward modeling and inversion of frequency-domain electromagnetic (EM) data. The forward modeling is based on unstructured-mesh finite element method and the inversion employs a Gauss–Newton optimization method. Supported data types are active-source EM (e.g., controlled-source EM, airborne EM, borehole EM) and natural source EM (e.g., magnetotelluric) data.
Tool Licensing and Access	The code is accessible by request through the developer: Piyoosh Jaysaval https://energyenvironment.pnnl.gov/staff/staff_info.asp?staff_num=3506
Model Input	Forward Modeling: 3D electrical conductivity model of the subsurface Inversion: Recorded EM data
Model Output	Forward Modeling: Simulated EM data Inversion: Inverted 3D electrical conductivity model of the subsurface
Risks Behavior Considered	Monitoring migration of CO_2 or brine through changes in the electrical conductivity.
Relevant Permitting Phase	All phases of a Class VI permit: pre- and post-injection characterization and monitoring
Class VI Permit Element Addressed	Site Characterization, Testing and Monitoring Plan, and Post Injection Site Care and Site Closure
How the Tool is Used	pGEMINI can be used to image subsurface conductivity for site characterization or changes in conductivity for monitoring CO_2 migration (Site Care).
Last Updated	March 2022
Ongoing Development	Yes. pGEMINI is a recently developed code, and new capabilities are being added.
Ease of Use	The tool does not have a graphical user interface but can be executed by providing input files created using a simple text editor. Computer programming skills are not required, but an understanding of geophysics, geology, and geophysical EM methods is needed for better applications.
Computational Speed	pGEMINI is massively parallelized to reduce computational wall-clock times for large-scale EM modeling and inversion problems.
Tool Verification	Numerical results are benchmarked against various published results and some of the benchmarking results are presented in Jaysaval et al. (2022).
Related References	Jaysaval, P.; Johnson, T.C. pGEMINI: Parallel Geophysical Electromagnetic Modeling and Inversion for Natural and Induced sources – 3-D Forward modeling for active source. *Computational Geosciences* under review **2022**. Jaysaval, P.; Knox, H.; Chojnicki, K.; Schwering, P.; Winn, C.; Hardwick, C.; Norbeck, J.; Hinz, N.; Matson, G.; Ayling, B.; Mlwasky, E.; Faulds, J. Feasibility Study of Magnetotelluric and Controlled-source Electromagnetic Methods for Geothermal Exploration at Steptoe Valley, NV. Poster presented at the Geothermal Rising Conference, 2021. https://doi.org/10.5281/zenodo.6326589

	Jaysaval, P.; Robinson, J. L.; Johnson, T.C. Stratigraphic identification with airborne EM methods at the Hanford Site, Washington. *Journal of Applied Geophysics* **2021,** *192*, 104398. https://doi.org/10.1016/j.jappgeo.2021.104398

A.3.6 RokDoc

Tool Name	RokDoc
Developer/Owner	Ikon Science
Tool Type	Geophysical Data Interpretation
Description	Geomechanical solutions for accelerating and improving subsurface predictions
Tool Licensing and Access	The tool is licensed through Flexlm tools on a license server. https://www.ikonscience.com/products/rokdoc/
Model Input	Seismic data and well log data
Model Output	Solutions include rock physics, reservoir characterization, pressure prediction, and real-time drilling monitoring
Relevant Permitting Phase	Site characterization, injection, and post injection
Class VI Permit Element Addressed	Site Characterization, Testing and Monitoring Plan
How the Tool is Used	This tool is used to perform fluid substitution modeling to determine the viability of using time-lapse seismic to monitor the CO_2 plume as part of the monitoring plan. This tool can also be used for reservoir characterization and interpretation of time-lapse seismic data.
Last Updated	June 2021, Version 6.6.3
Ongoing Development	The application is still under development with support. There is an active user community.
Ease of Use	The application has a graphical interface, and the user does not need programing skills. The user will need advanced knowledge of subsurface geoscience data.
Computational Speed	The speed varies depending on the size of the project and whether the data are networked or on a local drive.
Tool Verification	Verification can be found at https://www.ikonscience.com/products/rokdoc/
Related References	https://www.ikonscience.com/products/rokdoc/

A.4 GEOSPATIAL ANALYSIS

Mapping the surface footprint of a GCS site is a core requirement of the Class VI permitting process. Tools in this category are primarily used for mapping and analyzing spatial relationships.

A.4.1 Cumulative Spatial Impact Layers (CSIL)

Tool Name	Cumulative Spatial Impact Layers™ (CSIL)
Developer/Owner	National Energy Technology Laboratory; Developers: Lucy Romeo, Patrick Wingo
Tool Type	Geospatial Analysis
Description	Cumulative Spatial Impact Layers™ (CSIL) is a GIS-based tool that sums spatio-temporal datasets based on spatial overlap and numeric attributes. Developed as a desktop and online tool, CSIL applies multiple additive frameworks allowing users to analyze raster and vector datasets by calculating data, record, or attribute density. Providing an efficient and robust method for summarizing disparate, multi-format, multi-source geospatial data, CSIL addresses the need for a new integration approach and resulting geospatial product. The built-in flexibility of the CSIL tool allows users to answer a range of spatially driven questions. Use cases include addressing regulatory decision-making needs, risk analysis, economic modeling, and resource management.
Tool Licensing and Access	CSIL is currently trademarked by NETL. It can be freely downloaded from the Energy Date eXchange (EDX) website. Desktop tool citation: Romeo, L.; Wingo, P.; Nelson, J.; Bauer, J.; Rose, K. Cumulative Spatial Impact Layers™, Jan 24, 2019. https://edx.netl.doe.gov/dataset/cumulative-spatial-impact-layers. DOI: 10.18141/1491843
Model Input	The parameter information provided below is based on the current desktop version. Ultimately, the user needs only spatial data to complete a CSIL run. Ideally, they will understand of what the data represents, metadata, and a clear objective in running the CSIL tool. • Type of CSIL Analysis – There are three options the user can select: 1) "Create a Spatial-based CSIL (summarize data presence)" - quantifies the number of input spatial datasets that overlap within each grid cell over a spatial extent. Each dataset is represented in each cell by a 1 if present, or 0 if absent 2) "Create a Spatial-based CSIL (summarize data record density)" - counts the total number of records per each input spatial dataset that overlap within each grid cell over a spatial extent 3) "Create an Attribute-based CSIL (summarize data by numerical attribute)" - sums up the values from a common numeric attribute shared among input spatial datasets that overlap within each grid cell over a spatial extent • Input Folder or File Geodatabase – Path to a folder or file geodatabase (gdb) containing spatial data to be included in CSIL analysis. The CSIL tool will search this input path and all subsequent folders and geodatabases for spatial data, including shapefiles, feature classes, rasters, and feature raster datasets to be included in the CSIL run. • Spatial Reference System – (Optional) Projection to build the output CSIL layer in and reproject all spatial data within Input Folder or File Geodatabase into, as CSIL requires all data to be in the same spatial reference system (SRS). If not provided here and

	data are in different SRSs, CSIL will request information during runtime as needed. In addition, if a datum shift (i.e., geographic transformation) is required, the tool will generate a list of datum shifts for the user to select from while running. • Start Date – (Optional) If provided, the tool will search data for date-formatted attributes and query. Data with a date field will then be filtered starting with the date provided. If datasets have no attribute table, or no date field, they are assumed atemporal and will be included in subsequent processing steps. • End Date – (Optional) If provided, the tool will search data for date-formatted attributes and query. Data with a date field will then be filtered ending with the date provided. If a Start Date is provided, but no End Date, data with date attributes will be queried to only exact matches of the Start Date instead of a date range. If datasets have no attribute table, or no date field, they are assumed atemporal and will be included in subsequent processing steps. • Output CSIL – Output path and file name for output CSIL layer, which is currently set into a shapefile format. • Output Extent – (Optional) Vector polygon layer (feature class or shapefile) representing the spatial extent of the output CSIL to be created. Note that this will be reprojected into the SRS as needed. If not provided, the tool will derive this area from the input data, based on the largest spatial extent found. • Output Grid Cell Size – (Optional) Cell size (units-squared) of each grid cell of the output CSIL layer, spanning the Output Extent. Units of which are based on the linear units in the SRS. If not provided, the tool will calculate using ESRI's default approach.
Model Output	CSIL outputs a multivariate vector grid (polygon shapefile) that contains a field representing each input dataset, each category, and a total column. Categories are based on each dataset's parent folder or feature dataset if applicable. The total column is calculated as the sum of all datasets per grid cell. This value is calculated based on the selected CSIL analysis. In addition, a CSV dataset is produced as a field dictionary to map the fields in the output CSIL layer's attribute table to the input datasets and categories.
Risks Behavior Considered	Originally designed to understand the socio-economic and environmental impacts of oil spills following Deepwater Horizon, CSIL converts disparate spatial data into useful information. CSIL has been applied to model potential leakage risk, environmental risk, socio-economic impact, and induced seismicity. Based on the need and data provided, CSIL provides a multivariate vector grid to visualize data density, which could represent area vulnerability or risk presence.
Relevant Permitting Phase	During the Class VI permitting process CSIL could be applied at multiple steps throughout the process. It could be applied as an exploratory tool to screen sites for risk and opportunity. Applying spatial layers representing features pertinent for site characterization, CSIL could be used to map areas more optimally based on cost or infrastructure availability. Moreover, CSIL could be applied post-injection to visualize potential external risks, as an example.
Class VI Permit Element Addressed	Site Screening, Area of Review and Corrective Action Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	CSIL has been used as an exploratory and analysis tool for a variety of applications. These applications include summarizing potential socio-economic and environmental impacts to oil spills, providing a spatial analysis of anthropogenic and natural factors related to

	induced seismicity, visualizing potential leakage pathways, quantifying spatial uncertainty for geologic mapping, and mapping global oil and gas infrastructure.
Last Updated	Latest desktop release, October 2020 Latest online release, July 2021
Ongoing Development	Yes, currently working on a stand-alone desktop version of the tool, not reliant on ArcGIS software. The tool has an active user community and support for this tool is available.
Ease of Use	The desktop version of the CSIL tool is currently accessible through EDX and GitHub as an ArcGIS Toolbox complete with a user interface and help documentation. CSIL can be downloaded and ran through ArcGIS as an add-in toolbox. Users might need to run a dependency installer prior to use, based on their version of ArcGIS, but that is a simple double-click on an installer file. Users do not need any computer programming skills to use the tool, but they should understand the input spatial data the feed into the tool. The tool is built for GIS and non-GIS users alike and runs critical preprocessing checks and steps as needed (including putting all data into a common spatial reference system). The online versions of the CSIL tool are currently available through common operating platforms, which have limited user access. The online CSIL tools have a user interface and assist with documentation, but they are limited to the spatial area they run on and have been tailored for specific uses. These uses include quantifying potential impacts of offshore oil spills or summarizing data for National Environmental Policy Act analyses. All versions of the CSIL tool have been written in the widely used Python programming language. The desktop version requires access to the arcpy module (ArcGIS required), whereas online and the in-development standalone desktop versions apply open-source modules including gdal.
Computational Speed	The computational speed of CSIL depends on several factors: desktop versus online version, amount of input data, how preprocessed the input data is (i.e., is it all in the same spatial reference system or does it need to be projected), the area of the extent being analyzed, and the grid cell size. Computational speed for the desktop tool is discussed in the 2019 paper, Cumulative spatial impact layers: A novel multivariate spatio-temporal analytical summarization tool, where speeds range from 1 second to over 40 minutes, substantially faster than processing data using the same method manually.
Tool Verification	As a data-driven tool, results from CSIL are as accurate as the input data provided by the user. Moreover, users input the spatial extent and grid cell size into this multi-scale tool, so the spatial accuracy is based on user input.
Related References	Websites: Desktop tool on EDX tool – https://edx.netl.doe.gov/dataset/cumulative-spatial-impact-layers Online version of tools on Common Operating Platforms built for NETL, Bureau of Safety and Environmental Enforcement (BSEE), and Bureau of Ocean Energy Management (BOEM) (*limited access*) – https://edx.netl.doe.gov/cop/ Offshore Risk Modeling Suite - https://edx.netl.doe.gov/offshore/portfolio-items/risk-modeling-suite/ Tool publication: Romeo, L.; Nelson, J.; Wingo, P.; Bauer, J.; Justman, D.; Rose, K. Cumulative spatial impact layers: A novel multivariate spatio-temporal analytical summarization tool. *Transactions in GIS* **2019**.

	Original method discussed in publications: Bauer, J. R.; Nelson, J.; Romeo, L.; Eynard, J.; Sim, L.; Halama, J.; Rose, K.; Graham, J. *A Spatio-Temporal Approach to Analyze Broad Risks and Potential Impacts Associated with Uncontrolled Hydrocarbon Release Events in the Offshore Gulf Of Mexico*; NETL-TRS-2-2015; EPAct Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2015; p 60. https://edx.netl.doe.gov/dataset/a-spatio-temporal-approach-to-analyze-broad-risks-potential-impacts Romeo, L.; Bauer, J. R.; Rose, K.; Disenhof, C.; Sim, L.; Nelson, J.; Thimmisetty, C.; Mark-Moser, M.; Barkhurst, A. *Adapting the National Energy Technology Laboratory's Offshore Hydrocarbon Integrated Risk Assessment Modeling Approach for the Offshore Arctic*; NETL-TRS-3-2015; EPAct Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2015; p 40. https://edx.netl.doe.gov/dataset/adapting-the-netl-offshore-integrated-assessment-modeling-approach

A.5 GEOSTATISTICAL ANALYSIS

Predictions of the spatial extent of subsurface formations and features typically requires the geostatistical interpolation of sparce data. Tools in this category are designed to perform these geostatistical calculations.

A.5.1 Stanford Geostatistical Modeling Software (SGeMs)

Tool Name	SGeMs
Developer/Owner	Stanford/open-source
Tool Type	Geostatistical Analysis
Description	Open-source computer package for solving problems involving spatially related variables. It provides geostatistics practitioners with a user-friendly interface, an interactive 3D visualization, and a wide selection of algorithms.
Tool Licensing and Access	Open-source download: http://sgems.sourceforge.net/
Model Input	Geotechnical information, GIS data, map surfaces
Model Output	Maps, statistics
Risks Behavior Considered	Geostatistical analysis of geotechnical parameters and distribution, leakage
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
Last Updated	Open-source
Ongoing Development	Open-source
Related References	http://sgems.sourceforge.net/

A.5.2 Surfer

Tool Name	Surfer
Developer/Owner	Golden Software
Tool Type	Geostatistical Analysis
Description	Surfer is a grid-based mapping program that interpolates irregularly spaced XYZ data into a regularly spaced grid. Data metrics allow you to map statistical information about your gridded data, and surface area, projected planar area, and volumetric calculations can be performed quickly in Surfer. The grid files can be edited, combined, filtered, sliced, queried, and mathematically transformed, and cross-sectional profiles can also be computed and exported. Grids may also be imported from other sources, such as the United States Geological Survey (USGS). The grid is used to produce different types of maps including contour, color relief, and 3D surface maps among others. Many gridding and mapping options are available allowing you to produce the map that best represents your data.
Tool Licensing and Access	Commercial license: https://www.goldensoftware.com/products/surfer
Model Input	Geotechnical information
Model Output	Maps, gridded data, surfaces, trend analysis
Risks Behavior Considered	Leakage, storage resource, faults, fractures, boundaries
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
Last Updated	Surfer ® 21.2.192 (64-bit) Jul 6 2021
Ongoing Development	Commercial, regular updates
Related References	https://www.geometrics.com/software/golden-software-surfer/

A.6 PROJECT PLANNING

Tools in this category are primarily used to make high-level planning decisions for geologic carbon storage projects.

A.6.1 Designs for Risk Evaluation and Management (DREAM)

Tool Name	Designs for Risk Evaluation and Management (DREAM)
Developer/Owner	PNNL
Tool Type	Project Planning
Description	DREAM is a Java package that designs optimal combinations of sensors and geophysical surveys to monitor a reservoir or aquifer where some risk of potential contaminant leakage is expected.
Tool Licensing and Access	The DREAMv2 tool is publicly available under an open-source license, with a Java repository available at: https://github.com/pnnl/DREAM_V2 The DREAMv3 tool is currently available on a more limited basis for alpha testing.
Model Input	DREAM requires an ensemble of reservoir injection or aquifer leakage simulations with forecasts of the monitored properties (i.e., pressure, CO_2 saturation, salinity, stress/strain) as a function of space and time. These can be standard text output files from a multiphase flow simulator like NUFT or STOMP, or in the form of a TECPLOT or HDF5 file. If the monitoring design objective is plume and pressure front tracking, then reservoir CO_2 injection simulations are required. If the objective is groundwater quality monitoring, then aquifer brine and CO_2 leakage simulations are needed as input.
Model Output	DREAM outputs a set of proposed monitoring plans graphically within the user interface, and also produces a comma-delimited text file which the user can use to perform their own further analyses.
Risks Behavior Considered	DREAM was designed to help minimize the risk of unintended migration of CO_2 or brine through a legacy wellbore or a fracture in the caprock. There is no practical reason one could not use it to monitor for other types of groundwater risk cases such as nuclear waste storage sites, coal ash ponds, landfills, or concentrated livestock feeding operations.
Relevant Permitting Phase	Class VI site characterization and injection, operations monitoring, post-injection site care.
Class VI Permit Element Addressed	Site Characterization, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	The user would assemble their set of input files either by running their own STOMP or NUFT simulations, or by running any other reservoir or leakage simulation they choose, including NRAP-Open-IAM, and using the provided Python scripts to convert the outputs to HDF5 format. They would then run the DREAM executable (a JAR file) and use the GUI to select the directory where the inputs are stored. They would then respond to a series of prompts from the GUI, clarifying information about the types of sensors available such as their cost and their sensitivity to the monitored parameter, such as pressure or CO_2 saturation. The user would also specify where in the field monitoring sensors are and are not feasible to deploy (for example due to topography, land access, logistical constraints), and would define which optimization algorithm they would like DREAM to use.

	DREAM then runs the given optimization and provides a set of ideal monitoring plans tailored to the particular site.
Last Updated	The DREAMv2 GitHub release was last updated June 8, 2020. The DREAMv3 repository is still being actively developed, and was last updated October 15, 2021.
Ongoing Development	DREAMv3 is under active development and is in the process of alpha testing, and support from the development team is available.
Ease of Use	The GUI version has fewer features but has a user's manual with examples and a description of how to choose inputs and use outputs. The user would need some level of familiarity with geology and geomechanics but not expert-level knowledge. The GitHub Python library has documentation and examples but requires a basic level of familiarity with Python.
Computational Speed	The optimization is highly dependent on the size of the input files, and the complexity of the monitoring site. Some smaller runs complete on the order of less than a second, while large complex sites can run for several days.
Tool Verification	A set of unit and integration tests have been developed for QA/QC purposes. While a benchmark solution is not generally available for the more complex optimization problems that DREAM is developed for, the optimization algorithms have been tested against Monte Carlo and Grid Search methods and perform much more efficiently.
Related References	Bacon, D. H.; Yonkofski, C. M.; Brown, C. F.; Demirkanli, D. I.; Whiting, J. M. Risk-based post injection site care and monitoring for commercial-scale carbon storage: Reevaluation of the FutureGen 2.0 site using NRAP-Open-IAM and DREAM. *International Journal of Greenhouse Gas Control* **2019,** *90*, 102784. Huerta, N.; Bacon, D.; Carman, C.; Brown, C. F. *NRAP Toolkit Screening for CarbonSAFE Illinois–Macon County;* No. DOE-UIUC-29381; Univ. of Illinois at Urbana-Champaign, IL (United States); Illinois State Geological Survey, 2020. Vasylkivska, V.; Dilmore, R.; Lackey, G.; Zhang, Y.; King, S.; Bacon, D.; Chen, B.; Mansoor, K.; Harp, D. NRAP-Open-IAM: A Flexible Open-Source Integrated-Assessment-Model for Geologic Carbon Storage Risk Assessment and Management. *Environmental Modelling & Software* **2021,** *143*, 105114. Yonkofski, C. M.; Davidson, C. L.; Rodriguez, L. R.; Porter, E. A.; Bender, S. R.; Brown, C. F. Optimized, budget-constrained monitoring well placement using DREAM. *Energy Procedia* **2017,** *114*, 3649–3655. Yonkofski, C. M.; Gastelum, J. A.; Porter, E. A.; Rodriguez, L. R.; Bacon, D. H.; Brown, C. F. An optimization approach to design monitoring schemes for CO_2 leakage detection. *International Journal of Greenhouse Gas Control* **2016,** *47*, 233–239. Yonkofski, C.; Tartakovsky, G.; Huerta, N.; Wentworth, A. Risk-based monitoring designs for detecting CO_2 leakage through abandoned wellbores: An application of NRAP's WLAT and DREAM tools. *International Journal of Greenhouse Gas Control* **2019,** *91*, 102807.

A.6.2 FE/NETL Carbon Storage Cost Model

Tool Name	FE/NETL CO_2 Saline Storage Cost Model
Developer/Owner	NETL
Tool Type	Project Planning
Description	The CO_2 Storage Cost Model is an Excel®-based tool that estimates the first-year break-even price to store a tonne of CO_2 in a deep saline aquifer. The model has four interactive modules that serve as its foundation: Project Management, Financial, Geologic, and Activity Cost. The CO_2 Storage Cost Model incorporates the labor, equipment, technology, and financial instruments needed to be in compliance with U.S. EPA Underground Injection Control (UIC) Class VI regulations and Subpart RR of the Greenhouse Gas Reporting Rule. The purpose of this model is to mimic CO_2 storage operations to estimate the costs (e.g., capital, operating, financing, and revenue) associated with a potential CO_2 saline storage project; this model is not reservoir modeling software. Default parameters within the model are based on EPA's economic analysis of their Class VI regulations. These parameters include the storage project timeline—a CO_2 storage project has 30 years of injection operations followed by 50 years of PISC and site closure with up-front years for site selection, characterization, permitting, and construction reflecting a base case scenario.
Tool Licensing and Access	Open-Source. Can be downloaded from: https://edx.netl.doe.gov/dataset/fe-netl-co2-saline-storage-cost-model-2017
Model Input	• **Key_Inputs.** Key management decisions are entered in this tab including annual volume of CO_2 injected, years of injection, time span for other stages of a storage project, some two dimensional (2-D) and three dimensional (3-D) seismic parameters, well spacing for monitoring wells, and financial parameters defining the business scenario to be modeled. • **Financial Responsibility Inputs.** This tab contains modeler inputs for the Financial Responsibility (FR) instrument including the selection of the instrument and financial parameters for each instrument. The "Fin_Resp_Inputs" worksheet also includes output information pertaining to the costs of all components and instruments of FR with the results of the single formation being displayed in this tab. A multiple formation evaluation will display results for the last formation evaluated. • **Activity_Inputs**. This worksheet contains tables of modeler inputs that define costs of parameters related to the project. These items are divided into four table groups: (1) Parameters Consistent Across all Activities, (2) Activity-Specific Parameters, (3) Parameters Used in Activities across Multiple Stages, and (4) Well-Drilling Costs. • **Surface Equipment Cost**. Capital costs and annual operation and maintenance (O&M) costs for surface equipment/facility at a saline storage site are specified in this worksheet. Surface equipment includes a feeder pipeline; equipment/facility, roads, and buildings needed to operate the injection wells; and equipment and roads related to storage field operations. • **Back-End Cost Items**. This worksheet enables the modeler to fully audit and review the model calculations. It calculates the appropriate annual cost for each activity utilized in a storage project and posts this cost in the year(s) it is incurred. • **Drilling Costs**. This worksheet performs the calculations of drilling costs. • **Geologic Module**. This module includes the geologic database, storage coefficients, and geo-engineering equations and calculates CO_2 injectivity, number of CO_2 injection wells, and CO_2 plume area; the latter two are fundamental cost drivers for any CO_2

	storage project. It also calculates water withdrawal (production) from the CO_2 storage reservoir as well as subsequent treatment and disposal (injection) of water not rendered potable.
Model Output	• **Summary Output.** A summary of many important outputs of the model is within this tab. This worksheet also includes output information from the Project Management, Geologic, and Financial modules with the results of a single formation being displayed in this tab. A multiple formation evaluation will display results for the last formation evaluated. • **Cost Breakdown.** This tab uses data throughout the model to sum costs across different categories. These sums are used in some of the output the model produces.
Risks Behavior Considered	Financial Risks
Relevant Permitting Phase	Site Screening, Site Characterization, Injection Operations, Post-Injection Closure
Class VI Permit Element Addressed	Site Screening, Financial Assurance Demonstration, Well Construction Details
How the Tool is Used	The purpose of this model is to mimic CO_2 storage operations to estimate the costs associated with a potential CO_2 saline storage project; this model is not reservoir modeling software. The Storage Cost Model provides a flexible way to allow users to tailor the model to fit the requirements of each individual project by adjusting parameters in each stage (e.g., financial parameters or project lifetime). The storage project costs estimated by the model occur in one or more of the five stages of a storage project: site screening, site selection and site characterization, permitting and construction, operations, and PISC and site closure.
Last Updated	September 2017
Ongoing Development	Yes
Ease of Use	FE/NETL CO_2 Saline Storage Cost Model is developed in Excel with customized Visual Basic for Applications (VBA) programming language to extend its functionality. Users with Microsoft Excel and computer programming experience can access the complete functionality of the model. A customized ribbon is also available for users to run the model.
Computational Speed	A single formation calculation takes seconds to determine the CO_2 price making the Net Present Value (NPV) zero.
Tool Verification	The details of the model can be found here: https://www.netl.doe.gov/energy-analysis/details?id=2404
Related References	NETL. *FE/NETL CO_2 Saline Storage Cost Model*; U.S. Department of Energy, National Energy Technology Laboratory. Last Update: Sep 2017 (Version 3). https://www.netl.doe.gov/research/energy-analysis/search-publications/vuedetails?id=2403 Grant, T.; Morgan, D. *FE/NETL CO_2 Saline Storage Cost Model*; User's Manual; 2017. https://www.osti.gov/servlets/purl/1557137

A.6.3 SimCCS

Tool Name	SimCCS: Open-source software for designing CO_2 capture, transport, and storage infrastructure
Developer/Owner	Carbon Solutions, LLC.
Tool Type	Project Planning
Description	SimCCS is an open-source software developed to assist industry and governments in making CCS infrastructure decisions. The software accesses public- or user-provided CO_2 source, sink, and transportation data to create and solve an optimization problem to determine the most cost-effective CCS infrastructure design (e.g., minimizing costs or maximizing profits). The optimization problem is solved via a third-party optimization engine (e.g., C-Plex or Gurobi) on a local desktop computing platform. Users of SimCCS have the flexibility to adjust designs for changes in tax credits, CO_2 price, and address uncertainties associated with emission rates at sources and injection rates and capacities at sinks.
Tool Licensing and Access	SimCCS software is a proprietary software available through Carbon Solutions, LLC. https://www.carbonsolutionsllc.com/software/simccs/
Model Input	SimCCS addresses all parts of the CCS supply chain to find cost savings, revenue streams, and risks via three submodules: the optimization engine, the Cost Surface Multi-Layer Aggregation Program (CostMAP), and the Sequestration of CO_2 Tool (SCO_2T or "Scott"). The optimization engine brings together input data from the user, CostMAP, and SCO2T to model an end-to-end CCS supply chain that accounts for CO_2 capture, CO_2 pipeline transport, and CO_2 storage. • Capture data: The capture data includes parameters for each source location, including an ID, name, latitude/longitude location, fixed opening cost, variable operating cost, per unit capture cost, and a maximum CO_2 production rate. • Storage data: The storage data includes parameters for each storage location, including a label, latitude/longitude location, fixed opening cost for the entire location, variable operating cost for the entire location, fixed opening and variable operating costs for each well, injection cost, and a maximum capacity for each well and for the entire location. • Transport data: Weighted-cost surface data generated from CostMAP are used to determine the cost of building pipeline networks. Developing the weighted-cost surface involves laying a grid over the modeled domain and determining the cost of traversing from one cell to another. Traversing from cell-to-cell is a function of underlying topography (slope and aspect), land ownership (10 default classes), land use (16 default types), crossings (rail, river, and roads), existing pipeline rights-of-way (ROWs), and population density. These inputs are provided in SimCCS or users can use their own GIS raster files.
Model Output	Outputs from SimCCS include intermediate outputs (the pipeline candidate network and MPS file) and final solutions (SOL File and GIS shapefiles). • Candidate network: Unlike geographically fixed capture and storage facilities, CCS pipeline networks need to be modeled, since they do not yet exist in most areas. An intermediate output called the candidate pipeline is outputted as a GIS-shapefile from the SimCCS optimization engine based upon the weighted-cost surface generated in CostMAP. The candidate network is a subgraph of all possible pipeline routes between capture and storage facilities, calculated using shortest-path algorithms.

	• MPS file: Once source and storage locations are parameterized and a candidate pipeline network has been identified, the user is able to start formulating infrastructure design optimization problems. This formulation takes the form of mixed-integer linear programing (MIP) problem that is stored for the user in a Mathematical Programming System (MPS) file. • SOL file and GIS shapefiles: The SOL file contains solutions on which source and storage locations were opened, how much CO_2 was captured and stored, and where to purchase various sized pipelines. This information is visualized in the GUI. Costs are broken down by capture, transport, and storage and are also displayed for comparison purposes. SimCCS also generates GIS Shapefiles of this information, including source locations, storage locations, pipeline routes, and CO_2 flows.
Risks Behavior Considered	SimCCS does not explicitly consider risk but does allow users to avoid building pipelines in areas of their choosing (e.g., environmentally or socially sensitive areas).
Relevant Permitting Phase	Site Screening, Site Characterization, Injection Operations, Post-Injection Closure
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	SimCCS generates end-to-end CCS infrastructure solutions through a four-step workflow that can be characterized as inputs, problem creation, problem solving, and analysis. SimCCS inputs CO_2 capture, transport, and storage data to construct the MIP problem. The problem is solved and outputs can be analyzed in the SimCCS GUI or brought into third-part software, like a GIS, for further analysis.
Last Updated	August 2021
Ongoing Development	Yes
Ease of Use	SimCCS runs on any Java-enabled machine and requires no dependencies beyond what is packaged with the code to create the MIP. However, users do need an optimization solver on their local machine to solve the MIP.
Computational Speed	The computational costs of solving MIP problems can vary widely depending on the number of parameters. In SimCCS most solutions are solved quickly. However, as the size of the geography increases and the number of sources/sinks increase, computational efficiency declines. SimCCS developers are actively developing heuristics to improve efficiency.
Tool Verification	Components of SimCCS have been verified via various scientific papers (some listed below).
Related References	https://www.carbonsolutionsllc.com/ Hoover, B.; Yaw, S.; Middleton, R. CostMAP: an open-source software package for developing cost surfaces using a multi-scale search kernel. *International Journal of Geographical Information Science* **2020,** *34*, 520–538. Middleton, R. S.; Chen, B.; Harp, D. R.; Kammer, R. M.; Ogland-Hand, J. D.; Bielicki, J. M.; Clarens, A. F.; Currier, R. P.; Ellett, K. M.; Hoover, B. A.; McFarlane, D. N. Great SCO2T! Rapid tool for carbon sequestration science, engineering, and economics. *Applied Computing and Geosciences* **2020,** *7*, 100035.

	Middleton, R. S.; Yaw, S. P.; Hoover, B. A.; Ellett, K. M. SimCCS: An open-source tool for optimizing CO_2 capture, transport, and storage infrastructure. *Environmental Modelling & Software* **2020,** *124*, 104560.

A.7 RELEASE, TRANSPORT, AND RECEPTOR RESPONSE

Fate and transport modeling of CO_2 and brine through leakage pathways and into sensitive receptors is required to characterize the leakage risks at a GCS site. Tools in this category are primarily used to model CO_2 and brine leakage through leakage pathways and/or into potential receptors (e.g., shallow aquifers).

A.7.1 MODFLOW with MT3DMS/RT3D

Tool Name	Modular Three-Dimensional Finite-Difference Groundwater Flow Model (MODFLOW) with Multispecies Mass Transport in 3-Dimensions (MT3DMS) or Reactive Transport in 3-Dimensions (RT3D)
Developer/Owner	United States Geological Survey
Tool Type	Release, Transport, and Receptor Response
Description	A widely-used groundwater flow simulation tool that can simulate three-dimensional (3D) transport of a multiple solute species in flowing groundwater. Originally developed and released solely as a groundwater-flow simulation code when first published in 1984, MODFLOW's modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MODFLOW-related programs now includes capabilities to simulate coupled groundwater/surface-water systems, solute transport, variable-density flow (including saltwater), aquifer-system compaction and land subsidence, parameter estimation, and groundwater management.
Tool Licensing and Access	Open-source code can be freely downloaded here: https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model with no license needed.
Model Input	Initial concentration of solute species, hydrological parameters such as hydraulic head, hydraulic conductivity (kx, ky, and kz), transmissivity, storage coefficient, residual saturation, etc.
Model Output	Hydraulic head distribution (MODFLOW) and concentration distribution(s) (MT3DMS/RT3D) on a 3D grid
Risks Behavior Considered	Environmental risk to groundwater and surface water
Relevant Permitting Phase	Primarily Site characterization and in some instances, groundwater monitoring during injection
Class VI Permit Element Addressed	Site Characterization, Testing and Monitoring Plan
How the Tool is Used	The tool would be used to predict where leaks might manifest in groundwater and how they might be attenuated through groundwater flow. It would inform the level of risk to groundwater and where monitoring of groundwater should be most implemented.
Last Updated	The current version of MODFLOW 6 is version 6.2.2, released July 30, 2021.
Ongoing Development	The USGS Water Mission Area actively develops and supports the MODFLOW suite of programs. Ongoing efforts include providing maintenance and support for existing versions of MODFLOW such as MODFLOW 6, MODFLOW-2005, MODFLOW-NWT, MODFLOW-USG, MODPATH, MT3D-USGS, and related and supporting programs such as

	FloPy and PEST++. Current development efforts are focused on adding new capabilities to MODFLOW 6. These development efforts include: • A Basic Model Interface (BMI) for MODFLOW 6 to support easier coupling with other models such as those that simulate groundwater recharge, geochemical mixing, and optimization and management, as well as models that would benefit from tight coupling. • A Groundwater Transport (GWT) Model that works with structured or unstructured grids, the Newton formulation, and the advanced stress packages available in MODFLOW 6. • A new Buoyancy (BUY) Package that extends the Groundwater Flow (GWF) Model of MODFLOW 6 to represent variable-density groundwater flow. This new BUY Package makes it possible to simulate problems related to saltwater intrusion, deep-well injection, aquifer storage and recovery, and brine migration. • Extension of MODPATH to track particles in MODFLOW 6 models that use Discretization by Vertices (DISV) and fully unstructured (DISU) grids. • Parallelization of the MODFLOW 6 multi-model framework for High-Performance Computing (HPC) using the Message Passing Interface (MPI). Preliminary versions of MODFLOW 6 with this new capability have been used to solve groundwater models with billions of model cells. This new parallelization capability is being developed in a general manner that can be easily extended for future MODFLOW model types (for example GWT); applied at local, regional, and continental scales; and can be used on desktops and HPC systems. In addition to these ongoing efforts, future efforts may include development of new surface water, pipe network, and heat transport models. The USGS plans to continue these development efforts to meet the needs of the USGS, our stakeholders, and the needs of the hydrologic modeling community. Users are encouraged to track MODFLOW developments through our version-controlled MODFLOW 6 repository.
Ease of Use	MODFLOW is a command line executable program written in FORTRAN that reads ASCII text and binary input files and writes ASCII text and binary output files. Although experienced MODFLOW users may be able to create MODFLOW input files by hand, most MODFLOW users rely on a graphical user interface to prepare the input files and post-process the output files. The MODFLOW program itself does not generate contour plots or any other type of graphical output. These plots must be generated from MODFLOW results using other software programs. The USGS distributes several free pre- and post-processors for MODFLOW. Commercial GUIs are also available for sale by private vendors. Successful use of MODFLOW typically requires a college-level modeling course or professional training on groundwater modeling. In some situations, the USGS can provide training to governmental agencies with a cooperative agreement with the USGS; agencies can contact their cooperating USGS office for additional information. MODFLOW courses are also offered by several private companies.
Computational Speed	The model is generally designed for computational efficiency. Speeds are not limited in any way. It generally runs within minutes.
Tool Verification	https://www.epa.gov/sites/default/files/2015-05/documents/Draft-Risk-Modeling-Report-Appendix-A-September-11-2013.pdf https://www.wipp.energy.gov/library/cra/CRA-2014/References/Others/US_EPA_2006_TSD_for_Section_194_23_Models_and_Computer_Codes.pdf
Related References	https://www.usgs.gov/mission-areas/water-resources/science/modflow-and-related-programs?qt-science_center_objects=0#qt-science_center_objects

A.7.2 Semi-Analytical Leakage Solutions for Aquifers (SALSA)

Tool Name	SALSA (Semi-Analytical Leakage Solutions for Aquifers)
Developer/Owner	Abdullah Cihan/LBNL
Tool Type	Release, Transport, and Receptor Response
Description	SALSA computes pressure or head in aquifers and aquitards, leakage rates and cumulative leakages through abandoned wells for multilayered aquifer systems with multiple injection, pumping and leaky wells. Injection and extraction rates can change with time, and initially the system can be hydrostatic, overpressured, or underpressured.
Tool Licensing and Access	The code is accessible by request through the developer and LBNL. Abdullah Cihan: https://eesa.lbl.gov/profiles/abdullah-cihan/
Model Input	Layer-wise properties for aquifers and aquitards such as thicknesses, permeability, storativity, anisotropy ratio and initial heads. Also, coordinates of the wells, screen levels for injection and pumping wells with time-dependent injection and extraction rates, conductivity distribution along the leaky wells with options to identify cased, open and plugged segments.
Model Output	Time-dependent pressure or head changes in aquifers and aquitards, leakage rates and cumulative leakages at different aquifer-leaky well interfaces, contour plot for areal distribution of head or pressure changes in user-selected aquifers.
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Site screening, injection and post-injection pressure behavior in multilayered systems
Class VI Permit Element Addressed	Site Screening, Area of Review and Corrective Action Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	The tool can be used to estimate pressure front evolution in response to injection in multi-layered aquifer systems and the leakage risks through leaky paths. Leakage rates and cumulative leakages can be calculated in the presence of leaky abandoned wells, including leakages due to injection into already overpressured storage reservoirs.
Last Updated	The tool was last updated in September 2021.
Ongoing Development	The code is ready to use. The code has been used in several different research institutions, but there is not an active user community.
Ease of Use	No user interface currently, but the code can be built into NRAP Open-IAM in the future. The code uses one input text file and generates output files that can be directly dragged into the Tecplot software for plotting the results. The users do not need programing skills, but some basic knowledge about groundwater hydrology would be needed.
Computational Speed	The code runs very fast (seconds), because it is a mesh-free semi-analytical model.
Tool Verification	Verified extensively with existing analytical solutions for simpler problems and high-fidelity numerical models. These verifications were mostly documented in the published literature.
Related References	There is a user manual for the code, but it needs to be updated with the recent developments.

	Burton-Kelly, M. E.; Azzolina, N. A.; Connors, K. C.; Peck, W. D.; Nakles, D. V.; Jiang, T. Risk-based area of review estimation in overpressured reservoirs to support injection well storage facility permit requirements for CO_2 storage projects. *Greenhouse Gas Sci Technol* **2021,** *11,* 887–906. https://doi.org/10.1002/ghg.2098 Cihan, A.; Birkholzer, J.; Zhou, Q. Pressure Buildup and Brine Migration during CO_2 Storage in Multilayered Aquifers. *Ground Water* **2012**. doi: 10.1111/j.1745-6584.2012.00972.x Cihan, A.; Oldenburg, c. M.; Birkholzer, J. *Leakage in Abnormally Pressured Multilayered Aquifer Systems: Solutions Based on Laplace Transform and Matrix Calculus*; 2021 under preparation. Cihan, A.; Zhou, Q.; Birkholzer, J. Analytical Solutions for Pressure Perturbation and Fluid Leakage through Aquitards and Wells in Multilayered Aquifer Systems. *Water Resources Research* ***2011***. doi:10.1029/2011WR010721. Cihan, A.; Zhou*, Q.;* Birkholzer*, J. T.;* Kraemer, S. R. Flow in horizontally anisotropic multilayered aquifer systems with leaky wells and aquitards. *Water Resources Research* **2013,** *50. doi:10.1002/2013WR013867.* Oldenburg, C. M.; Cihan, A.; Zhou, Q.; Fairweather, S.; Spangler, L. H. Geologic carbon sequestration injection wells in overpressured storage reservoirs: estimating area of review. *Greenhouse Gases: Science and Technology* **2016.** doi:10.1002/ghg.1607.

A.7.3 Tfrack

Tool Name	Tfrack
Developer/Owner	Quanlin Zhou (LBNL)
Tool Type	Release, Transport, and Receptor Response
Description	The Tfrack code in MATLAB can analytically predict evolution of fracture length, spacing, aperture, and pattern of thermal fractures around vertical and horizontal injection wells (as well as hydraulic fractures or faults). Thermal fractures are induced and propagated by significant cooling and thermal stress caused by CO_2 injection through/into deep hot formations. They create leakage flow paths in caprock for injected CO_2. This type of leakage risk has been overlooked in the CCS community for site permitting and operation.
Tool Licensing and Access	The website for free download is under development Quanlin Zhou: https://eesa.lbl.gov/profiles/quanlin-zhou/
Model Input	One, two, or three dimensionless model parameters: effective confining stress, wellbore radius, and horizontal stress ratio are needed for half-plane thermal fractures from a hydraulic fracture, radial thermal fractures around a horizontal well, or longitudinal thermal fractures around a vertical well, respectively.
Model Output	Fracture length, spacing, aperture, and pattern of half-plane, radial, and longitudinal thermal fractures, as functions of time for a specific application
Risks Behavior Considered	A new type of leakage risk caused by CO_2 leakage through longitudinal thermal fractures out of injection wells in sealing formations; a new risk of reduced storage capacity and efficiency in a thick storage formation or stacked storage formations caused by focused CO_2 flow through thermal fractures
Relevant Permitting Phase	Applicable to site screening, site characterization, and injection of a Class VI permit
Class VI Permit Element Addressed	Area of Review and Corrective Action Plan, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan
How the Tool is Used	In the current Class VI permitting workflow, hydraulic fracturing is avoided by limiting injection pressure to be less than fracturing pressure (without consideration of cooling-induced thermal stress). This tool focuses on predicting thermal fractures and related leakage risks for injection and post-injection periods.
Last Updated	The tool was last updated October 1, 2021
Ongoing Development	The development of the tool is completed, but it does not have an active user community. Promotion of the applications of the tool is key to permitting.
Ease of Use	No graphical user interface. The code is in MATLAB, and users can run the tool as a black box or use derived type curves without a computer.
Computational Speed	This tool is a collection of analytical solutions, and is computationally fast.
Tool Verification	The tool has been verified for accuracy by excellent agreements with numerical modeling results. The verifications were documented in three related journal publications (see below):
Related References	Chen, B.; Zhou, Q. Analytical prediction of thermal fracturing around horizontal wells. *Geophysical Research Letters* **2021** (submitted).

	Chen, B.; Zhou, Q. Scaling behavior of thermally driven fractures in deep low-permeability reservoirs: a plane strain model with 1-D heat conduction. *Journal of Geophysical Research - Solid Earth* **2021,** *126*, 2021JB022964 (under revision). Chen, B.; Zhou, Q. Scaling behavior of thermally driven longitudinal fractures along a vertical well: a plane strain model with radial heat conduction. *Journal of Geophysical Research - Solid Earth* **2021** (submitted).

A.8 RESERVOIR SIMULATION

Simulating the behavior of the subsurface CO_2 plume and corresponding pressure response is a fundamental requirement of the Class VI permitting process. Tools in this category were designed to simulate the complex physics associated with multiphase flow in porous media.

A.8.1 Aquifer Injection Modeling Toolbox (AIM Toolbox)

Tool Name	AIM Toolbox
Developer/Owner	Developer: Christian Johnson and Inci Demirkanli (PNNL) Owner: Region 8 EPA (Wendy Cheung)/ORD (Rick Wilkins)
Tool Type	Reservoir Simulation
Description	The audience for this web application is permitting authorities or operators who do not have modeling experience. The Aquifer Injection Modeling Toolbox ("AIM Toolbox") software is a user-friendly app that provides a collection of analytical solutions suitable for evaluating the potential extent of the area impacted by subsurface injection operations with minimal data input. While specifically designed to evaluate brine disposal operations (e.g., produced water from oil and gas operations that would be disposed into UIC Class IID wells), it can provide a first cut evaluation of visualizing the extent of an injected plume in a GIS map to assess potential vulnerable areas within the Area of Review. It is also well suited to apply for an expansion of the Class II aquifer exemption and demonstrate that an appropriately sized area is exempted such that the CO_2 plume and pressure front remain within the approved exempted area. The app currently contains five analytical and semi-analytical solutions to delineate the area that can potentially be impacted by subsurface operations that range from simple volume fill-up, incorporation of natural hydraulic gradient, and consideration of the density differential between injectate and formation fluids. The app also places the plume relative to existing aquifer exemptions.
Tool Licensing and Access	The app is licensed for government use only. Initial deployment is at: https://socrates.pnnl.gov/epa-rare-aim/index.html As of April 2022, the app will be available on the EPA Office of Research and Development website: https://www.epa.gov/sites/default/files/js-scripts/aim-toolbox/index.html
Model Input	Depending upon the model selected, the input parameters may include: well location, groundwater direction, natural hydraulic gradient and dispersivity, flow rate, injection duration, injectate specific gravity, aquifer thickness, porosity, hydraulic conductivity, and specific storage.
Model Output	The output is both in numeric and visual form.
Risks Behavior Considered	Siting issues
Relevant Permitting Phase	Site Screening
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Aquifer Exemption Expansion
How the Tool is Used	Provides a quick comparison against applicant-submitted models or during pre-application process, allowing assessment of potential siting issues. User can also change input parameter such as project duration.

Last Updated	Spring 2021
Ongoing Development	The app is completed, however as funding becomes available, there may be additional development, such as adding a data layer to include injection and production wells from state and EPA databases.
Ease of Use	The tool has a graphical user interface and is very simple to use. No programming knowledge is required. The utility of this app is in the ease of its use.
Computational Speed	Computational speeds are nearly instantaneous.
Tool Verification	Model verification includes comparison of outputs to known results or results from independent methods. PNNL has developed a robust QA document that can be shared.
Related References	Additional information can be found at: https://www.pnnl.gov/projects/aim-toolbox, including user guide.

A.8.2 CMG GEM

Tool Name	CMG GEM
Developer/Owner	Computer Modelling Group LTD. (CMG)
Tool Type	Reservoir Simulation
Description	GEM is a reservoir dynamic flow simulator that accounts the equation of state (EOS) for compositional reservoir modeling. Physical processes that occur during CO_2 storage are integrated in the simulator.
Tool Licensing and Access	License purchased from CMG: https://www.cmgl.ca/gem
Model Input	Static geologic model input, known as reservoir description Reservoir fluids components Rock-fluid types, known as relative permeability for each rock type Reservoir initial conditions, including petrophysical properties, initial reservoir pressure, and temperature conditions Numerical settings for accuracy and computational efficiency Well data and recurrent injection/production data When incorporating geochemical interactions, aqueous chemical equilibrium, mineral dissolution, and precipitation reactions from Thermo/Phreeqc/Minteq Geo-Chemistry database need to be selected and defined.
Model Output	Simulator generates .sr3 file and text format .out file
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Site screening, site characterization, area of review (AOR) evaluation, injection, and post injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	CMG is used to simulate site-specific injection capacity, fluid movement, and pressure changes. The output is then used to determine CO_2 plume and AO CMG can also be used to evaluate geochemical reactions and their potential impacts on injectivity.
Last Updated	The latest version is October 2020.
Ongoing Development	Versions are updated periodically. There is no active user community. Support is available.
Ease of Use	The tool has a graphical user interface. Computer-programming skills are not needed. An understanding of reservoir fluid flow physics and reservoir simulation techniques is needed to run the tool.
Computational Speed	GEM is designed for computation efficiency. Simulation time depends on the size and the type of the model—typically 8–24 hours. Geochemical models can take a longer time to complete. Computational speeds can be limited by availability of sufficient clusters/nodes on the server.

Tool Verification	The tool has been used for several years throughout the oil and gas industry.
Related References	A list of websites, manuals, and publications that provide additional insight into the tool include the following: Resources available on https://www.cmgl.ca/gem Class, H.; Ebigbo, A.; Helmig, R.; Dahle, H. K.; Nordbotten, J. M.; Celia, M. A.; Audigane, P.; Darcis, M.; Ennis-King, J.; Fan, Y.; Flemisch, B.; Gasda, S. E.; Jin, M.; Krug, S.; Labregere, D.; Naderi Beni, A.; Pawar, R. J.; Sbai, A.; Thomas, S. G.; Trenty, L.; Wei, L. A benchmark study on problems related to CO_2 storage in geologic formations. *Computational Geosciences* **2009,** *13*. https://doi.org/10.1007/s10596-009-9146-x Nghiem, L.; Sammon, P.; Grabenstetter, J.; Ohkuma, H. Modeling CO_2 storage in aquifers with a fully-coupled geochemical EOS compositional simulator; Paper presented at the SPE/DOE Symposium on Improved Oil Recovery, Tulsa, Oklahoma, April 2004. https://doi.org/10.2118/89474-MS Nghiem, L.; Shrivastava, V. K.; Tran, D.; Kohse, B.; Frederick, H.; Hassam, M.; Yang, C. Simulation of CO_2 Storage in Saline Aquifers; Paper presented at the SPE/EAGE Reservoir Characterization and Simulation Conference, Abu Dhabi, UAE, October 2009. https://doi.org/10.2118/125848-MS

A.8.3 ECLIPSE

Tool Name	ECLIPSE
Developer/Owner	Schlumberger
Tool Type	Reservoir Simulation
Description	The ECLIPSE simulator offers a robust set of numerical solutions for fast and accurate prediction of dynamic behavior for different reservoirs and development schemes including black oil, compositional, thermal finite-volume, and streamline simulation. By choosing from a wide range of add-on options—such as local grid refinements, coalbed methane, gas field operations, advanced wells, reservoir coupling, and surface networks—simulator capabilities can be tailored to meet ones needs and enhance reservoir modeling capabilities.
Tool Licensing and Access	Commercial: https://www.software.slb.com/products/eclipse#sectionFullWidthTable
Model Input	Geological description, Rock properties like porosity, permeability, mechanical properties, etc., fluid properties like equation of state, viscosity, etc.
Model Output	Pressure, saturation, stress, fracture growth, etc.
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Site screening, site characterization, Injection and post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan, Stimulation Program
How the Tool is Used	The tool can be used to run simulations to determine the extent of the plume. Multiple simulations can be run by varying uncertain parameters.
Last Updated	2020
Ongoing Development	Yes
Ease of Use	There is a graphical user interface. Training courses are offered.
Computational Speed	Computationally expensive
Tool Verification	Yes
Related References	Archer Daniels Midland CCS1 Class VI Permit Documents: https://www.epa.gov/sites/default/files/2021-05/documents/adm_ccs1_attachment_b_-_aor_and_ca_plan_-_final.pdf Archer Daniels Midland CCS2 Class VI Permit Documents https://www.epa.gov/uic/archer-daniels-midland-ccs2-class-vi-permit-documents

A.8.4 EASiTool

Tool Name	EASiTool
Developer/Owner	Seyyed A. Hosseini/The University of Texas at Austin
Tool Type	Reservoir Simulation
Description	Tool is developed in MATLAB platform (comes independent of installing MATLAB) and uses semi-closed form analytical equations to estimate CO_2 saturation and pressure plume evolution with time.
Tool Licensing and Access	Free, contact developer: https://www.jsg.utexas.edu/researcher/seyyed_hosseini
Model Input	Model inputs are average formation properties (permeability, porosity, pressure, temperature, salinity, relative permeability, etc.)
Model Output	Number of injection wells needed to inject given CO_2 volume, pressure, and saturation plume. Tool is providing some rough estimates of NPV and formation fracture pressure as well.
Relevant Permitting Phase	Site screening
Class VI Permit Element Addressed	Site Screening, Area of Review and Corrective Action Plan
How the Tool is Used	This tool uses homogenized formation properties to estimate radial extension of the CO_2 plume and associated elevated pressure. Model inputs are average formation properties (permeability, porosity, pressure, temperature, salinity, relative permeability, etc.) where model is using advanced analytical solutions for closed and open boundary condition reservoirs to estimate pressure build up in multi-well injection scenarios. Tool is capable of providing tornado charts for sensitivity analysis.
Last Updated	2017
Ongoing Development	No new development, but this tool has a very active user base with lots of feedback received over years. However, funding from DOE ended in 2017.
Ease of Use	Very easy, single interface
Computational Speed	Very fast, in seconds
Tool Verification	Results are compared with full-physics simulators and published in peer-reviewed literature.
Related References	Hosseini, S. A.; Ganjdanesh, R.; Seunghee, K. *Enhanced Analytical Simulation Tool (EASiTool) for CO2 Storage Capacity Estimation and Uncertainty Quantification*; 2018. https://doi.org/10.2172/1463329

A.8.5 Finite Element Heat and Mass Transfer Code (FEHM)

Tool Name	Finite Element Heat & Mass Transfer Code (FEHM)
Developer/Owner	Los Alamos National Laboratory (LANL)
Tool Type	Reservoir Simulation
Description	FEHM is a reservoir simulator with capability to simulate coupled thermal-hydrological-mechanical-chemical processes that take place in the subsurface during various energy and environmental applications. It has proved to be a valuable asset on a variety of projects of national interest including: environmental remediation of the Nevada Test Site, the LANL Groundwater Protection Program, geologic CO_2 sequestration, enhanced geothermal energy (EGS) programs, oil and gas production, nuclear waste isolation, and arctic permafrost. Subsurface physics has ranged from single-fluid/single-phase fluid flow when simulating basin scale groundwater aquifers to complex multi-fluid/multi-phase fluid flow that includes phase change with boiling and condensing in applications such as unsaturated zone surrounding nuclear waste storage facility or leakage of CO_2/brine through faults or wellbores. The numerical method used in FEHM is the control volume method (CV) for fluid flow and heat transfer equations which allows FEHM to exactly enforce energy/mass conservation; while an option is available to use the finite element (FE) method for displacement equations to obtain more accurate stress calculations. In addition to these standard methods, an option to use FE for flow is available, as well as a simple finite difference scheme.
Tool Licensing and Access	Open-Source Available at https://github.com/lanl/FEHM Website: https://fehm.lanl.gov
Model Input	Site specific reservoir models parameters based on geologic model for the site
Model Output	Time-dependent 3D reservoir variables including pressure, saturation, temperature, and in case of mechanical modeling stress and displacements
Risks Behavior Considered	Can be used to simulate and predict: 1) time-dependent leakage of CO_2 and brine through wellbores and faults as part of leakage risk assessment, and 2) time-dependent displacements and stress changes as part of induced seismicity risk assessment
Relevant Permitting Phase	Site Screening, Site Characterization, Injection Operations, Post-Injection Closure
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan
Last Updated	2021
Ongoing Development	Yes
Related References	Chen, B.; Harp, D. R.; Lu, Z.; Pawar, R. J. On Reducing Uncertainty in Geologic CO_2 Sequestration Risk Assessment by Assimilating Monitoring Data. *International Journal of Greenhouse Gas Control* **2020,** *94*. Dempsey, D.; Kelkar, S.; Pawar, R. Passive injection: A strategy for mitigating reservoir pressurization, induced seismicity and brine migration in geologic CO_2 storage. *International Journal of Greenhouse Gas Control* **2014,** *28*, 96–113.

	Dempsey, D.; Kelkar, S.; Pawar, R.; Keating E. Coblentz, Modeling caprock bending stresses and their potential for induced seismicity during CO_2 injection. *International Journal of Greenhouse Gas Control* **2014,** *22*, 223–236. Harp, D. R.; Pawar, R. J.; Carey, J. W.; Gable, C. W. Reduced order models for transient CO_2 and brine leakage along abandoned wellbores from geologic carbon sequestration reservoirs. *International Journal of Greenhouse Gas Control* **2016,** *45*, 150–162. Harp, D.; Onishi, T.; Chu, S.; Chen, B.; Pawar, R. Development of quantitative metrics of plume migration at geologic CO_2 storage sites. Greenhouse Gases Science & Technology **2019,** *0*, 1–16. Hyman, J. D.; Jimenez-Martinez, J.; Gable, C.; Stauffer, P.; Pawar, R. Characterizing the impact of network heterogeneity on the injection of super critical CO_2 into fractured caprock. *Transport in Porous Media* **2020,** *131*, 9315–955. Keating, E. H.; Harp, D. R.; Dai, Z.; Pawar, R. J. Reduced order model for assessing CO_2 impacts in shallow unconfined aquifers. *International Journal of Greenhouse Gas Control* **2016,** *46*, 187–196. Singh, M.; Chaudhari, A.; Stauffer, P. H.; Pawar, R. J. Simulation of gravitational instability and thermo-solutal convection during the dissolution of CO_2 in deep storage reservoirs, *Water Resources Research* **2020,** *56*, e2019WR026126. https://doi.org/10.1029/2019WR026126

A.8.6 GEOSX

Tool Name	GEOSX
Developer/Owner	Lawrence Livermore National Laboratory, Stanford University, and Total
Tool Type	Reservoir Simulation
Description	GEOSX is an open-source, multi-physics simulator. It enriches the physics used in industrial simulations, allowing complex fluid flow, thermal, and geomechanical effects to be handled in a seamless manner. It has highly scalable algorithms for solving these coupled systems, and improved workflows for modeling faults, fractures, and complex geologic formations.
Tool Licensing and Access	GEOSX is open-source and released under an LGPL-v2.1 license http://www.geosx.org/
Model Input	Rock properties like porosity, permeability, mechanical properties, etc.; fluid properties like equation of state, viscosity, etc.
Model Output	Pressure, saturation, stress, fracture growth, etc.
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Injection and post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Post Injection Site Care and Site Closure Plan
How the Tool is Used	The tool can be used to run simulations to determine the extent of the plume. Multiple simulations can be run by varying uncertain parameters.
Last Updated	2021
Ongoing Development	Yes
Ease of Use	No graphical user interface. Some level of proficiency with running codes via command line is perhaps necessary
Computational Speed	Run time is dependent on several factors. It is computationally expensive and has to be run in parallel on multiple cores.
Tool Verification	Different aspects of the software have been benchmarked. Details can be found at http://www.geosx.org/
Related References	https://arxiv.org/abs/2105.09468 http://www.geosx.org/

A.8.7 Heat and Salinity Transport (HAST)

Tool Name	Heat and Salinity Transport (HAST)
Developer/Owner	Abdullah Cihan/LBNL
Tool Type	Reservoir Simulation
Description	HAST computes pressure, salinity and temperature changes in subsurface by solving three coupled nonlinear partial differential equations for pressure, salt mass fraction, and temperature using the Finite Volume method.
Tool Licensing and Access	The code is accessible through the developer and LBNL. Abdullah Cihan: https://eesa.lbl.gov/profiles/abdullah-cihan/
Model Input	Model geometry, numerical grid (1D, 2D, and 3D Cartesian, or 2D axisymmetric cylindrical coordinates), hydrogeological and thermal properties in the domain, and initial and boundary conditions, provided through a single input file
Model Output	Time-dependent pressure, salinity and temperature as both contour data and observation point data (user-selected). Users can also obtain brine leakage fluxes at any arbitrary selected points.
Risks Behavior Considered	Brine leakage risk
Relevant Permitting Phase	Site screening, injection and post-injection
Class VI Permit Element Addressed	Site Screening, Area of Review and Corrective Action Plan, Post-injection Site Care and Site Closure Plan
How the Tool is Used	The tool can be used to estimate evolution of pressure and brine leakage risks for a wide range of pressure, salinity, and temperature conditions. Natural attenuation of brine leaking into USDWs can be simulated accurately.
Last Updated	The tool was last updated in June 2021. The earlier versions of the code did not include heat transport.
Ongoing Development	The development was mainly completed, but a user manual needs to be developed. There is no active user community. The code has been used by graduate students and postdocs.
Ease of Use	No user interface. The code uses one input text file and generates output files that can be directly dragged into Tecplot software for plotting the results. The users do not need programing skills, but some basic knowledge about heat and mass transport in subsurface and modeling is needed.
Computational Speed	The code is partially parallelized and may be efficiently used to solve complex 3D problems. It typically runs faster compared to the multiphase simulators, because this is a single-phase flow model of freshwater and saltwater mixing.
Tool Verification	Verified with analytical solutions, other numerical models and laboratory data. Some of these verifications were documented in the published literature.
Related References	There is currently no published user manual for the code. The following references include either descriptions or applications of the code:

	Agartan, E.; Cihan, A.; Illangasekare, T. H.; Birkholzer, J. T.; Zhou, Q. Mixing and Trapping of Dissolved CO_2 in Deep Geologic Formations with Shale Layers. *Advances in Water Resources* **2017,** *105*, 67–81. Cihan, A.; Oldenburg, C. M.; Birkholzer, J. *Leakage in Abnormally Pressured Multilayered Aquifer Systems: Solutions Based on Laplace Transform and Matrix Calculus*; 2021 under preparation. (Presents model comparisons of the codes HAST and SALSA with each other) Cihan, A.; Petrusak, R.; Bhuvankar, P.; Birkholzer, J. T.; Alumbaugh, D.; Trautz, R. Permeability decline by clay fine migration around a low-salinity fluid injection well. *Groundwater* **2021.** https://doi.org/10.1111/gwat.13127 Siirila-Woodburn, E. R.; Cihan, A.; Birkholzer, J. T. A risk map methodology to assess the spatial and temporal distribution of leakage into groundwater from Geologic Carbon Storage. *International Journal of Greenhouse Gas Control* **2017,** *59*, 99–109.

A.8.8 MATLAB Reservoir Simulation Tool (MRST)

Tool Name	MATLAB Reservoir Simulation Tool (MRST)
Developer/Owner	SINTEF Digital
Tool Type	Reservoir Simulation
Description	MRST is not primarily a simulator, but it is developed as a research tool for rapid prototyping and demonstration of new simulation methods and modeling concepts. The toolbox offers a wide range of data structures and computational methods you can easily combine to make your own custom-made modelling and simulation tools. MRST offers comprehensive black-oil and compositional reservoir simulators capable of simulating industry-standard models and also contains graphical user interfaces for post-processing simulation results. The software is organized into: • A minimal core module offering basic data structures and functionality • A large set of add-on modules offering discretizations, solvers, physical models, and a wide variety of simulators and workflow tools The modules contain many tutorial examples that explain and showcase how MRST can be used to make general or fit-for-purpose simulators and workflow tools. Using MATLAB for reservoir simulation may seem strange at first, but most of the tools and simulators are quite efficient and can be applied to surprisingly large and complex models (several real datasets are supplied with the software). For more computationally challenging cases, the open-source OPM Flow simulator from the Open Porous Media initiative is recommended.
Tool Licensing and Access	Open-source, can be used with MATLAB and Octave. https://www.sintef.no/projectweb/mrst/
Model Input	Dependent on the MRST module used.
Model Output	Dependent on the MRST module used.
Risks Behavior Considered	Leakage risk, environmental risk
Relevant Permitting Phase	Site screening, site characterization, injection, post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post Injection Site Care and Site Closure Plan
How the Tool is Used	MRST is, as the name implies, a toolbox that contains many of the features associated with reservoir simulators such as visualization, solvers, and grid processing/generation, but it is not a stand-alone/black-box simulator. It assumes that the user is comfortable working "under the hood" and knows how to choose the right tools for the right job. For running an Eclipse-type input file directly, review the "simulateSPE1" example under ad-blackoil for a minimal working example.
Last Updated	September 13, 2021
Ongoing Development	MRST is still under development and new versions are published twice a year.
Ease of Use	The tool requires knowledge of the MATLAB/Octave programming language to run.

Computational Speed	MRST is not optimized for speed.
Tool Verification	https://www.sintef.no/projectweb/mrst/documentation/
Related References	https://www.sintef.no/projectweb/mrst/download/

A.8.9 Nexus

Tool Name	Nexus
Developer/Owner	Landmark
Tool Type	Reservoir simulation
Description	Software suite for reservoir simulation equips reservoir engineers with the integrated modeling capabilities needed to assess, validate, plan, and execute asset development optimization.
Tool Licensing and Access	Commercial license: https://www.landmark.solutions/Nexus-Reservoir-Simulation
Model Input	Reservoir information, geotechnical parameters, saturation data, injection data, etc.
Model Output	Simulated pressure, flow rates, saturation changes
Risks Behavior Considered	Induced seismicity, storage resource
Relevant Permitting Phase	All
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Injection Well Plugging Plan and Post-Injection Site Care and Site Closure Plan
Last Updated	2021
Ongoing Development	Commercial, regular updates
Related References	https://www.landmark.solutions/Nexus-Reservoir-Simulation

A.8.10 Nonisothermal, Unsaturated-saturated Flow and Transport (NUFT)

Tool Name	Nonisothermal, Unsaturated-saturated Flow and Transport (NUFT)
Developer/Owner	Lawrence Livermore National Laboratory
Tool Type	Reservoir Simulation
Description	NUFT is a 3D multi-phase non-isothermal flow and transport model for both saturated and unsaturated simulations. It has been extensively applied to groundwater cleanup (especially thermal alternatives), deep geologic processes, including high level nuclear waste repositories and subsurface sequestration of CO_2. In the CSS context it has been used for reservoir-scale reactive flow modeling of CO_2 injection, transport, and storage. It has also been used to understand the impact of leaked CO_2 on aquifers.
Tool Licensing and Access	Lawrence Livermore National Security, LLC. Can be licensed from: https://ipo.llnl.gov/technologies/software/nuft
Model Input	Porosity, permeability, clay fraction, clay correlation length, mineralogy of geological formation, initial brine composition, reservoir pressure and CO_2 saturation, leakage location and flux
Model Output	CO_2 saturation, TDS, and pressure in shallow groundwater aquifers. Can be coupled to geophysical models to obtain geophysical monitoring data
Risks Behavior Considered	Leakage risk and impact
Relevant Permitting Phase	Injection and post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-injection Site Care and Site Closure Plan
How the Tool is Used	The tool can be used to run simulations to determine pressure, the extent of the plume, concentration of species, etc. Multiple simulations can be run by varying input parameters.
Last Updated	2019
Ongoing Development	Yes
Ease of Use	No graphical user interface. Some level of proficiency with running codes via command line is necessary
Computational Speed	Run time is dependent on several factors. It is computationally expensive and has to be run in parallel on multiple cores.
Tool Verification	Yes. Some of the verification is shown in the reference below
Related References	Hao, Y.; Sun, Y.; Nitao, J. J. *Chapter 9: Overview of NUFT: A versatile numerical model for simulating flow and reactive transport in porous media*; 2010. doi:10.2172/948987.

A.8.11 PFLOTRAN

Tool Name	PFLOTRAN
Developer/Owner	Glen Hammond (PNNL)/Multi-lab collaboration
Tool Type	Reservoir Simulation
Description	PFLOTRAN is an open-source, state-of-the-art massively parallel subsurface flow and reactive transport code. PFLOTRAN solves a system of generally nonlinear partial differential equations describing multiphase, multicomponent, and multiscale reactive flow and transport in porous materials. The code is designed to run on massively parallel computing architectures as well as workstations and laptops. Parallelization is achieved through domain decomposition using the PETSc (Portable Extensible Toolkit for Scientific Computation) libraries. PFLOTRAN has been developed from the ground up for parallel scalability and has been run on up to 2^{18} processor cores with problem sizes up to 2 billion degrees of freedom. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with experienced domain scientists, without which PFLOTRAN's sophisticated process models would not exist. The reactive transport equations can be solved using either a fully implicit Newton-Raphson algorithm or the less robust operator splitting method.
Tool Licensing and Access	https://www.pflotran.org/index.html
Model Input	Model domain, rock properties, boundary conditions, component properties, reaction rates
Model Output	Spatial and temporal changes in pressure, CO_2 saturation, and constituent concentrations.
Risks Behavior Considered	Leakage risk, environmental risk
Relevant Permitting Phase	Site screening, site characterization, injection, post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post Injection Site Care and Site Closure Plan
How the Tool is Used	PFLOTRAN can be used as a reservoir simulation tool for a GCS project.
Last Updated	November 11, 2021
Ongoing Development	Yes
Ease of Use	The tool does not have a graphical user interface but may be executed by providing an input file created using a simple text editor. Computer programming skills are not required but an understanding of geology is.
Computational Speed	PFLOTRAN simulations are designed to be run in parallel, which greatly reduces computational speeds.
Tool Verification	https://www.pflotran.org/documentation/
Related References	https://www.pflotran.org/index.html

A.8.12 STOMP-CO2

Tool Name	STOMP-CO2
Developer/Owner	PNNL
Tool Type	Reservoir Simulation
Description	The STOMP-CO2 simulator solves three coupled conservation equations: water mass, CO_2 mass, and salt mass; with the potential for aqueous and gas mobile phases and a precipitated salt solid phase. STOMP-CO2E additionally solves the energy equation. The ECKEChem Module, used to simulate geochemical reactions, is available for STOMP-CO2.
Tool Licensing and Access	https://www.pnnl.gov/get-stomp
Model Input	Domain grid, rock zonation, porosity, permeability, saturation function, relative permeability function, injection and/or legacy well characteristics, initial and boundary conditions
Model Output	Spatial and temporal distribution of dissolved, gaseous or supercritical CO_2, brine salinity, pressure, temperature, aqueous species concentrations, rock mineral volumes
Risks Behavior Considered	Leakage risk, environmental risk
Relevant Permitting Phase	Site screening, site characterization, injection, post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post Injection Site Care and Site Closure Plan
How the Tool is Used	As an example, STOMP-CO2 was used for the FutureGen 2.0 UIC permit application to develop models of CO_2 injection and CO_2 leakage at the site. AOR: https://archive.epa.gov/region5/water/uic/futuregen/web/pdf/attachament-b.pdf PISC: https://archive.epa.gov/region5/water/uic/futuregen/web/pdf/attachment-e-2.pdf Monitoring: Vermeul, V. R.; Amonette, J. E.; Strickland, C.E.; Williams, M. D.; Bonneville, A. An overview of the monitoring program design for the FutureGen 2.0 CO_2 storage site. *International Journal of Greenhouse Gas Control* **2016,** *51*, 193–206. 10.1016/j.ijggc.2016.05.023. Since then, the capability to simulate leakage through legacy wells has been added.
Last Updated	October 15, 2021
Ongoing Development	STOMP is still under development, has an active user community, and support for the tool is available at https://www.pnnl.gov/projects/stomp
Ease of Use	The tool does not have a graphical user interface, but may be executed by providing an input file created using a simple text editor. Users do not need computer programming skills to use STOMP-CO2, but some knowledge of hydrogeology is required.
Computational Speed	Computational speed is inversely proportional to the number of grid cells, time steps, and components selected by the user.
Tool Verification	Example applications comparing STOMP results to published benchmark problems are provided with the source code.

Related References	https://www.pnnl.gov/projects/stomp https://stomp-userguide.pnnl.gov

A.8.13 TOUGH3-ECO2N/M or iTOUGH2-ECO2N/M

Tool Name	TOUGH3-ECO2N/M or iTOUGH2-ECO2N/M
Developer/Owner	Lawrence Berkeley National Laboratory
Tool Type	Reservoir Simulation
Description	The TOUGH ("Transport Of Unsaturated Groundwater and Heat") suite of software codes are multi-dimensional numerical models for simulating the coupled transport of water, vapor, non-condensable gas, and heat in porous and fractured media. Developed at the Lawrence Berkeley National Laboratory (LBNL) in the early 1980s primarily for geothermal reservoir engineering, the suite of simulators is now widely used at universities, government organizations, and private industry for applications to nuclear waste disposal, environmental remediation problems, energy production from geothermal, oil and gas reservoirs as well as gas hydrate deposits, geological carbon sequestration, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and mechanical processes in permeable media. The TOUGH suite of simulators is continually updated, with new equation-of-state (EOS) modules being developed, and refined process descriptions implemented into the TOUGH framework (see the overview of the TOUGH development history). Notably, EOS property modules for mixtures of water, NaCl, and CO2 has been developed and is widely used for the analysis of geologic carbon sequestration processes.
Tool Licensing and Access	The tool is licensed through Berkeley lab marketplace at: https://marketplace.lbl.gov/
Model Input	Model domain, discretized grids, hydrological parameters of the geological formation, operational parameters (e.g., injection rate), characteristic curves (e.g., relative permeability and capillary pressure functions)
Model Output	Pressure, temperature and CO_2 saturation (or mass fraction is it is fully liquid saturated) within the model domain
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Injection, post-injection
Class VI Permit Element Addressed	Site Screening, Area of Review and Corrective Action Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	Identify questions to be addressed, collect site data, build site model, calibrate the model (match model output to observed data), use the calibrated model to predict
Last Updated	Officially 2017
Ongoing Development	The tool has an active user community. Researchers update the tools occasionally for their research need. Like any other large simulation codes, when occasionally a bug is suspected, the development team will work on fixing the bug. The development team provides short courses on a regular basis for the tool. There is also a user forum where the user community and development team try to provide support.
Ease of Use	The tool has commercial graphical user interfaces. Users should have a basic understanding of numerical models and multiphase flow to use the tool. Computer programming skills are not required but may be helpful. The tool is written in Fortran. Basic knowledge on compiling a computer code may be helpful unless the user has someone else to help this aspect.

Computational Speed	The tool can handle runs in parallel. The speed depends on the problem size and the difficulty of the problem itself. Understanding in numerical models may help to design a problem that has a good balance between the efficiency and accuracy of the problem required.
Tool Verification	Related documentation and research paper can be found at https://tough.lbl.gov/documentation/
Related References	Pan, L.; Spycher, N.; Doughty, C.; Pruess, K. *ECO2N V2.0: A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl and CO_2*; Report LBNL-6930E; Lawrence Berkeley National Laboratory, Berkeley, CA, Feb 2015. A list of websites, manuals, and publications that provide additional insight into the tool. Pruess, K. *ECO2M: A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl, and CO_2, Including Super- and Sub-Critical Conditions, and Phase Change Between Liquid and Gaseous CO_2*; Report LBNL-4590E; Lawrence Berkeley National Laboratory, Berkeley, CA, 2011. Pruess, K. *ECO2N: A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl, and CO2;* Report LBNL-57952; Lawrence Berkeley National Laboratory, Berkeley, CA, 2005. (superseded by Pan et al., 2015).

A.8.14 TOUGH-FLAC

Tool Name	TOUGH-FLAC
Developer/Owner	Jonny Rutqvist at LBNL and co-workers have developed the linking of TOUGH2 and FLAC3D
Tool Type	Reservoir Simulation
Description	TOUGH-FLAC is based on the linking of TOUGH-family multiphase fluid flow and heat transport simulators with the FLAC3D geomechanics simulator.
Tool Licensing and Access	The user would need a TOUGH2 or TOUGH3 license from LBNL (https://tough.lbl.gov/) and a FLAC3D license from Itasca Consulting Group (http://www.itascacg.com/software/FLAC3D). There is currently no formal license developed for the coupling routines between TOUGH2 and FLAC3D, has only been provided under research collaborations.
Model Input	Model geometry, properties for fluid flow (e.g., porosity, permeability), thermal (e.g., thermal conductivity) and geomechanics (e.g., Elastic modulus), initial conditions (pressure, temperature, stress), boundary conditions (e.g., fixed pressure, temperature, displacement, stress, flow)
Model Output	Distribution and evolution of fluid flow, pressure, thermal flow, temperature, stress, strain, and displacements
Risks Behavior Considered	Leakage risks through caprock and along faults, induced seismicity, well integrity
Relevant Permitting Phase	Site characterization, injection, post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post Injection Site Care and Site Closure Plan, Stimulation Program
How the Tool is Used	After initial site screening, the tool can be used for evaluating geomechanical performance of an injection site, to identify areas of concern, e.g., faults, caprock, basement for the potential of induced seismicity or leakage, including fault activation.
Last Updated	It is continuously updated and applied to a wide-range of problems related to subsurface coupled processes.
Ongoing Development	Yes
Ease of Use	The FLAC3D codes has a graphical interface that can be used for pre- and post-processing. TOUGH2 output such as pressure, saturation, and temperature that can be displayed in the FLAC3D graphical interface. The user needs a geosciences background, with experience in coupled thermal-hydraulic-mechanical modeling. The user does not need advanced programming skills.
Computational Speed	Latest versions included TOUGH3 and FLAC3D V7, includes parallel processing and can run few million gridblocks if desired.
Tool Verification	Each of the components TOUGH2 and FLAC3D have been extensively verified and validated as documented in user's manuals and other documents. The TOUGH-FLAC couplings has been verified and published in an extensive number of peer-reviewed publications.
Related References	For FLAC3D: http://www.itascacg.com/software/FLAC3D For TOUGH: https://tough.lbl.gov/

	General for TOUGH-FLAC and linking: Cappa, F.; Rutqvist, J. Impact of CO_2 geological sequestration on the nucleation of earthquakes. *Geophysical Research Letters* **2011,** *38*, L17313. Cappa, F.; Rutqvist, J. Modeling of coupled deformation and permeability evolution during fault reactivation induced by deep underground injection of CO_2. *International Journal of Greenhouse Gas Control* **2011,** *5*, 336–346. Cappa, F.; Rutqvist, J. Seismic rupture and ground accelerations induced by CO_2 injection in the shallow crust. *Geophysical Journal International* **2012,** *190*, 1784–1789. Cappa F.; Rutqvist, J.; Yamamoto, K. Modeling crustal deformation and rupture processes related to upwelling of deep CO_2 rich fluids during the 1965–1967 Matsushiro Earthquake Swarm in Japan. *Journal of Geophysical Research* **2009,** *114*, B10304. Figueiredo, B.; Tsang, C. F.; Rutqvist, J.; Bensabat, J.; Niemj A. Coupled hydro-mechanical processes and fault reactivation induced by CO_2 Injection in a three-layer storage formation. *International Journal of Greenhouse Gas Control* **2015,** *39*, 432–448. Jeanne, P.; Guglielmi, Y.; Cappa, F.; Rinaldi, A. P.; Rutqvist, J. The effects of lateral property variations on fault-zone reactivation by fluid pressurization: application to CO_2 pressurization effects within major and undetected fault zones. *Journal of Structural Geology* **2014,** *62*, 97–108. Kim, H.-M.; Rutqvist, J.; Bae, W.-S. Sensitivity analysis for fault reactivation in potential CO2-EOR site with multi-layers of permeable and impermeable formations. *Geosystem Engineering* **2014,** *17*, 253–263. Konstantinovskaya, E.; Rutqvist, J.; Malo, M. CO_2 storage and potential fault instability in the St. Lawrence Lowlands sedimentary basin (Quebec, Canada): Insights from coupled reservoir-geomechanical modeling. *International Journal of Greenhouse Gas Control* **2014,** *22*, 88–110. Lee, J.; Min, K.-B.; Rutqvist, J. Probabilistic analysis of fracture reactivation associated with deep underground CO_2 injection. *Rock Mechanics and Rock Engineering* **2013,** *46*, 801–820. Mazzoldi, A.; Rinaldi, A. P.; Borgia, A.; Rutqvist, J. Induced seismicity within geologic carbon sequestration projects: Maximum earthquake magnitude and leakage potential. *International Journal of Greenhouse Gas Control* **2012,** *10*, 434–442. Pruess, K.; García, J.; Kovscek, J. T.; Oldenburg, C.; Rutqvist, J.; Steefel, C.; Xu, T. Code Intercomparison Builds Confidence in Numerical Simulation Models for Geologic Disposal of CO_2. *Energy* **2004,** *29*, 1431–1444. Rinaldi, A. P.; Rutqvist, J. Modeling of deep fracture zone opening and transient ground surface uplift at KB-502 CO_2 injection well, In Salah, Algeria. *International Journal of Greenhouse Gas Control* ***2013***, *12*, 155–167. Rinaldi, A. P.; Jeanne, P.; Rutqvist, J.; Cappa, F.; Guglielmi, Y. Effects of fault-zone architecture on earthquake magnitude and gas leakage related to CO_2 injection in a multilayered sedimentary system. Greenhouse Gases: Science and Technology **2014,** *4*, 99–120. Rinaldi, A. P.; Rutqvist, J.; Cappa F. Geomechanical effects on CO_2 leakage through fault zones during large-scale underground injection. *International Journal of Greenhouse Gas Control* **2014,** *20*, 117–131. Rinaldi, A. P.; Vilarrasa, V.; Rutqvist, J.; Cappa F. Fault reactivation during CO_2 sequestration: Effects of well orientation on seismicity and leakage. *Greenhouse Gas Sciences and Technology* **2015,** *5*, 1–12.

	Rutqvist, J.; Tsang, C.-F. A study of caprock hydromechanical changes associated with CO_2 injection into a brine aquifer. *Environmental Geology* **2002,** *42*, 296–305. Rutqvist J. Status of the TOUGH-FLAC simulator and recent applications related to coupled fluid flow and crustal deformations. *Computers & Geosciences* **2011,** *37*, 739–750. Rutqvist, J. The geomechanics of CO_2 storage in deep sedimentary formations. *International Journal of Geotechnical and Geological Engineering* **2012,** *30*, 525–551. Rutqvist, J.; Birkholzer, J.; Cappa, F.; Tsang, C.-F. Estimating maximum sustainable injection pressure during geological sequestration of CO_2 using coupled fluid flow and geomechanical fault-slip analysis. *Energy Conversion and Management* **2007,** *48*, 1798–1807. Rutqvist, J.; Birkholzer, J. T.; Tsang, C. F. Coupled Reservoir-Geomechanical Analysis of the Potential for Tensile and Shear Failure Associated with CO_2 Injection in Multilayered Reservoir-Caprock Systems. *Int. J. Rock Mech. & Min. Sci* **2008,** *45*, 132–143. Rutqvist, J.; Cappa, F.; Rinaldi, A. P.; Godano, M. Modeling of induced seismicity and ground vibrations associated with geologic CO_2 storage, and assessing their effects on surface structures and human perception. *International Journal of Greenhouse Gas Control* **2014,** *24*, 64–77. Rutqvist, J.; Vasco, D.; Myer, L. Coupled reservoir-geomechanical analysis of CO_2 injection and ground deformations at In Salah, Algeria. *Int. J. Greenhouse Gas Control* **2010,** *4*, 225–230. Rutqvist, J.; Wu, Y.-S.; Tsang, C.-F.; Bodvarsson, G. A Modeling Approach for Analysis of Coupled Multiphase Fluid Flow, Heat Transfer, and Deformation in Fractured Porous Rock. *Int. J. Rock Mech. & Min. Sci.* **2002,** *39*, 429-442.

A.8.15 TOUGHREACT

Tool Name	TOUGHREACT
Developer/Owner	Lawrence Berkeley National Laboratory
Tool Type	Reservoir Simulation
Description	TOUGHREACT is a numerical simulation program for chemically reactive non-isothermal flows of multiphase fluids in porous and fractured media, developed by introducing reactive chemistry into the multiphase flow code TOUGH2.
Tool Licensing and Access	The tool is licensed through LBNL at website: https://tough.lbl.gov/software/toughreact/ and distributed via Berkeley Lab Marketplace.
Model Input	Model inputs include hydrological information of the aquifer/reservoir such as porosity, permeability, and geochemical information of the system such as groundwater composition and mineralogical composition.
Model Output	The model generates the spatial and temporal distribution of pressure, temperature, saturation, and concentrations of chemical components.
Risks Behavior Considered	The model simulates the leakage risk and other environmental risk such as the change of groundwater in response to the leakage of CO_2.
Relevant Permitting Phase	For Class VI permit the tool can be used for all the phases ranging from site screening, site characterization, injection to post-injection, especially if geochemical changes are of concern.
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post Injection Site Care and Site Closure Plan
How the Tool is Used	The tool can be used to quantify hydrological and geochemical changes at any phases of the permit in conjunction with site characterization and monitoring.
Last Updated	A major update of the code was done in 2014.
Ongoing Development	The tool has been widely used both domestically and international for many underground engineering applications and has been supported by the scientist from LBNL.
Ease of Use	The tool does not have a graphical user interface, but a graphical interface had been developed by third party. Users does not need computer programming skills to use the tool, but knowledge on the underground hydrology and geochemistry is needed.
Computational Speed	The model has been upgraded for computational efficiency and one of the most efficient codes for simulating multiphase flow and reactive transport. Computation time is usually not a problem, but the simulation can be time consuming if the problem is very big and complicated.
Tool Verification	The tool been verified by analytical solution and testing problems, which is documented in the manual of the code.
Related References	The manual can be found on the website: https://tough.lbl.gov/software/toughreact/

A.8.16 Two-Phase Flow Model (TPFLOW)

Tool Name	TPFLOW (Two-Phase Flow Model)
Developer/Owner	Abdullah Cihan/LBNL
Tool Type	Reservoir Simulation
Description	TPFLOW computes pressure and saturation changes in subsurface by solving the coupled nonlinear partial differential equations for pressure and saturation using the Finite Volume method.
Tool Licensing and Access	The code is accessible through the developer and LBNL. Abdullah Cihan: https://eesa.lbl.gov/profiles/abdullah-cihan/
Model Input	Model geometry, numerical grid (1D, 2D, and 3D Cartesian, or 2D axisymmetric cylindrical coordinates), hydrogeological and two-phase flow properties (relative permeability and capillary pressure functions) in the domain, and initial and boundary conditions, provided through a single input file
Model Output	Time-dependent pressure and saturation as both contour data and observation point data (user-selected). Users can also obtain leakage fluxes at any arbitrary selected points.
Risks Behavior Considered	CO_2 leakage risk
Relevant Permitting Phase	Site screening, injection, and post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan
How the Tool is Used	The tool can be used to estimate evolution of pressure and saturation in subsurface.
Last Updated	The tool was last updated in March 2021.
Ongoing Development	The development was mainly completed, but a user manual needs to be developed. There is no active user community. The code has been used by graduate students and postdocs.
Ease of Use	No user interface. The code uses one input text file and generates output files that can be directly dragged into Tecplot software for plotting the results. The users do not need programing skills, but some basic knowledge about two-phase flow in subsurface and modeling is needed.
Computational Speed	The code is partially parallelized and it may be used to simulate CO_2 migration efficiently. Because the phase changes of CO_2 (sc-liq-gas-ice) and chemical reactions are not included, the code may be computationally more efficient compared to other multiphase simulators taking into account those processes. The code also has a version that can be run as a vertically-integrated model (semi-3D model), which might be used for modeling a single-layer reservoir with varying thickness.
Tool Verification	Verified with analytical solutions, other numerical models and laboratory data. Some of these verifications were documented in the published literature.
Related References	There is currently no published user manual for the code. The following references include either descriptions or applications of the code:

	Cihan, A.; Birkholzer, J. T.; Illangasekare, T. H.; Zhou, Q. A modeling approach to represent hysteresis in capillary pressure-saturation relationship based on fluid connectivity in void space. *Water Resources Research* **2014,** *50*. doi:10.1002/2013WR014280. Cihan, A.; Birkholzer, J. T.; Trevisan, L.; Gonzalez-Nicolas, A.; Illangasekare, T. H. Investigation of representing hysteresis in macroscopic models of two-phase flow in porous media using intermediate scale experimental data. *Water Resources Research* **2017,** *53*, 199–221. doi: 10.1002/2016WR019449. Cihan, A.; Birkholzer, J. T.; Bianchi, M. Optimal Well Placement and Brine Extraction for Pressure Management during CO_2 Sequestration, *International Journal of Greenhouse Gas Control* **2015,** *42*, 175–187. Cihan, A.; Bhuvankar, P.; Birkholzer, J. T. *Risk of wellbore leakage to shallow aquifers in geologic carbon sequestration: Numerical studies on the effects of CO_2 property changes in multilayered systems*; under preparation, 2021. Cihan, A.; Wang, S.; Tokunaga, T. K.; Birkholzer, J. T. The role of capillary hysteresis and pore-scale heterogeneity in limiting the migration of buoyant immiscible fluids in porous media. *Water Resources Research* **2018,** *54*, 4309–4318. González-Nicolás, A.; Trevisan, L.; Illangasekare, T. H.; Cihan, A.; Birkholzer, J. T. Enhancing Capillary Trapping Effectiveness through Proper Time Scheduling of Injection of Supercritical CO_2 in Heterogeneous Formations. *Greenhouse Gases: Science and Technology* **2017,** *7*, 339–352.

A.9 RESOURCE ESTIMATION

Estimating the CO_2 storage capacity of a reservoir is necessary to characterize its potential for GCS. Tools in this category accept general information about a potential storage interval and return an estimate of the quantity of CO_2 that can be stored in the formation.

A.9.1 Storage Prospective Resource Estimation Excel Analysis (CO_2 SCREEN)

Tool Name	CO_2-SCREEN (Storage prospeCtive Resource Estimation Excel aNalysis)
Developer/Owner	National Energy Technology Laboratory: Angela Goodman, Sean Sanguinito, Foad Haeri, Grant Bromhal
Tool Type	Resource Estimation
Description	CO_2-SCREEN (Storage prospeCtive Resource Estimation Excel aNalysis) is a tool developed by the U.S. DOE's NETL to provide prospective carbon storage resource estimates in subsurface formations to establish the scale of carbon capture and storage activities for governmental policy and commercial project decision-making. CO_2-SCREEN is coded in Python with a Java based graphical user interface which provides robust probabilistic estimates within an easy-to-use framework. CO_2-SCREEN is capable of generating prospective carbon storage estimates for various geologic formations including saline, shale, and residual oil zones.
Tool Licensing and Access	Open-source: Can be downloaded from: https://edx.netl.doe.gov/dataset/co2-screen
Model Input	The CO_2-SCREEN tool accepts user inputs for physical parameters and storage efficiency factor terms, which differ as a function of formation type. Physical parameters are geologic reservoir properties (e.g., area, thickness, porosity, etc.) that are used to calculate the total volume of a formation or region of interest while storage efficiency factors (e.g., net-to-total thickness, effective-to-total porosity, etc.) reduce the total volume to only the volume available and accessible to CO_2 storage. The physical parameter data are dependent on formation type based on how CO_2 is stored. CO_2 is stored as a free phase for all formation types (saline, shale, residual oil zones) and required physical parameters include total area, gross thickness, total porosity, and temperature, and pressure of the CO_2 injection depth. Because of the higher clay and organic content in shales, CO_2 can be stored as a sorbed phase. To account for this, additional physical parameters include total organic content, Langmuir slope, and Langmuir y-intercept. In residual oil zones, a significant portion of CO_2 can be stored as a dissolved phase in the residual oil and additional physical parameters include irreducible water saturation, residual oil saturation, and concentration of CO_2 in oil. All physical parameter inputs require mean values, and a standard deviation can be provided to account for uncertainties. The tool automatically calculates density of CO_2 based on pressure and temperature inputs. Efficiency factor ranges are also dependent on formation type. For the most accurate CO_2 storage estimations, it is recommended that region-specific data are used for efficiency factor ranges. Since these data are not always readily available, CO_2-SCREEN has the unique capability to provide users efficiency factor ranges based on reservoir modeling and numerical simulations. For saline and residual oil zone formations, efficiency factors have been simulated for a variety of depositional environments (IEA, 2009). Users can select the depositional environment most relevant to their dataset to auto-populate a set of efficiency factor ranges. For shale formations, well-scale efficiency factors (effective-to-total-porosity and effective-to-total-sorption) were

	simulated as a function of injection time and users can select an injection time to auto-populate these values. These ranges can be further modified or entered manually to account for specific datasets.
Model Output	CO_2-SCREEN is a software tool that is coded in Python with a Java based graphical user interface. CO_2-SCREEN applies user entered data into embedded CO_2 storage equations (developed by the U.S. DOE) and uses Monte Carlo simulation to calculate probability estimates for prospective CO_2 storage capacity. Another key feature of CO_2-SCREEN is its ability to estimate CO_2 storage resources for a gridded formation. Data from multiple wells can be entered for the physical parameters into separate spatially divided grid cells to account for geologic heterogeneity within a single formation. By incorporating specific ranges for storage efficiency factor terms on a "grid cell by grid cell" basis, the tool can provide more localized storage estimates and minimize uncertainties associated with formation heterogeneity.
Relevant Permitting Phase	Site Screening, Site Characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	The CO_2-SCREEN tool provides a user-friendly platform for estimating the prospective CO_2 storage potential of geologic formations at the national-, regional-, basin- and formation-scale. The tool can be applied at the initial screening stages of a project using only limited publicly available geophysical data to provide a preliminary estimate. The tool can be used to refine the estimate and reduce its uncertainty as the project progresses to the commercial scale as site-specific geophysical data become more readily available. It also provides a consistent method to calculate CO_2 storage potential while allowing for direct comparison of prospective CO_2 storage estimates between a variety of organizations including government agencies and independent research studies.
Last Updated	June 28, 2021
Ongoing Development	Yes
Ease of Use	CO_2-SCREEN is a software tool that is coded in Python with a Java based graphical user interface. It is intended to be easy to use and is free to use.
Computational Speed	Simulations take between 30 and 60 seconds to complete.
Tool Verification	No
Related References	Azenkeng, A.; Mibeck, B. A. F.; Kurz, B. A.; Gorecki, C. D.; Myshakin, E. M.; Goodman, A. L.; Azzolina, N. A.; Eylands, K. E.; Butler, S. K. An Image-based Equation for Estimating the CO_2 Storage Resource Capacity of Organic-rich Shale Formations. *International Journal of Greenhouse Gas Control* **2020,** *98*, 103038 Goodman, A.; Sanguinito, S.; Levine, J. Prospective CO_2 Saline Resource Estimation Methodology: Refinement of Existing DOE-NETL Methods Based on Data Availability. *International Journal of Greenhouse Gas Control* **2016,** *54*, 242–249. Goodman, A.; Hakala, A.; Bromhal, G.; Deel, D.; Rodosta, T.; Frailey, S.; Small, M.; Allen, D.; Romanov, V.; Fazio, J.; Huerta, N.; McIntyre, D.; Kutchko, B.; Guthrie, G. U.S. DOE methodology for the development of geologic storage potential for

	carbon dioxide at the national and regional scale. *Int. J. of Greenhouse Gas Control* **2011,** *5*, 952–965. Goodman, A.; Bromhal, G.; Strazisar, B.; Rodosta, T.; Guthrie, W.; Allen, D.; Guthrie, G. Comparison of methods for geologic storage of carbon dioxide in saline formations. *International Journal of Greenhouse Gas Control* **2013,** *18*, 329–342. Levine, J. S.; Fukai, I.; Soeder, D. J.; Bromhal, G.; Dilmore, R. M.; Guthrie, G. D.; Rodosta, T.; Sanguinito, S.; Frailey, S.; Gorecki, D.; Peck, W.; Goodman, A. L. U.S. DOE NETL Methodology for Estimating the Prospective CO_2 Storage Resource of Shales at the National and Regional Scale. *Int. J. of Greenhouse Gas Control* **2016,** *51*, 81–94. Myshakin, E.; Singh, H.; Sanguinito, S.; Bromhal, G.; Goodman, A. Simulated Efficiency Factors for Estimating the Prospective CO_2 Storage Resource of Shales. *International Journal of Greenhouse Gas Control* **2018,** *76*, 24–31. Myshakin, E.; Singh, H.; Sanguinito, S.; Bromhal, G.; Goodman, A. Flow Regimes and Storage Efficiency of CO_2 Injected into Depleted Shale Reservoir. *Fuel* **2019,** *246*, 169–177. Sanguinito, S.; Goodman, A.; Sams, J. CO_2-SCREEN Tool: Application to the Oriskany Sandstone to Estimate Prospective CO2 Storage Resource. *International Journal of Greenhouse Gas Control* **2018**, *75*, 180–188. Sanguinito, S.; Singh, H.; Myshakin, E.; Goodman A.; Dilmore, R.; Grant, T.; Morgan, D.; Bromhal, G.; Warwick, P. D.; Brennan, S. T.; Freeman, P. A.; Karacan, C. O.; Gorecki, C.; Peck, W.; Burton-Kelly, M.; Dotzenrod, N.; Frailey, S.; Pawar, R. U.S. DOE NETL methodology for estimating the prospective CO_2 storage resource of residual oil zones at the national scale. *International Journal of Greenhouse Gas Control* **2020,** *96*, 103006. Sanguinito, S.; Goodman, A.; Haeri, F. *CO_2 Storage prospeCtive Resource Estimation Excel aNalysis (CO_2-SCREEN) User's Manual*; DOE/NETL-2020/2133; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Pittsburgh, PA, 2020; p 36. DOI: 10.2172/1617640.

A.9.2 Offshore CO_2 Saline Storage Calculator

Tool Name	Offshore CO_2 Saline Storage Calculator
Developer/Owner	National Energy Technology Laboratory; Developers: Lucy Romeo, Patrick Wingo, Aaron Barkhurst, Burt Thomas, Kelly Rose
Tool Type	Resource Estimation
Description	The Offshore CO_2 Saline Storage Calculator applies the logic of the Offshore CO_2 Saline Storage (OCSS) Methodology to calculate long-term storage resource (in gigatons) distributions for offshore saline environments. The OCSS Methodology (Cameron et al., 2018) was developed by tailoring the U.S. DOE methodology (Goodman et al., 2016) for offshore environments. The OCSS Methodology accounts for how CO_2 density changes with the overlying water column, and how the unlithified, more porous and permeable sediment behaves differently in marine saline geologic formations. Built in Python 3.7, this stand-alone tool uses all possible combinations of input variables (i.e., reservoir area, height, porosity, efficiency) to calculate storage potential. Furthermore, the tool enables the application of spatial data to define key variables, such as area, while also accounting for setback distances from potential leakage pathways.
Tool Licensing and Access	Desktop version of the tool is available for download on Energy Data eXchange. Citation: Romeo, L.; Wingo, P.; Barkhurst, A.; Thomas, R.; Rose, K. Offshore CO_2 Saline Storage Calculator, 2020. https://edx.netl.doe.gov/dataset/offshore-co2-saline-storage-calculator DOI: 10.18141/1607787
Model Input	Data representing reservoir area, height, porosity, lithology and depositional environment, microscopic and volumetric displacement, and efficiency are needed to run the Calculator. A dataset of interpreted petrophysical well logs was developed and this data was applied (Bean et al., 2020) with Subsurface Trend Analysis™ STA domains representing areas of similar geologic histories (Mark-Moser et al., 2020; Rose et al., 2020) to evaluate geologic storage potential in the Northern Gulf of Mexico. These data are available for further application. Bean, A.; Romeo, L.; Justman, D.; DiGiulio, J.; Miller, R.; Cameron, E.; Rose, K. Petrophysical Well Log Interpretation Dataset, Mar 5, 2020. https://edx.netl.doe.gov/dataset/petrophysical-well-log-interpretation-dataset, DOI: 10.18141/1560053 Mark-Moser, M.; Miller, R.; Rose, K.; Bauer, J. Subsurface Trend Analysis Domains for the Northern Gulf of Mexico; 2020. https://edx.netl.doe.gov/dataset/subsurface-trend-analysis-domains-for-the-northern-gulf-of-mexico doi:10.18141/1606228 Rose, K. K.; Bauer, J. R.; Mark-Moser, M. A systematic, science-driven approach for predicting subsurface properties. *Interpretation* **2020,** *8*, T167–T181. Input Parameters • Data Table – Data table (CSV or TXT file) containing numeric fields associated with inputs. • Net Height – Field from Data Table representing the height (meters, kilometers, feet, or miles) of the sands available for storage beneath a shale sea. • Total Height – Field from Data Table representing the total height (meters, kilometers, feet, or miles) of the reservoir.

	• Lithology and Depositional Environment(s) – A range of porosity efficiency (portion of pore space in the sands available for storage) based on selected lithology and depositional environment(s) (Gorecki et al., 2009).
	• Total Porosity – Field from Data Table representing the total fraction of porosity in the sands.
	• Volumetric Displacement – Field from Data Table representing the fraction of pore space adjacent to the injection point that is contacted by CO_2 (Gorecki et al., 2009); can be based on lithology and depositional environment(s).
	• Microscopic Displacement – Field from Data Table representing the fraction of brine-filled pore volume that can be replaced by CO_2 (Gorecki et al., 2009); can be based on lithology and depositional environment(s).
	• CO_2 Density
	  o Density – Field from Data Table representing CO_2 densities (kilograms per cubic meter) at reservoir mid-depths.
	  or
	  o Temperature at Seafloor – Constant temperature (Celsius or Fahrenheit) at the seafloor of the Total Area of the saline formations.
	  o Temperature Gradient – Subseafloor temperature (Celsius or Fahrenheit) gradient per depth (meters, kilometers, feet, or miles).
	  o Top Reservoir Depth – Field in Data Table representing top reservoir depth(s) (meters, kilometers, feet, or miles) at the base of the sealing shale.
	  o Bottom Reservoir Depth – Field in Data Table representing bottom reservoir depth(s) (meters, kilometers, feet, or miles).
	  o Water Depth
	    ▪ Water Depth Field – Field in Data Table representing water depth(s) (meters, kilometers, feet, or miles).
	    or
	    ▪ Bathymetry Raster – Continuous rater representing water depth (meters, kilometers, feet, or miles).
	    ▪ Latitude – Field in Data Table representing Y coordinate (decimal degrees in geographic coordinate system) of well log location.
	    ▪ Longitude - Field in Data Table representing X coordinate (decimal degrees in geographic coordinate system) of well log location.
	    or
	    ▪ Constant Water Depth – Water depth (meters, kilometers, feet, or miles) to be associated with all reservoir logs.
	• Area
	  o Net Area Field – Field in Data Table representing area(s) (meters-, kilometers-, feet-, or miles-squared) of the offshore saline formations available for storage.
	  o Total Area Field – Field in Data Table representing total area (meters-, kilometers-, feet-, or miles-squared) of the offshore saline formation.
	  or
	  o Spatial Extent – Polygon shapefile representing total area of the offshore saline formation.

	- Leakage Pathway(s) – Subsurface features (point, line, or polygon shapefile(s)) or proxies at the seafloor where if injected CO_2 could migrate upward from the subsurface and into the water column (faults, chemosynthetic communities). - Minimum Buffer Size – Minimum setback distance (meters, kilometers, feet, or miles), will be used to buffer leakage pathway data. - Maximum Buffer Size – Maximum setback distance (meters, kilometers, feet, or miles), will be used to buffer leakage pathway data. - Step Buffer Size – Step sizes (meters, kilometers, feet, or miles) from Minimum Buffer Size to Maximum Buffer Size. <u>Output Parameters</u> - Output Directory – Existing folder to where all outputs will be stored. - Filename – Output file (CSV or TXT) containing variables for all computation combinations. An additional file with "SummaryReport" preceding the Filename, will be exported, which contains count and percentile values for both overall efficiency and storage potential (gigatons). - Distribution Graph Outputs – (Optional) Distribution histograms (PNG) and data used to build histograms (CSV) can be output for any or all variables. Variables to export distribution graphs from include storage resource distribution, area efficiency, porosity efficiency, microscopic displacement, total height, CO_2 density, efficiency, height efficiency, volumetric displacement, total area, and total porosity. - Spatial Outputs – (Optional) Shapefiles representing net area(s) and buffered leakage pathways can be exported if spatial data was provided to run the tool.
Model Output	The tool automatically outputs two files. The first is a table where each record represents a different combination to compute gigatons of storable CO_2 and each field represents a variable (Area Efficiency, Height Efficiency, Porosity Efficiency, Volumetric Displacement, Microscopic Displacement, Saline Efficiency, Total Area (m^2), Total Height(m), Total Porosity (kg/m^3), CO_2 density, and gigatons of storable CO_2. The second automatic output is a summary report containing count and percentiles (10^{th}, $50^{th,}$ 90^{th}) for overall efficiency and CO_2 storage potential. The tool also has a series of optional outputs, including distribution graphs, and spatial data outputs, if applicable. For each distribution graph output, an associated CSV data table with the associated values are also output. In addition, if users select to Calculate CO_2 density values, a distribution histogram by CO_2 phase and associate table will also be automatically output. If spatial data has been used to calculate Net and Total Area, the spatial output options will be made available. These outputs are spatial data layers (shapefiles) representing Net Area or the Buffered Leakage Pathways.
Risks Behavior Considered	Leakage risk
Relevant Permitting Phase	Site Screening, Area of Review and Corrective Action Plan
Class VI Permit Element Addressed	Area of Review
How the Tool is Used	The Offshore CO_2 Saline Storage Calculator can be applied to calculate potential long-term storage distributions for an area of interest. This tool can take information from interpreted petrophysical well logs, reservoir data, leakage pathway data, and regulatory setback distance to quantify resource storage potential for safe saline CO_2 storage.

Last Updated	Desktop Version – February 2021 Online Version – October 2021
Ongoing Development	Yes, this tool is being developed as an online version for integration into GeoCube and the NETL Common Operating Platform.
Ease of Use	The desktop and online versions of the tools have a similar graphical user interface with help information readily accessible. Users do not need any computer programming skills to run the tool, but should have a comprehensive understanding of their input data and the area where they are hoping to calculate storage efficiency for. Moreover, though this Calculator was built specifically for offshore saline environments, it was written in Python using stand-alone libraries, and could be adapted for other regions and scales of interest.
Computational Speed	As a data-driven tool, the more input data results in longer runtimes. The logic of the tool runs all possible variable combinations for efficiency, then again to calculate total storage values. Furthermore, the runtime for the desktop tool is dependent on local computational capabilities. Running the tool for around 50 to 100 data records at a time is recommended. The tool is capable of handling more, though the runtime will increase exponentially substantially.
Tool Verification	Outcomes of this data-driven tool can currently be verified using data comparison, comparison to similar studies, and peer-review. Further validation can be assessed following the practice of long-term geologic saline storage of CO_2, which is not yet available for the northern Gulf of Mexico.
Related References	Method and Calculator Papers: Cameron, E.; Thomas, R.; Bauer, J.; Bean, A.; DiGiulio, J.; Disenhof, C.; Galer, S.; Jones, K.; Mark-Moser, M.; Miller, R.; Romeo, L.; Rose, K. *Estimating Carbon Storage Resources in Offshore Geologic Environments*; NETL-TRS-14-2018; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Albany, OR, 2018; p 32. DOI: 10.18141/1464460. https://edx.netl.doe.gov/dataset/estimating-carbon-storage-resources-in-offshore-geologic-environments Goodman, A.; Sanguinito, S.; Levine, J. S. Prospective CO_2 saline resource estimation methodology: Refinement of existing US-DOE-NETL methods based on data availability. *International Journal of Greenhouse Gas Control* **2016,** *54*, 242–249. Gorecki, C. D.; Sorensen, J. A.; Bremer, J. M.; Knudsen, D.; Smith, S. A.; Steadman, E. N.; Harju, J. A. Development of storage coefficients for determining the effective CO_2 storage resource in deep saline formations. In SPE International Conference on CO_2 Capture, Storage, and Utilization; OnePetro, 2009. Romeo, L.; Thomas, R.; Mark-Moser, M.; Bean, A.; Bauer, J.; Rose, K. Data-driven spatially informed offshore carbon storage efficiency and storage resource methodology. *International Journal of Greenhouse Gas Control*, in preparation. This tool is featured in: Bauer, J.; Justman, D.; Mark-Moser, M.; Romeo, L.; Creason, C.G.; Rose, K. Exploring beneath the basemap. Wright, D. J., Harder, C., Ed.; In *GIS for Science: Applying Mapping and Spatial Analytics*, Vol 2; Esri Press: Redlands, CA, 2020; pp. 51–67. https://www.gisforscience.com/chapter5/

A.10 RISK ASSESSMENT

Risk assessment is a necessary element of the Class VI permitting process. Tools in this category are used to identify and/or quantify the risks associated with geologic carbon storage.

A.10.1 FEMA HAZUS

Tool Name	FEMA Hazus
Developer/Owner	FEMA open-source
Tool Type	Risk Assessment
Description	FEMA HAZUS provides standardized tools and data for estimating risk from earthquakes, floods, tsunamis, and hurricanes. Hazus models combine expertise from many disciplines to create actionable risk information that increases community resilience. Hazus software is distributed as a GIS-based desktop application with a growing collection of simplified open-source tools. Risk assessment resources from the Hazus program are always freely available and transparently developed.
Tool Licensing and Access	Open-source: https://www.fema.gov/flood-maps/products-tools/hazus
Model Input	GIS data, land use, maps, surface feature maps
Model Output	Risk analysis
Risks Behavior Considered	Leakage, storage resource, faults, fractures, boundaries
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Financial Assurance Demonstration, Testing and Monitoring Plan, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan
Last Updated	2021
Ongoing Development	Maintained by FEMA
Related References	https://www.fema.gov/flood-maps/products-tools/hazus

A.10.2 National Risk Assessment Partnership Open-Source Integrated Assessment Model (NRAP-Open-IAM)

Tool Name	The NRAP Open-Source Integrated Assessment Model (NRAP-Open-IAM)
Developer/Owner	National Risk Assessment Partnership, Phase II
Tool Type	Risk Assessment
Description	NRAP-Open-IAM is an open-source Integrated Assessment Model (IAM) developed by the National Risk Assessment Partnership (NRAP) to perform risk assessment for geologic CO_2 storage (GCS). The goal of NRAP-Open-IAM is to extend beyond risk assessment into risk management, containment assurance, and decision support. NRAP-Open-IAM builds on many years of NRAP tool development for risk assessment, including the NRAP-IAM-CS also developed by the NRAP project. The NRAP-Open-IAM builds on the functionality of NRAP-IAM-CS within an open-source Python framework allowing NRAP-Open-IAM to: 1) take advantage of standard Python libraries and other open-source analytical libraries written in Python; 2) be applied on multiple platforms; 3) have more flexible options of selecting modules for a specific study; and 4) give advanced users the option to modify the IAM to fit their need as well as enhancing the potential for community contributions to the software. The implementation of the reduced-order models and analytical tools within the NRAP-Open-IAM makes the risk assessment process computationally efficient enough to simulate an operational CO_2 storage site, potential events and various scenarios in a probabilistic/ensemble manner. The NRAP-Open-IAM is equipped with capabilities to: 1) inform monitoring design; 2) assess model concordance to measured field data; 3) evaluate mitigation alternatives; and 4) provide probabilistic risk assessment and update the risk as new data becomes available.
Tool Licensing and Access	Open-Source. Can be downloaded from: https://edx.netl.doe.gov/nrap/nrap-open-iam/ https://gitlab.com/NRAP/OpenIAM
Model Input	NRAP-Open-IAM models are created by linking reduced-order representations of sophisticated component models together into a complete GCS system. Each component model describes the structure or flow behavior in a critical element of a GCS site. Component models are modular and are designed to be interchangeable. Users build NRAP-Open-IAM models by selecting component models and specifying inputs that represent the characteristics of their GCS site. Inputs to NRAP-Open-IAM component models can either be specified as a single value or a range of values. If a range of values is identified for some model inputs, these values will be randomly sampled when stochastic simulations are run. The component models of NRAP-Open-IAM are organized into four major categories: • Stratigraphy. The stratigraphy component details the structure of the GCS system. Stratigraphy inputs include the number of shale and aquifer layers in the model, the thicknesses of these layers, and the thickness of the reservoir. • Reservoir. The reservoir component describes the conditions in the reservoir during the simulation time period. NRAP-Open-IAM is not a reservoir simulator. However, users can simulate a simplified CO_2 injection using the simple and analytical reservoir components. Inputs for these models include reservoir characteristics (permeability, porosity, thickness, extent), CO_2 and brine characteristics (density, viscosity), and injection rate. More sophisticated reservoir behavior can be included in the NRAP-Open-IAM by including simulation results from a high-fidelity numerical simulator as a look up table.

	• Leakage pathway. The leakage pathway component simulates the upward flow of CO_2 and brine out of the reservoir. NRAP-Open-IAM contains multiple interchangeable leakage pathway components that can simulate flow through cemented and uncemented wells, seals, and faults. Users must specify the properties of the leakage pathway, which vary depending on its type. For example, the inputs for the cemented wellbore component are the well radius, the permeability of the well cement, and the permeability of potential thief zones. • Receptor. The receptor component simulates either the flow of CO_2 and brine in an aquifer (shallow or deep) or the atmosphere. Aquifer component models consider geochemical reactions and predict the size of CO_2 and brine impact plumes. A number of aquifer components exist that represent different types of aquifers (e.g., carbonate, deep alluvium). Model inputs for each aquifer component are different but typically include general characteristics of the formation, such as its thickness, depth, porosity, permeability, and anisotropy. The atmosphere component simulates CO_2 dispersion after leakage out of the ground. Inputs for the atmosphere component include ambient pressure and temperature, wind velocity, CO_2 source temperature, and coordinates of potential receptors.
Model Output	Outputs are created separately by each component of an NRAP-Open-IAM model: • Reservoir. The outputs of the simple and analytical reservoir component models are the pressure at the top of the reservoir, the CO_2 saturation, and the mass of CO_2 in the reservoir. • Leakage pathway. Outputs from each leakage pathway component include CO_2 and brine leakage rates to any of the specified overlying aquifers. • Receptor. Outputs for aquifer component models typically include impact plume dimensions (radius in x, y, and z directions) for various metrics including: pH, total dissolved solids, pressure, and dissolved CO_2. The atmosphere component model outputs are flags at receptors indicating whether CO_2 concentrations have exceeded a pre-defined critical value and the critical downwind distance from the source. Component models in NRAP-Open-IAM are linked so the outputs from one component can serve as the inputs to another. However, outputs from any component model used in a simulation can be exported. Simulations in NRAP-Open-IAM are run in either a forward (one realization) or stochastic (multiple realization) manner. Outputs for all model realizations can be exported at the end of a simulation.
Risks Behavior Considered	Leakage risk/containment assurance
Relevant Permitting Phase	Site Screening, Site Characterization, Injection Operations, Post-Injection Closure
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan
How the Tool is Used	NRAP-Open-IAM is generally used in conjunction with a high-fidelity reservoir simulation software. Outputs from reservoir simulations are brought in to NRAP Open-IAM as lookup tables and used as a basis for system models that simulate leakage at the site. The tool is useful for: 1) characterizing leakage risks for a proposed injection plan, 2) calculating a risk-based area of review, 3) justifying the length of a post-injection site care period, and 4) evaluating various risk mitigation plans.
Last Updated	May 2021

Ongoing Development	Yes
Ease of Use	NRAP-Open-IAM is written in the widely used Python programming language. Users with computer programming experience can access the complete functionality of NRAP-Open-IAM. A graphical user interface is also available for NRAP Open-IAM that allows users without computer programming experience to access the base functionality of the code.
Computational Speed	NRAP-Open-IAM models are comprised of lookup tables, reduced-order models, and analytical models than can be run concurrently on different processors (in parallel). It was intentionally designed for computational efficiency to enable the stochastic simulation of thousands of model realizations.
Tool Verification	The component models of NRAP-Open-IAM have been verified. Details of verification are provided here: https://gitlab.com/NRAP/OpenIAM
Related References	Bacon, D. H.; Yonkofski, C. M. R.; Brown, C. F.; Demirkanli, D. I.; Whiting, J. M. Risk-based post injection site care and monitoring for commercial-scale carbon storage: Reevaluation of the FutureGen 2.0 site using NRAP-Open-IAM and DREAM. *International Journal of Greenhouse Gas Control* **2019,** *90*, 102784. Harp, D. R.; Curtis M. Oldenburg, C.M.; Pawar, R. A metric for evaluating conformance robustness during geologic CO_2 sequestration operations. *International Journal of Greenhouse Gas Control* **2019,** *85*, 100–108. Lackey, G.; Vasylkivska, V.; Huerta, N.; King, S.; Dilmore, R. (2019), Managing well leakage risks at a geologic carbon storage site with many wells. *International Journal of Greenhouse Gas Control* ***2019***, *88*, 182–194. https://doi.org/10.1016/j.ijggc.2019.06.011 Vasylkivska, V.; Lackey, G.; Zhang, Y.; Bacon, D., Chen, B., Mansoor, K., Yang, Y.; King, S.; Dilmore, R.; Harp, D. NRAP-Open-IAM: A Flexible Open Source Integrated Assessment Model for Geologic Carbon Storage Risk Assessment and Management. *Environmental Modeling & Software* **2021,** *143*, 105114. https://doi.org/10.1016/j.envsoft.2021.105114

A.10.3 Spatially Integrated Multivariate Probabilistic Assessment (SIMPA)

Tool Name	SIMPA (Spatially Integrated Multivariate Probabilistic Assessment) Tool
Developer/Owner	National Energy Technology Laboratory
Tool Type	Risk Assessment
Description	SIMPA Tool is a Python-based fuzzy logic tool designed to help assess the likelihood of fluid and/or gas migration pathways throughout the subsurface. The SIMPA tool helps users develop and apply fuzzy logic to various datasets to construct knowledge-based inferential rules that reduce uncertainty and results in a visual representation depicting the likelihood of potential fluid and/or gas migration pathways. SIMPA results spatially describe the potential magnitude and extent of natural and anthropogenic subsurface pathways, for areas with little or no data, to help evaluate potential subsurface hazards to improve storage assessments and critical information for improving industry decisions related to the use of various CCS methods and technologies.
Tool Licensing and Access	Creative Commons Attribution – available for download on EDX. https://edx.netl.doe.gov/dataset/simpa-tool
Model Input	Any number of rasterized coverage layers associated with surface or subsurface risks and hazards One or more sets of fuzzy logic rules (can be authored in tool) One or more sets of combinatorial/output rules (can be authored in tool)
Model Output	Any number of output raster layers, whose composition and count are dependent on the fuzzy logic and output rules applied An output raster recording the number of no-data values found at a given pixel coordinate A .csv containing the above information in a tabular form
Risks Behavior Considered	Tool helps identify areas with high structural complexity and a greater likelihood for leakage pathways. This information can aid in planning and permitting efforts, as well as support human health and environmental risk mitigation efforts.
Relevant Permitting Phase	Primarily designed for site screening, but with additional information could support site characterization and post-injection
Class VI Permit Element Addressed	Site Characterization, Site Characterization, Area of Review and Corrective Action Plan, Testing and Monitoring Plan, Post-Injection Site Care and Site Closure Plan
How the Tool is Used	Tool could be used to understand risks associated with geologic structure (faults, fractures, formation thickness and extents), water resources (aquifers, water wells), and legacy oil and gas well infrastructure
Last Updated	April 16, 2020
Ongoing Development	The tool has limited support for addressing minor issues. Current user community is predominately within DOE.
Ease of Use	A graphical user interface is offered, along with tool support to help users determine and set fuzzy logic inferential rules to produce model outputs. Experience with geospatial data, especially raster data formats is preferred.
Computational Speed	SIMPA's processing steps are SIMD-style algorithms and are designed to be run on any number of threads and CPU cores in parallel. The performance increases dramatically as

	the number of pixels gets larger when compared to running serially. For a problem with 27,335 pixels, the average parallel run takes under a minute on the same hardware where a serial/single-threaded version takes over 10 minutes to run. Theoretically, there may be computational speed limits, but they have not been hit yet.
Tool Verification	The fuzzy logic portions have been tested enough for confidence in its use. The tool is general purpose enough that scenario-specific validation will depend on the data being used, and the rules being applied.
Related References	SIMPA Tool: https://edx.netl.doe.gov/dataset/simpa-tool SIMPA Publication: https://www.sciencedirect.com/science/article/pii/S0191814120300857 Use case datasets: structural and wellbore: https://edx.netl.doe.gov/dataset/oklahoma-structural-complexity-data

A.10.4 The Evidence Support Logic Application (TESLA)

Tool Name	The Evidence Support Logic Application (TESLA)
Developer/Owner	Quintessa
Tool Type	Risk Assessment
Description	The technique of Evidence Support Logic implemented in Quintessa's TESLA software is intended to support decision-makers and modelers in their sense-making when faced with extensive information processing requirements. In summary, evidence support logic involves systematically breaking down the question or hypothesis under consideration into a logical hypothesis model the elements of which expose basic judgments and opinions relating to the quality of evidence associated with a particular interpretation or proposition, in addition to establishing the level of confidence that can be placed in the relevant judgments. By independently evaluating confidence "for" and "against" propositions on the basis of evidence, uncertainty (and/or conflict) is captured and the sensitivity of the results to that uncertainty can be evaluated.
Tool Licensing and Access	Commercial: https://www.quintessa.org/software/downloads-and-demos/tesla-2.1.1
Model Input	A logical hypothesis model, sources of evidence for these hypotheses, uncertainty
Model Output	Confidence in the inputted hypotheses (Ratio plot, Tornado plot, Tree display, Flow lines)
Risks Behavior Considered	Leakage, storage resource, faults, fractures, and any other risks at a GCS site that a user defines
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Financial Assurance Demonstration, Emergency and Remedial Response Plan
Last Updated	2012
Ongoing Development	Maintained by Quintessa
Related References	https://www.quintessa.org/software/downloads-and-demos/tesla-2.1.1

A.11 SEISMIC AND GEOMECHANICAL RISK

Underground injection of CO_2 causes a pressure increase that can increase the risk of triggering seismic events or inducing fractures in existing formations. Tools in this category are used to characterize the seismic and geomechanical risks associated with underground CO_2 injection.

A.11.1 Athena Data Management

Tool Name	Athena Data Management System
Developer/Owner	Nanometrics
Tool Type	Seismic and Geomechanical Risk
Description	The Athena Data Management System allows one to browse up-to-date event catalogues, view all recorded event source parameters and waveforms, select and download sections of the catalogue, plot frequency/magnitude relationships for event clusters, examine maps showing distribution of ground motions from each recorded event and track network seismicity rate to manage risks associated with induced seismicity in real time. It is integrated with real-time monitoring that tracks probabilistic estimates of future maximum magnitude and seismicity rate.
Tool Licensing and Access	Commercial: Contact Nanometrics at https://www.nanometrics.ca/services/passive-seismic-monitoring/athena-data-management-system Open-source version called ORION being developed as part of NRAP and SMART
Model Input	High-precision catalog of seismic events, magnitudes, injection rate
Model Output	Short-term seismic hazard assessment
Risks Behavior Considered	Seismic Hazard
Relevant Permitting Phase	Monitoring plan and risk mitigation
Class VI Permit Element Addressed	Testing and Monitoring Plan, Emergency and Remedial Response Plan, Stimulation Program
How the Tool is Used	It is a service that is provided to operators. The operator is given a link to look at the dashboard, but there is no ability for users to "interact" or change properties.
Ongoing Development	Yes
Ease of Use	Comes with a graphical user interface. Programming skills may not be needed to learn the software.
Computational Speed	It is reasonably fast and near real time
Related References	https://www.nanometrics.ca/services/passive-seismic-monitoring/athena-data-management-system

A.11.2 Fault Slip Potential

Tool Name	Fault Slip Potential
Developer/Owner	Stanford Center for Induced and Triggered Seismicity and ExxonMobil/XTO
Tool Type	Seismic and Geomechanical Risk
Description	Fault slip potential (FSP) is a software to predict the probability of fault slip to occur in response to pore pressure increase due to injection.
Tool Licensing and Access	Get added to the mailing list and follow instructions for downloading: https://scits.stanford.edu/software
Model Input	Stress model (stress gradients, or A-phi model parameters), fault interpretation (location, length, strike, kinematics), hydrological model (reservoir thickness, porosity, permeability, or user defined model specifying pressure increase), injection well specifications (location, injection volume), uncertainty (distribution of the parameters)
Model Output	Probability of faults to slip
Risks Behavior Considered	Seismic risk
Relevant Permitting Phase	Site screening, Pre-injection, Monitoring
Class VI Permit Element Addressed	Site Screening, Site Characterization, Testing and Monitoring Plan, Stimulation Program
How the Tool is Used	See description above
Ongoing Development	Yes
Ease of Use	Comes with a graphical user interface. Programming skills may not be needed to learn the software.
Related References	Walsh, F. R.; Zoback, M. D. Probabilistic assessment of potential fault slip related to injection-induced earthquakes: Application to north-central Oklahoma, USA. *Geology* **2016,** *44*, 991–994. doi: https://doi.org/10.1130/G38275.1 https://scits.stanford.edu/software https://scits.stanford.edu/file/fullmeetingvideomp4

A.11.3 RiskCat

Tool Name	RiskCat
Developer/Owner	Bill Foxall and Jean Savy
Tool Type	Seismic and Geomechanical Risk
Description	RiskCat determines the seismic hazard and risk based on seismic catalogs. RiskCat uses SynHaz to determine the ground motion internally to determine the risk at a specified location.
Tool Licensing and Access	The tool is available on gitlab: https://gitlab.com/NRAP/RiskCat
Model Input	Seismic catalogs (timing, magnitude, location) and seismic source parameters if possible
Model Output	Hazard and risk curves, i.e., probabilities of exceeding certain values of accelerations or risk values
Risks Behavior Considered	Seismic hazard and risk
Relevant Permitting Phase	With simulated catalogs, the tool can be used during the site screening. With recorded catalogs, the tool can determine the increase of hazard and risk during the injection and post-injection.
Class VI Permit Element Addressed	Site Screening, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan
How the Tool is Used	With simulated catalogs, the tool can be used during the site screening. With recorded catalogs, the tool can determine the increase of hazard and risk during the injection and post-injection.
Last Updated	It was uploaded to GitLab in 2020
Ongoing Development	Support for the tool exists in theory, but it is not always straightforward
Ease of Use	Basic knowledge of seismic catalogs and risk calculations are needed to run the tool. Knowledge of how to manipulate input files is needed.
Computational Speed	Model is not optimized for speed
Tool Verification	No
Related References	Gitlab includes a manual: https://gitlab.com/NRAP/RiskCat

A.11.4 RSQSim

Tool Name	RSQSim
Developer/Owner	James H. Dieterich and Keith Richards-Dinger at UC Riverside
Tool Type	Seismic and Geomechanical Risk
Description	RSQsim is 3D boundary-element code incorporating rate-state fault friction to simulate long sequences of earthquakes in interacting fault systems. It can simulate seismic events based on the interaction of tectonic loading, stress changes due to earthquake occurrence, and external pressure and/or stress histories (e.g., those that arise from anthropogenic sources). The external pressure and/or stress histories must be calculated externally and provided to RSQSim by means of an addition input file containing the pressure and/or stress for every fault element as a function of time.
Tool Licensing and Access	A github distribution is in the works. It is currently not publicly available, only through contact with the developers. https://profiles.ucr.edu/james.dieterich https://profiles.ucr.edu/app/home/profile/keithrd
Model Input	The primary input parameters: Fault constitutive/material parameters (including rate-state parameters, absolute shear and normal stresses, elastic moduli, a fault model, and long-term average slip rates for all fault elements). In the simplest form, a fault file should contain the x, y, z location of the centers of the fault elements, strike, dip, rake, and slip rate for each element. The RSQSim source code includes scripts to prepare fault models based on standardized input in the UCERF3 fault model format (based on fault surface trace information) or planar fault structures (including those with fractal roughness or segmentation). Faults can be discretized into rectangular to triangular elements that better represent surfaces with complex geometries. RSQSim also accepts spatially variable constitutive and/or material parameters provided via an input file with a value for each fault element. External pressure and/or stress histories should be provided in a similar fashion.
Model Output	RSQSim produces a seismic catalog with occurrence times, magnitudes, rupture area, stress drop, event location, seismic moment, and slip per fault element. Additional information is also provided for the entire fault system at user-specified intervals. This information includes the shear and normal stress, slip speed, and slip-state evolution.
Risks Behavior Considered	Induced and natural seismicity hazard estimation
Relevant Permitting Phase	Site screening, pre-injection, operational management
Class VI Permit Element Addressed	Site Screening, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan, Stimulation Program
How the Tool is Used	RSQSim uses site-specific (local and/or basin-scale) reservoir, flow, material, fault location/geometry, and constitutive parameters and external pressure/stress history to compute the seismic response to the operation.
Last Updated	RSQSim is actively undergoing development
Ongoing Development	RSQSim is actively undergoing development

Ease of Use	The installation of the tool and the tool itself require programming skills. RSQSim is run on the command line or can be executed through user-generated wrappers in their preferred programming language. Built-in postprocessing scripts are written in R. RSQSim requires expert-level user knowledge.
Computational Speed	Computational costs scale with the number of fault elements. RSQSim is highly-parallelized (via openMPI) and optimized to run on super-computer platforms.
Tool Verification	https://pubs.geoscienceworld.org/ssa/srl/article-abstract/83/6/983/315277/RSQSim-Earthquake-Simulator
Related References	https://pubs.geoscienceworld.org/ssa/srl/article-abstract/83/6/983/315277/RSQSim-Earthquake-Simulator Kroll, K. A.; Cochran, E. S. Stress Controls Rupture Extend and Maximum Magnitude of Induced Earthquakes. *Geophysical Research Letters* **2021**. DOI: 10.1029/2020GL092148. Kroll, K. A.; Buscheck, T. A.; White, J. A.; Richards-Dinger, K. B. Testing the Efficacy of Active Pressure Management as a Tool to Mitigate Induced Seismicity. *International Journal of Greenhouse Gas Control* **2019**. Kroll, K. A.; Richards-Dinger, K. B.; Dieterich, J. H. 2017. Sensitivity of Induced Seismic Sequences to Rate-and State- Frictional Processes. *Journal of Geophysical Research: Solid Earth* **2017,** *122*. Dieterich, J. H.; Richards-Dinger, K. B.; Kroll., K. A. Modeling Injection- induced Seismicity With the Physics-based Earthquake Simulator RSQSim. *Seismological Research Letters* **2015,** *86*, 1102-1109.

A.11.5 Seismogenic Index Model

Tool Name	Seismogenic Index Model
Developer/Owner	The theory is developed by Shapiro and collaborators. Codes for the model have been developed by different people.
Tool Type	Seismic and Geomechanical Risk
Description	Seismogenic index characterizes the seismic response of a rock to a unit volume of injected fluid. It has been used by Nanometrics in their Athena Seismicity Portal and in various publications demonstrating the on-going hazard evolution in areas like Oklahoma
Tool Licensing and Access	Open-source: https://github.com/amignan/rseismTLS https://github.com/RyanJamesSchultz/SeismogenicIndex
Model Input	Seismic catalog and an injection rate
Model Output	Estimate of short-term forecast of the number of seismic events and seismic hazard
Risks Behavior Considered	Seismic Hazard
Relevant Permitting Phase	Monitoring plan and risk mitigation
Class VI Permit Element Addressed	Site Screening, Post-Injection Site Care and Site Closure Plan, Emergency and Remedial Response Plan, Stimulation Program
How the Tool is Used	Requires expert user interaction with R and/or MATLAB
Last Updated	The Github accounts listed above were last updated in 2020 and 2018, respectively
Ongoing Development	Unknown
Ease of Use	Code is in R or Matlab, some level of programming experience would be needed
Computational Speed	Can be run in real-time, provided that a good seismicity catalog exists
Tool Verification	There are publications on the model, not sure about tool implementation. The github site has some readme files about the code.
Related References	Shapiro, S. A.; Dinske, C.; Langenbruch, C.; Wenzel, F. Seismogenic index and magnitude probability of earthquakes induced during reservoir fluid stimulations. *The Leading Edge* **2010,** *29*, 304–309. doi: https://doi.org/10.1190/1.3353727

A.11.6 Short-Term Seismic Forecasting Tool (STFS)

Tool Name	Short-Term Seismic Forecasting Tool (STSF)
Developer/Owner	Corinne Layland-Bachmann at LBNL
Tool Type	Seismic and Geomechanical Risk
Description	The Short-Term Seismic Forecasting (STSF) tool uses site-specific catalogs of measured seismicity to forecast future event frequency over the short term. The STSF tool uses a model developed for the decay of aftershocks of large seismic events to determine the event rate in future time bins. This model is adapted with a term to modify the background seismicity rate above a pre-determined magnitude threshold as a function of injection-related parameters (e.g., injection rate or bottom-hole pressure). This injection-related seismicity forecasting capability can be a valuable tool to complement stoplight approaches for induced seismicity risk planning and permitting.
Tool Licensing and Access	Tool is available on EDX: https://edx.netl.doe.gov/nrap/short-term-seismic-forecasting-stsf/
Model Input	Seismic catalog (timing and magnitude at a minimum), injection parameter (such as injection rate, downhole pressure, etc.)
Model Output	Seismicity rates for given time and magnitude bins
Risks Behavior Considered	Induced seismicity
Relevant Permitting Phase	Injection, post-injection
Class VI Permit Element Addressed	Testing and Monitoring Plan, Stimulation Program
How the Tool is Used	Aid decision-making during active injection
Last Updated	2018
Ongoing Development	Tool is being integrated into a bigger dashboard, tool is still being supported, tool has active users
Ease of Use	Tool runs as a graphical user interface, but only on Linux and Mac computers. Can be used with a pearl script for more advanced users.
Computational Speed	Speed is not optimized. Steps can take from seconds to minutes and a whole simulation depends on the problem size.
Tool Verification	Not the tool, but the method has been verified in Bachmann et al. (2011)
Related References	Manual: https://edx.netl.doe.gov/dataset/short-term-seismic-forecasting-stsf-reduced-order-model-rom-tool-users-guide-version-2016-11-1-0-4 Bachmann, C. E.; Wiemer, S.; Woessner, J.; Hainzl, S. Statistical analysis of the induced Basel 2006 earthquake sequence: introducing a probability-based monitoring approach for Enhanced Geothermal Systems. *Geophysical Journal International* **2011,** *186*, 793–807.

A.11.7 State of Stress Analysis Tool (SOSAT)

Tool Name	State of Stress Analysis Tool (SOSAT)
Developer/Owner	NRAP/PNNL/Jeff Burghardt
Tool Type	Seismic and Geomechanical Risk
Description	The State of Stress Analysis Tool (SOSAT) is a Python package that helps analyze the state of stress in the subsurface using various types of commonly available characterization data such as well logs, well test data such as leakoff and minifrac tests, regional geologic information, and constraints on the state of stress imposed by the existence of faults and fractures with limited frictional shear strength. It employs a Bayesian approach to integrate these data into a probability density function for the principal stress components.
Tool Licensing and Access	The tool is publicly available. There is a version with a GUI accessible at: https://edx.netl.doe.gov/nrap/state-of-stress-analysis-tool-sosat/ And there is an open-source Python library available at: https://github.com/pnnl/SOSAT The Python library has more features, but currently no graphical user interface.
Model Input	Well logs, well tests, regional stress observations
Model Output	Probability distribution for the state of stress at a point in the subsurface, as well as a probability estimate for the risk of hydraulic fracturing or fault activation at a point as a function of pore pressure
Risks Behavior Considered	Leakage by hydraulic fracturing or fault slip in sealing formations, and induced seismicity
Relevant Permitting Phase	Class VI site characterization and injection
Class VI Permit Element Addressed	Site Characterization, Stimulation Program
How the Tool is Used	The tool would be used to assemble all geomechanical characterization data for a site into a probabilistic estimate of the state of stress, which can then be used to estimate the probability of tensile or shear failure of caprock, which can be used to determine the maximum safe injection pressure. The tool could also be used to evaluate probability of fault activation, on known faults or on an assumed unknown critically oriented fault, which is useful for evaluating the risk of induced seismicity.
Last Updated	The GitHub site hosts a development branch and tagged releases. The repository has a set of quality control checks that are evaluated with every update and new tests are regularly written as new features are added. The last tagged release was April 26, 2021.
Ongoing Development	The tool is still under active development. There is a user community forum on the NETL EDX site, and support from the developer is available.
Ease of Use	The graphical user interface version has fewer features, but it has a user's manual with examples and a description of how to choose inputs and use outputs. The user would need some level of familiarity with geology and geomechanics, but not expert level knowledge. The GitHub Python library has documentation and examples but requires a basic level of familiarity with Python.

Computational Speed	The calculations at each point only take a few minutes. With the Python library it is possible to construct depth profiles and 2D maps, in this case each spatial location requires a few minutes so that calculations could take an hour or so.
Tool Verification	There are continuous integration tests that check accuracy and consistency of results as the tool is updated. A few of these compare against analytical solutions, but in other cases where statistical sampling techniques (rejection sampling, Markov Chain Monte Carlo) are used there are no analytical solutions, so the tests check for changes in the results introduced by code modifications.
Related References	Appriou, D. *Assessment of the geomechanical risks associated with CO_2 injection at the FutureGen 2.0 Site;* PNNL-28657; Pacific Northwest National Laboratory, Richland, WA, 2019. https://www.pnnl.gov/publications/assessment-geomechanical-risks-associated-co2-injection-futuregen-20-site Burghardt, J. A.; Appriou, D. State of Stress Uncertainty Quantification and Geomechanical Risk Analysis for Subsurface Engineering. In Proceedings of the 55st US Rock Mechanics / Geomechanics Symposium; paper number ARMA-2021-2129; 2021. https://onepetro.org/ARMAUSRMS/proceedings-abstract/ARMA21/All-ARMA21/ARMA-2021-2129/468335 Burghardt, J. Geomechanical Risk Assessment for Subsurface Fluid Disposal Operations. *Rock Mechanics and Rock Engineering* **2018,** *51,* 2265–2288.

A.12 WELL TEST AND LOG INTERPRETATION

A variety of well logging and testing techniques exist that provide insight into the characteristics of subsurface formations. Tools in this category are used to interpret and organize diverse well testing and logging information.

A.12.1 IHS WellTest

Tool Name	IHS WellTest
Developer/Owner	IHS/Fekete
Tool Type	Well Test and Log Interpretation
Description	Software for conducting gas and oil pressure transient analysis and serves as an everyday well test data interpretation tool
Tool Licensing and Access	Commercial license: https://ihsmarkit.com/products/welltest-reserve-pta-software.html
Model Input	Well test pressure, flow rates, reservoir information
Model Output	Reservoir parameters, permeability, porosity, transmissivity, reservoir features, injection pressures
Risks Behavior Considered	Injectivity, leakage, storage resource, faults, fractures, boundaries
Relevant Permitting Phase	Site characterization, monitoring, operations, closure
Class VI Permit Element Addressed	Site Characterization, Area of Review and Corrective Action Plan, Financial Assurance Demonstration, Well Construction Details, Testing and Monitoring Plan, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan
Last Updated	Routine updates
Ongoing Development	Commercial, regular updates
Related References	https://ihsmarkit.com/products/welltest-reserve-pta-software.html

A.12.2 Interactive Petrophysics (IP)

Tool Name	Interactive Petrophysics (IP)
Developer/Owner	Lloyd's Register. Starting in 1760, Lloyd's Register is one of the world's leading providers of professional services for engineering and technology.
Tool Type	Well Test and Log Interpretation
Description	IP offers a complete, cost-effective industry-standard solution to detailed formation evaluation (porosity, permeability, capillary pressure, fluid saturation, and volumetrics) using deterministic, probabilistic, and machine learning approaches. IP is a very popular petrophysical data processing and interpretation software in the energy industry. It is robust, stable, and user-friendly. It is fully customizable and external codes (e.g., Python) can be imported into it. As per IP website, it is used in >85 countries by >500 companies and >107 universities.
Tool Licensing and Access	Lloyd's Register. Commercial license: https://www.lr.org/en-us/ip-well-analysis-software/
Model Input	Any kind of open hole and cased hole wireline logs, logging-while-drilling logs, rock core data (porosity, permeability, saturation, geomechanics), core images, and previous user interpretations, etc. It offers analysis of pore pressure, wellbore stability, casing and cement quality, and live analysis of wellsite log data.
Model Output	Robust multi-well processing and interpretation, and customizable visualization of formation lithology, clay volume, total porosity, effective porosity, fluid saturation, geomechanical properties, rock physics, fractures, saturation height, and uncertainties. IP offers Monte Carlo simulation for reservoir properties used in volumetrics calculation. In addition, IP's machine learning module offers classification of rock types and prediction of missing curves.
Risks Behavior Considered	Monte Carlo simulation of uncertainty analysis of rock and fluid properties
Relevant Permitting Phase	Site screening (very relevant), site characterization (very relevant), injection, post-injection
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	User imports petrophysical log and core data and analyzes the caprock and reservoir properties in both deterministic and probabilistic approaches. The derived properties are then used in volumetric calculations. The tool also provides Tornado charts showing the sensitivities of all model input.
Last Updated	2021
Ongoing Development	The tool is robust and stable. The company regularly updates the software with new modules and approaches.
Ease of Use	The tool has a user-friendly graphical user interface (including 1D, 2D, and 3D plots). The users do not need any computer programming skills. Interested and advanced users can import their codes (e.g., Python) into this software and run their own algorithms for 1,000s of wells. It offers 24/7 customer support.
Computational Speed	IP is very fast, and it does not take more than a few seconds for advanced petrophysical analysis.

Tool Verification	Results are compared with rock core data inside and outside the software and published in peer-reviewed literature.
Related References	https://www.lr.org/en-us/ip-well-analysis-software/ https://www.youtube.com/watch?v=mmc5TF6L3_I (Official YouTube videos of IP)

A.12.3 Neuralog

Tool Name	Neuralog
Developer/Owner	Neuralog Pro
Tool Type	Well Test and Log Interpretation
Description	NeuraLog transforms scanned images into usable digital data.
Tool Licensing and Access	https://www.neuralog.com/well-log-digitizing-software-neuralog/ https://www.neuralog.com/request-license/
Model Input	Raster well logs - Standard color, grayscale or b/w TIFF, JPEG, PDF or BMP image
Model Output	LAS 1.2; LAS 2.0 (Log ASCII Standard) - digital log curve data AutoCAD DXF; IHS PETRA ASCII Well Data; Tab Delimited ASCII
Risks Behavior Considered	No risks or behaviors
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan
How the Tool is Used	NeuraLog creates straightened and depth-registered digital images for geological applications. The software includes a comprehensive set of tools such as automated curve tracing, lithology data capture, interactive log display, image warp and stretch correction to improve the quality of digital log data.
Last Updated	January 31, 2020
Ongoing Development	It has an active user community; support for the tool is available
Ease of Use	Operating system Windows 7/8/10; no need for computer programming skills to use the tool
Computational Speed	The model is designed for computational efficiency
Related References	https://www.neuralog.com/product_brochures/Neuralog-Products-Solutions.pdf

A.12.4 Strater

Tool Name	Strater
Developer/Owner	Golden Software
Tool Type	Well Test and Log Interpretation
Description	Visualize and analyze subsurface data as well logs, boreholes, and cross sections
Tool Licensing and Access	Commercial: https://www.goldensoftware.com/products/strater
Model Input	Well log information, LAS files, well specifications
Model Output	Borehole logs, well designs, geologic cross sections
Risks Behavior Considered	Well integrity, geohazards, geologic variability
Relevant Permitting Phase	Site screening, site characterization
Class VI Permit Element Addressed	Site Screening, Site Characterization, Area of Review and Corrective Action Plan, Well Construction Details, Injection Well Plugging Plan, Post-Injection Site Care and Site Closure Plan
Last Updated	Version 5.7.1094.
Ongoing Development	Commercial, regular updates
Related References	https://www.goldensoftware.com/products/strater

A.12.5 Techlog

Tool Name	Techlog
Developer/Owner	Schlumberger
Tool Type	Well Test and Log Interpretation
Description	Incorporates data acquired from near-wellbore environments (e.g., geophysical well logs, core data, etc.) to assist users in performing petrophysical analyses and geologic interpretation tasks.
Tool Licensing and Access	Commercial proprietary software. Licensing options purchased via communication with Schlumberger. https://www.software.slb.com/products/techlog
Model Input	Geophysical well log data, core data, geologic formation tops, and wellhead data
Model Output	Synthetic geophysical well log data, well correlations, graphics, and interpretations
Risks Behavior Considered	Parameter uncertainty/sensitivity analysis
Relevant Permitting Phase	Site screening, site characterization, and application preparation
Class VI Permit Element Addressed	Site Screening, Site Characterization
How the Tool is Used	Techlog can be used to evaluate and interpret wellbore information in the nearby region after collecting site-specific data and to create inputs for 3D geologic modeling. It can also be used to generate figures for reporting/permit application activities.
Last Updated	June 30, 2021 (latest major release)
Ongoing Development	Schlumberger develops, supports, and maintains the software. It is a standard tool in the oil and gas industry.
Ease of Use	The tool has an interactive graphical user interface. No programming skills are required, but Python can be utilized in Techlog workflows. Well log interpretation experience is recommended before use.
Computational Speed	Petrophysical modeling can generate loads of varying sizes on computational resources. Machine learning and data analysis tasks performed with the software could potentially lead to long computational times. Basic tasks (loading well logs, viewing well logs, basic interpretation/analysis) are generally not computationally intensive.
Tool Verification	The tool has been used for several years throughout the oil and gas industry.
Related References	https://www.software.slb.com/products/techlog https://www.software.slb.com/products/product-library-v2?product=Techlog&tab=Case%20Studies

A.13 WELL DESIGN

Class VI wells must be appropriately designed to handle the proposed CO_2 injection. Tools in this category are primarily used to aid well design (e.g., sizing of casings).

A.13.1 PIPESIM

Tool Name	PIPESIM
Developer/Owner	Schlumberger
Tool Type	Well Design
Description	PIPESIM is a steady state multi-phase flow simulator used for designing wells, pipelines, or a network of wells and pipelines. The tool incorporates flow modeling, heat transfer, and fluid behavior to help size and optimize well and pipeline systems.
Tool Licensing and Access	It can be downloaded from Schlumberger Information Solutions (SIS) website. License needs to be purchased from SIS. https://www.software.slb.com/products/pipesim
Model Input	Pressure boundary conditions (start and/or end), reservoir properties (porosity, depth, permeability, skin, etc.), fluid flow rates
Model Output	Bottomhole pressure vs. depth for various tubing-casing programs, pipeline diameter and length depending on flowrates and terrain, fluid mass/temperature/phase streams between network components (wells/pipelines)
Risks Behavior Considered	BHP modeling can potentially and indirectly be used to understand risk of over pressuring the formation (seismicity)
Relevant Permitting Phase	Site screening, feasibility study, design/FEED, permitting
Class VI Permit Element Addressed	Site Screening, Well Construction Details, Injection Well Plugging Plan
Last Updated	2020
Ongoing Development	The tool is commercially available and widely used
Related References	Technical Papers - https://www.software.slb.com/products/product-library-v2?product=PIPESIM&tab=Technical%20Papers Case Studies - https://www.software.slb.com/products/product-library-v2?product=PIPESIM&tab=Case%20Studies

NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO_2). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

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