NRAP-Open-IAM User's Guide

Release alpha 2.6.1-22.09.30

V. Vasylkivska, S. King, D. Bacon, D. Harp, E. Lindner, S. Baek, E. Keating, Y. Yang, Y. Zhang, B. Chen, K. Mansoor

Sep 28, 2022

CONTENTS:

CHAPTER

ONE

OBTAINING NRAP-OPEN-IAM

1.1 Introduction

NRAP-Open-IAM is an open-source Integrated Assessment Model (IAM) for Phase II of the National Risk Assessment Partnership (NRAP). The goal of this software is to go beyond risk assessment into risk management and containment assurance. NRAP-Open-IAM is currently in active development and is available for testing and feedback only.

As this is a prototype of software being actively developed, we are seeking any feedback and/or issue reports. An online feedback form can be found here: https://docs.google.com/forms/d/e/1FAIpQLSed5mcX0OBx1dLNmYGbmS4Vfc0mdOLapIzFqw-6vHoho9B19A/viewform?usp=sf_link

Issue reports and feedback can be left at the forum on NETL's Energy Data eXchange webpage for NRAP-Open-IAM: https://edx.netl.doe.gov/workspace/forum/nrap-tools/topic?t=nrap-tools-nrap-open-iam or on GitLab issues page for NRAP-Open-IAM: https://gitlab.com/NRAP/OpenIAM/-/issues?sort=created_date&state=opened

If you have been given access to the code indirectly and would like to be notified when updates are available for testing, please contact the development team to be added to our email list.

1.2 Downloading NRAP-Open-IAM

NRAP-Open-IAM tool and examples can be downloaded from a public GitLab repository located at https://gitlab.com/NRAP/OpenIAM. In addition to that, the copy of the tool can be obtained through NETL's Energy Data eXchange website: https://edx.netl.doe.gov/dataset/nrap-open-source-iam by requesting an access through e-mail addressed to NRAP@netl.doe.gov. The NRAP-Open-IAM is distributed as a zip file that can be extracted in the location specified by user. If the NRAP-Open-IAM was downloaded from the GitLab repository, the folder name may have the repository's current hash appended to it. Feel free to rename the folder something simple like *NRAPOpenIAM* to simplify the navigation.

1.3 Installing NRAP-Open-IAM

The NRAP-Open-IAM requires Python version 3.9 or greater to operate. If you need to install Python, we describe all steps of the installation process below.

General Installation Guide:

- Extract the tool files from the provided/downloaded zip.
- Navigate to the *installers* folder within the recently unzipped directory.
- Navigate to the folder corresponding to the operating system that you are utilizing.
- Follow instructions file located in the folder for your operating system.

For Windows: The file *Installation_Instructions_Windows.txt* describes steps required to install needed Python packages for the proper work of NRAP-Open-IAM.

For macOS: The file *Installation_Instructions_macOS.txt* describes steps user needs to follow in order to install required Python packages.

For Linux OS: Linux users are assumed to know the installation commands for their specific version of Linux needed to install required tools. The file *Installation_Instructions_Linux.txt* specifies the needed software and package dependencies.

For alternative installation of Python the following packages are needed: `NumPy`, `SciPy`, `PyYAML`, `Matplotlib`, `Pandas`, `TensorFlow` (of version 2.6), `Keras`, `scikit-learn`, `Pmw`, `pip`, and `six`. In most cases (mainly dependent on the platform and Python distribition) the required libraries can be installed using `pip` or `conda` package managers. Additional libraries recommended to run Jupyter notebooks and scripts illustrating work of NRAP-Open-IAM are `IPython` and `Jupyter`.

On macOS and Linux machines the gfortran compiler needs to be present/installed to compile some of the NRAP-Open-IAM code (macOS users can find gfortran here: (https://gcc.gnu.org/wiki/GFortranBinariesMacOS)).

After the proper version of Python is installed, the NRAP-Open-IAM can be set up and tested. **Note: If Python was installed through Anaconda please use Anaconda prompt instead of command prompt for setup and tests.** In the NRAP-Open-IAM distribution folder find and open the sub-folder *setup*. Next, open a command prompt/Anaconda prompt in the *setup* folder (on Windows, this can be done by holding Shift and right clicking inside the folder when no file is selected, then selecting `Open command window here`; alternatively, one can navigate to the folder *setup*, type `cmd` in the address bar of the file browser and hit Enter to open the command prompt there). (On Windows, Anaconda prompt can be found in the programs menu under submenu `Anaconda3 (64-bit)`.) Run the setup script by entering the command:

```
python openiam_setup_tests.py
```

in the command prompt/Anaconda prompt. This will test the version of Python installed on the system. Next the setup script will test the versions of several Python libraries that the NRAP-Open-IAM depends on. The setup script will compile several Fortran libraries needed for some component models on Mac and Linux. Users of Windows OS will be provided with the compiled libraries. Finally, the setup script will run the test suite to see if the NRAP-Open-IAM has been installed correctly. If the results printed to the console indicate errors during the testing the errors have to be resolved before the NRAP-Open-IAM can be used. When contacting the developers to resolve problems please include all output from the setup script or test suite runs.

1.4 Testing installation

After setup the test suite can be run again by entering the NRAP-Open-IAM *test* directory in a terminal and typing:

```
python iam_test.py
```

Test results will be printed to the terminal. The setup script run during the installation process uses the same test suite after testing whether the necessary Python libraries are installed, and compiling the NRAP-Open-IAM libraries.

CHAPTER

TWO

GETTING STARTED

The NRAP-Open-IAM has several ways for a user to build and run simulations, including graphical user interface (GUI), text based control files and python scripts. The simplest way to build and run simulations for NRAP-Open-IAM is the GUI. This guide will primarily focus on using the GUI to interact with the NRAP-Open-IAM. To launch the GUI open a command prompt in the *source/GUI* directory and type:

```
python NRAP_OPENIAM.py
```

2.1 Conceptual model

Within the NRAP-Open-IAM the system model is divided up into components that are loosely coupled together. As the first step during setup of NRAP-Open-IAM simulation, we specify a few simulation parameters that affect all components and as the second step we build the system model by adding the components we want.

2.2 GUI Operation

When the GUI is first opened a disclaimer screen will be shown followed by the main interface.

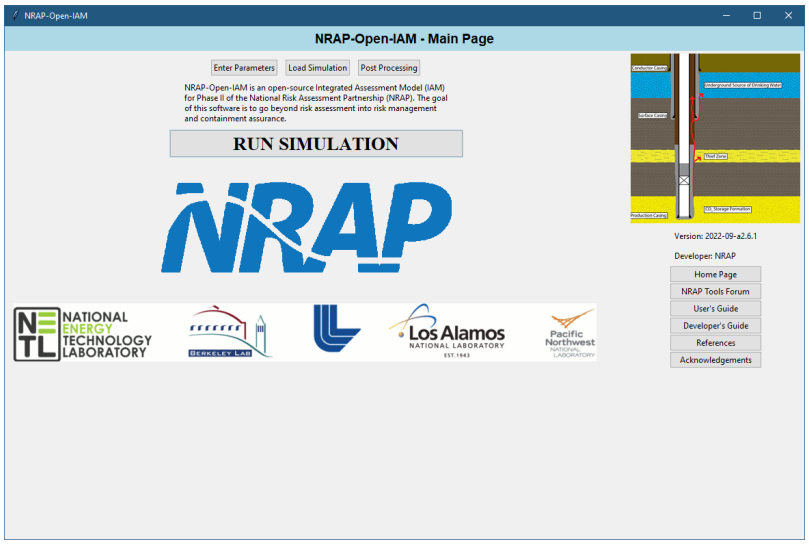


Fig. 2.1: Main NRAP-Open-IAM Interface

To begin building a model click on the **Enter Parameters** button. The process of building a model consists of entering basic model parameters, defining the geologic stratigraphy of the site, then adding a component model for each component of the system to be modeled. Therefore, the first tab that user would see after clicking the **Enter Parameters** button is the model parameters view.

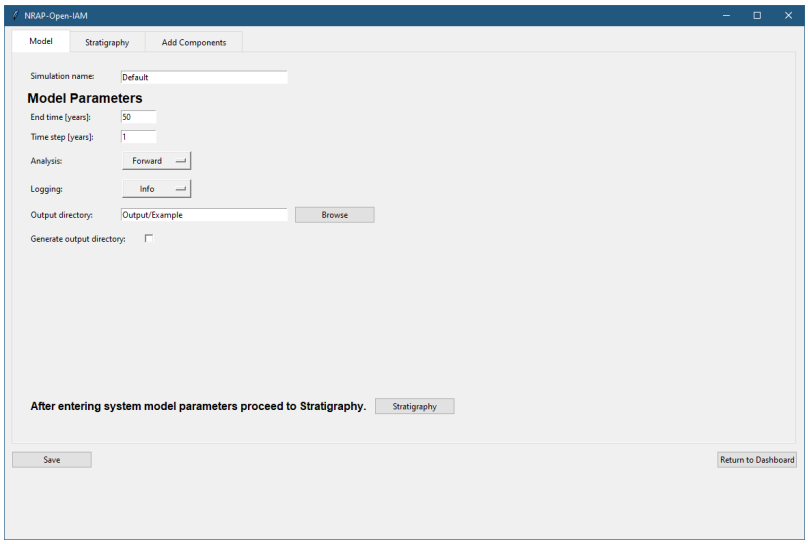


Fig. 2.2: Model Parameters View

Start by defining a `Simulation name` for the model: the name also will be used as the name of the file containing details of NRAP-Open-IAM simulation. Time should be entered in years. The `End time` is the number of years during which the simulation will be run. A uniform time step will be taken during the simulation specified by the `Time step` entry (typically 1 year time steps are used). The NRAP-Open-IAM can perform three types of simulations and/or analysis: `Forward`, `LHS`, and `Parstudy`. `Forward` analysis runs a single deterministic scenario. `LHS` (abbreviation for Latin Hypercube Sampling) is the type of random parameters sampling used to run stochastic simulations. `Parstudy` (short for parameter study analysis) divides user-defined range for each stochastic variable into equally spaced subdomains and selects parameter value from each subdomain. `Parstudy` analysis is useful for studying the effects of several variables on the components outputs but the number of realizations grows exponentially with the number of variables.

The NRAP-Open-IAM creates a log file with each simulation run: the level of information being logged in can be set by changing value of `Logging` entry. In general, the default level of `Info` would contain the most useful messages. A `Debug` (debugging) level of `Logging` will contain more information about component model connections, setup and calls, but will produce very large files and should be avoided for large simulations. `Warn` (warning) and `Error` levels can be used if log file sizes become an issue.

The NRAP-Open-IAM will save all the simulation results to the specified `Output directory`. In text field corresponding to `Output directory` user needs to enter a path to the folder where the output will be saved. In the case the entered path does not exist the empty directory will be created if box `Generate output directory` is checked. Additionally, if the provided path is not absolute, it is assumed that it starts in the NRAP-Open-IAM root folder. A `{datetime}` stamp can be added to the folder name so that each run of a particular simulation will be saved separately, otherwise results from a previous run will be overwritten by subsequent runs until the output folder is changed. After setting up the model parameters proceed to the Stratigraphy tab.

In the Statigraphy tab model parameters related to the stratigraphy of the CO_2 storage site are defined. All coordinate systems are assumed to have units of meters and are defined by the reservoir component used. Model parameters for the stratigraphy and appropriate components are defined by either assigning a fixed value or random distribution to vary over. For the LHS analysis parameters defined with a distribution will be sampled from that distribution. For forward simulation all parameters should be specified with a fixed value. See the *Stratigraphy Component* section of this document for a list of all available parameters and their definitions.

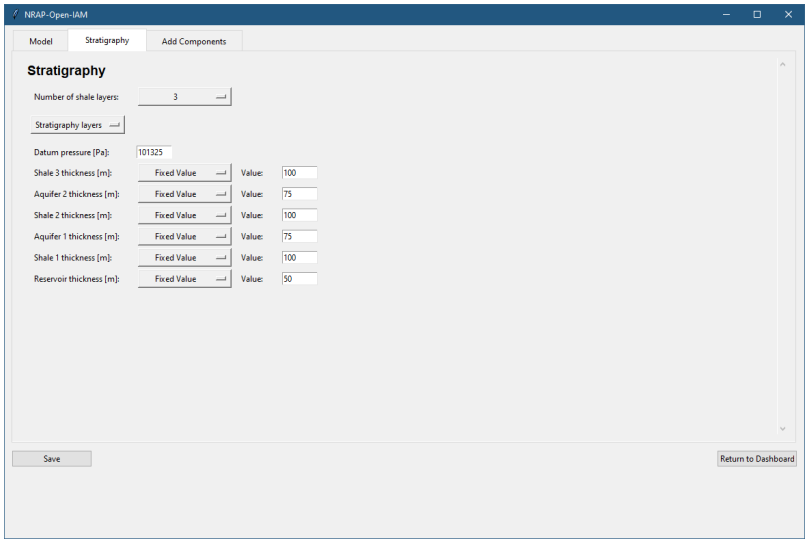


Fig. 2.3: Stratigraphy View

2.2.1 Adding Component Models

The NRAP-Open-IAM is designed in a way so that only the components of interest need to be modeled in the system. Generally, a simulation will be built from the deepest component upward (reservoir, wellbore, aquifer, etc.). To add a component, first give it a name (each component must have a unique name). Next select the type of component model to be used. When adding subsequent components, a connection to existing components can be specified.

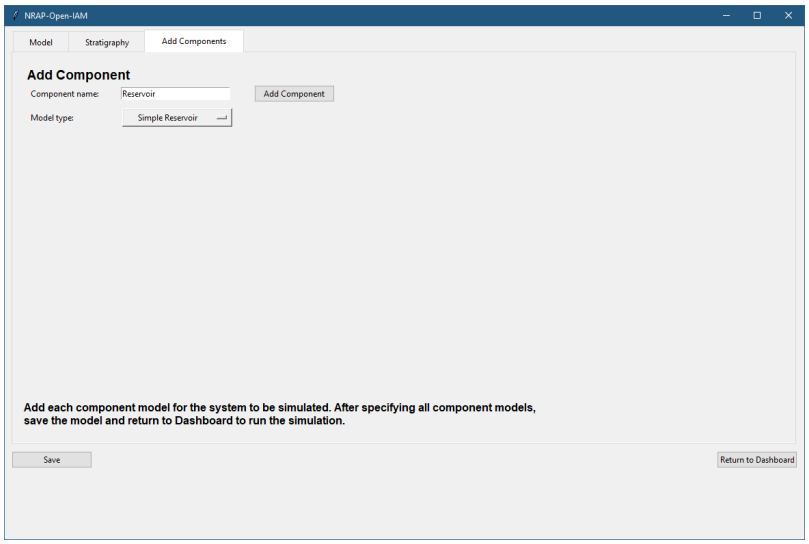


Fig. 2.4: Adding a Component Model

Each component model has component-specific input parameters and outputs. Parameters can be specified to be sampled from different distributions, or take on default values. When running a forward model parameters should only be specified as fixed values. When running a parameter study the parameters to vary should be specified as having a uniform distribution and minimum and maximum values. For stochastic simulations, any distributions can be specified. Parameter and output definitions can be found in the specific component model parameter section.

If a component is specified that needs input from another component but the deeper component is not to be part of the

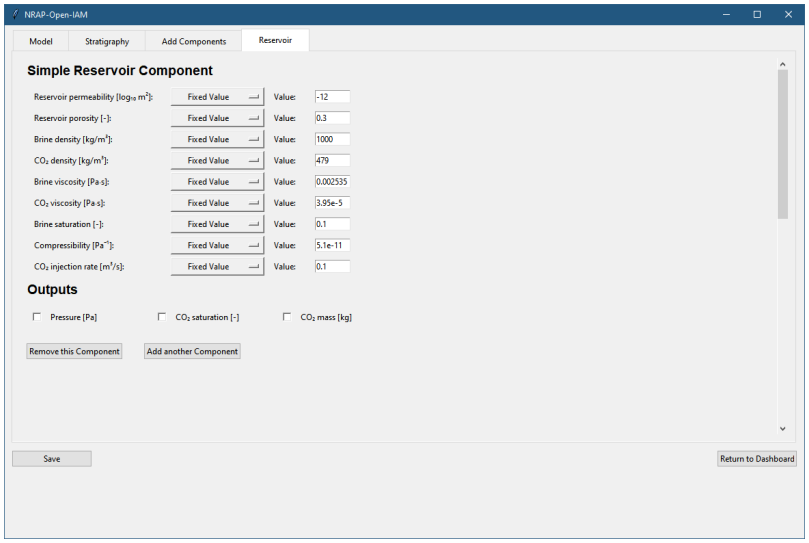


Fig. 2.5: Setup of Reservoir Component

model (i.e. specifying a wellbore model without a reservoir model), dynamic parameters can be used for the component model input. For dynamic parameters a value must be specified for each time step in the simulation. Values can be entered manually separated by a comma, or entered by providing path to the file containing the data. Some components require specification of which layer in the stratigraphy they represent (such as an aquifer model).

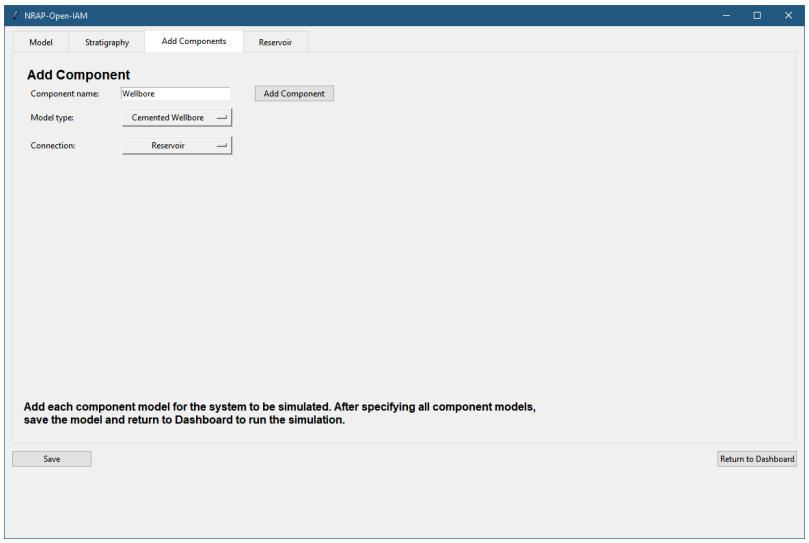


Fig. 2.6: Adding Second Component

After a given component is specified, subsequent component can be added to the system model. When all required components have been added, save the model and return to the dashboard. The system model can then be run using the **RUN SIMULATION** button on the main dashboard.

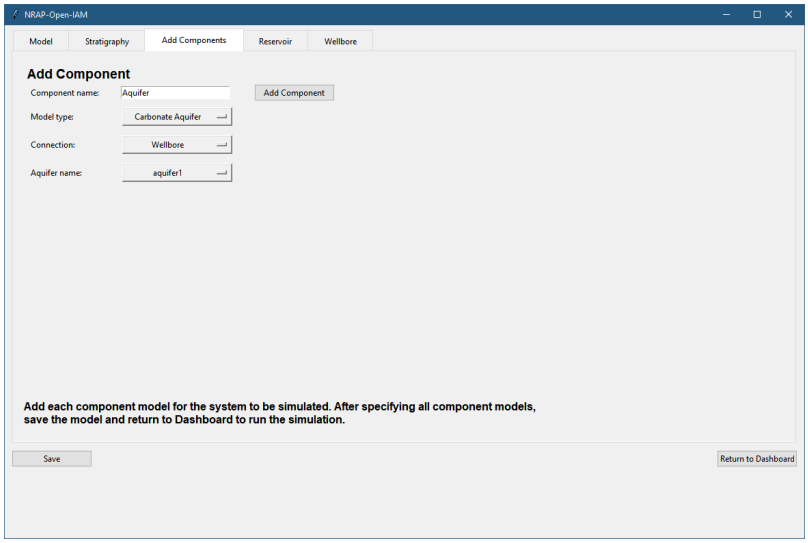


Fig. 2.7: Adding a Component Model with Connection and a Stratigraphy Selection

2.2.2 GUI Setup Examples

In the folder *examples*, there is a subfolder *GUI_Files* with example simulation files that can be loaded into the GUI and run by the NRAP-Open-IAM. To run one of the provided examples select **Load Simulation** on the main dashboard of the GUI. In the file browser that appears, navigate to the *GUI_Files* subfolder of the *examples* folder and select the first example file *01_Forward_SR_CW.OpenIAM*. This example runs a simple forward model with a Simple Reservoir component providing an input to a Cemented Wellbore component. When the file is loaded into the GUI, the parameters of the simulation can be investigated. After the simulation is complete the user can proceed to the post-processing step (by clicking **Post Processing** on the main dashboard of the GUI) to visualize and, for some scenarios, analyze the obtained results. Post Processing tab has a folder selection button which allows user to select (output) folder containing results of simulation. Note that the selection of the folder (and loading of results) might fail if the simulation did not finish successfully. In this case it is recommended to check file *IAM_log.txt* within the output folder containing useful (debug, info, warning or error) messages produced during the simulation. File names of the GUI setup examples distributed with the tool contain shortcuts that would help the user to figure out the featured components and type of analysis.

The second example file *02_LHS_SR_MSW.OpenIAM* is a stochastic simulation of system model containing a Simple Reservoir and a Multisegmented Wellbore components. Example illustrates Latin hypercube sampling approach applied to the parameters of the setup model. The number of realizations run is 30.

The third example file *03_LHS_LUT_MSW.OpenIAM* illustrates use of a Lookup Table Reservoir and Multisegmented Wellbore components. The lookup tables data set utilized in the example for the Lookup Table Reservoir component is based on the simulation for Kimberlina oil field ([19]).

The fourth example file *04_LHS_DP_MSW.OpenIAM* illustrates Latin hypercube sampling approach applied to a Multisegmented Wellbore component. The pressure and CO_2 saturation required as inputs of the component are provided in the form of arrays. This form of input arguments is called dynamic parameters, i.e. parameters that change in time.

The system model setup in the fifth example file *05_LHS_SR_OW_CA.OpenIAM* illustrates application of three component models: Simple Reservoir, Open Wellbore and Carbonate Aquifer. It estimates the impact the leakage of fluids through the wellbore has on the aquifer overlying the storage reservoir.

2.3 Control Files

Control files are a method of getting user input into the NRAP-Open-IAM for setting up a simulation scenario. Control files use a YAML format. Any line in the control file starting with a pound sign (#) is a comment and is ignored by the program. The basic format of the control file is a parameter name followed by a colon, space, and a value. For objects with several parameters the object name is followed by a colon and the underlying parameters are listed on the consecutive lines tabbed in. For example, consider this partial file:

```
#NRAP-Open-IAM Control File example
#-------------------------------------------------
ModelParams:
    EndTime: 50
    TimeStep: 1.0
    Analysis: forward
    Components: [SimpleReservoir1,
                 CementedWellbore1]
    OutputDirectory: ../../output/example_{datetime}
    Logging: Debug
Stratigraphy:
    shale1Thickness:
        min: 500.0
        max: 550.0
        value: 525.0
    shale2Thickness:
        min: 450.0
        max: 500.0
        value: 475.0
    aquifer1Thickness:
        vary: False
        value: 22.4
    reservoirThickness:
        vary: False
        value: 51.2
```

Here, the first two lines are comments that are not read by the code. The third line defines the keyword `ModelParams` which describes parameters of the system model. The subsequent lines contain parameters of `ModelParams`. A `ModelParams` section is required in all NRAP-Open-IAM control files. The `EndTime` keyword defines the ending time for the simulation in years (50 years in the example). The `TimeStep` parameter defines the length of a time step (1 year in the example). The type of analysis being run is a `forward` (deterministic) simulation. Other possible options for `Analysis` parameter are `lhs` for Latin Hypercube Sampling analysis and `parstudy` for a parameter study. The `Components` parameter is a required entry that contains a list of component model names that are defined later in the file. The component list will always begin with a square bracket '[' followed by each of the component names that make up the system separated by a comma ',' and closed by a square bracket ']'. The names of the components are listed in the order they are supposed to be run. The next keyword `OutputDirectory` defines a directory for the output to be written into. The output directory can be appended with a keyword `{datetime}`. When a simulation is run, the `{datetime}` keyword will be replaced with the date and time of the simulation run. Note that the `{datetime}` keyword is optional: if it is omitted subsequent runs of the simulation will overwrite past results. That is, if there is a need to keep all results from re-running an NRAP-Open-IAM case, the `{datetime}` keyword will easily facilitate this; if re-running an NRAP-Open-IAM case should overwrite previous results, the `{datetime}` keyword should be omitted. In the output folder the NRAP-Open-IAM places a copy of the input file, all outputs from the component models written to text files, and *.png* images for all graphics. The last keyword `Logging` defines what level of logging information is written out to the logging files. Options for `Logging` levels are `Debug`, `Info`, `Warning`, and `Error`. `Info` is the default level (if no `Logging` keyword is given the logging will be set to `Info`) and will give you a valuable

information about when parameters go outside of permitted ranges and when there are problems in the program. Debug is a good option if you have problems with your IAM model and want more information to explore the causes.

The next keyword section of the file is the required `Stratigraphy` section. In this section any model parameters related to the stratigraphy of the CO_2 storage site is defined. Any parameters for the stratigraphy are defined here with either a deterministic value or a range to vary over. A fixed value of any given parameter can be specified with the `vary: False` and `value: ###` specification shown here or simply `parameterName: ###`. The `min` and `max` specification gives a range for the parameter to vary over if an analysis is done over multiple realizations. See the *Stratigraphy Component* section of this document for a list of all available parameters.

The next sections of the input file defines every component model in the component model list specified earlier in the control file. The first component listed in the example is SimpleReservoir1 defined as follows

```
#-------------------------------------------------
# SimpleReservoir1 is a user defined name for component;
# the type SimpleReservoir is the ROM model name
#-------------------------------------------------
SimpleReservoir1:
    Type: SimpleReservoir
    Parameters:
        injRate: 0.1
    Outputs: [pressure,
              CO2saturation]
```

This section of the file defines a `SimpleReservoir` Component model named *SimpleReservoir1* to be part of the system model. The name *SimpleReservoir1* can be replaced with any other name defined by user, but will not be a part of the system model unless it is an element of the components list described in the previous section `ModelParams`. The `Type` is a keyword that defines the component model to be used and must match up with one of the component models currently available in the NRAP-Open-IAM. The `Parameters` section defines parameters of the component model. Description of parameters available for the user to specify can be found in the *Components Description* chapter of the current documentation. The component model parameters are specified in the same fashion as the Stratigraphy parameters. The `Outputs` specifies the observations of the component model that will be output from the simulation. Please refer to the *Components Description* chapter of this document to see which parameters and outputs are available for user specification in the control file.

Generally, dynamic (time-varying) input to component models comes from the output of other connected component models (e.g., the pressure and saturation as an input to a wellbore leakage model comes from a reservoir model). In some instances there may be a need to study a component model without the other attached component models feeding the input. In this case dynamic input can be specified with the `DynamicParameters` keyword. Under the `DynamicParameters` section each input name is specified followed by a list of values (enclosed in square brackets []) of the same length as the number of time points (a value for each time point, including an initial value). See files *ControlFile_ex7a.yaml* and *ControlFile_ex7b.yaml* for example of control files utilizing dynamic input for some components.

The next section of the input file is similar to the previous section and defines the next component model *CementedWellbore1*.

```
#-------------------------------------------------
CementedWellbore1:
    Type: CementedWellbore
    Connection: SimpleReservoir1
    Number: 4
    Locations:
        coordx: [100, 540]
        coordy: [100, 630]
    RandomLocDomain:
```

(continues on next page)

(continued from previous page)

```
        xmin: 150
        xmax: 250
        ymin: 200
        ymax: 300
    Parameters:
        logWellPerm:
            min: -14.0
            max: -12.0
            value: -13.0
    Outputs: [CO2_aquifer1,
              CO2_aquifer2,
              CO2_atm,
              brine_aquifer1,
              brine_aquifer2]
```

In this part of the example, `CementedWellbore` type component model is specified. There are four wellbores of this type being added with `Number: 4`: two of the locations are given in the `Locations` part and other two are generated randomly within the domain specified in `RandomLocDomain` part.

Unknown wellbore locations can be generated by specifying more wellbores (with *Number: `) than the number of known wellbore locations. To control the location of the random well placement, a ``RandomLocDomain`* section need to be used as

```
    RandomLocDomain:
        xmin: 150
        xmax: 250
        ymin: 200
        ymax: 300
```

This specification will limit the x-coordinate of random wells to be between 150 and 250, and the y-coordinate to be between 200 and 300. Sampling will be from a uniform distribution on the domain defined by `xmin` (`ymin`) and `xmax` (`ymax`).

All coordinate systems are assumed to have units of meters and are defined by the reservoir component used. Known wells will be placed first; after all known well coordinates are used wells will be placed within the random wells domain.

Known wellbore coordinates are entered as a comma separated list. There must be a comma between each coordinate. Random wellbores generated in an area when more wells are specified than number of known coordinates. After completing the model parameters proceed to the Stratigraphy tab.

The next keyword is `WellboreLocations`. This keyword defines its own section and is not part of the `ModelParams` section (it is not a sub-keyword in `ModelParams`). In this section the x and y coordinates (`coordx` and `coordy`, respectively) of two leaky wellbores are given. Coordinates are assumed to be given in units of meters. For the SimpleReservoir component model the default injection location is at [0, 0]. For the Lookup Table based reservoir component the wellbore locations should fall within the domain of the reservoir simulations.

See *ControlFile_ex3.yaml* for additional example using random well placement and *ControlFile_ex4.yaml* for example using only known well locations.

The last section of the input file is used to specify a graphical output

```
#-------------------------------------------------
# Plot setup part of the control file
#-------------------------------------------------
Plots:
```

(continues on next page)

(continued from previous page)

```
    CO2_Leakage1:
        TimeSeries: [CO2_aquifer1]
        subplot:
            ncols: 2
            use: True
    CO2_Leakage2:
        TimeSeries: [CO2_aquifer2]
        subplot:
            ncols: 2
            use: True
    Pressure_plot:
        TimeSeries: [pressure]
        subplot:
            ncols: 2
            use: True
            SimpleReservoir1_000.pressure: 'Pressure at well #1'
            SimpleReservoir1_001.pressure: 'Pressure at well #2'
            SimpleReservoir1_002.pressure: 'Pressure at well #3'
            SimpleReservoir1_003.pressure: 'Pressure at well #4'
        Title: Reservoir Pressure at Wellbore Location
```

Here, three plots are being requested. The firsts two plots will illustrate the CO_2 leakage to the shallow aquifer and the thief zone aquifer; the third plot will illustrate the pressures in the reservoir for the four wellbore locations specified earlier in the control file. *CO2_Leakage1*, *CO2_Leakage2* and *Pressure_plot* are the user defined names of the three plots to be created: these will also be used as the filenames of the figures saved in the output directory. `TimeSeries` is a keyword that instructs the program to plot the observation data as a time series plot. The values to be plotted (*CO2_aquifer1*, *CO2_aquifer2* and *pressure* above) have to be defined in the control file as outputs from one of the specified component models. Each plot will have a title corresponding to the values plotted. A user defined title can be specified with the `Title` keyword (as illustrated for the *Pressure_plot*) in the given plot section. For each aquifer the CO_2 leakage rates for all wells will be plotted on the same figure but on different subplot. If each observation is to be plotted on a separate subplot, the `subplot` keyword with `use` set to `True` must be specified, as illustrated in the example setup. Additionally, the `ncols` keyword (under `subplot` section) can be used to set the number of subplot columns to use. The number of rows is controlled by the number of different values (observations) to plot over the number of columns. Each subplot will be given a (default) title of the variable plotted unless specified by user. The default title names can be replaced with the user defined ones by using the full observation name as a key and the desired title as the value under `subplot` section as shown in the setup of *Pressure_plot*.

The example file described here can be found in the *examples/Control_Files* directory with the filename *ControlFile_ex1.yaml*. To run this example, open a command prompt in the *examples/Control_Files* directory and run the command:

```
python ../../source/openiam/openiam_cf.py --file ControlFile_ex1.yaml
```

Note: use \ on Windows and / on Mac and Linux.

Other example control files can be found in the same directory. They can be run by replacing the file name in the above command with the user specified one.

2.4 Output

Output is written to the folder specified in the model definition with the `Output directory`. If the path to the output directory is not absolute (i.e., does not containt the drive letter) it is assumed to start from the NRAP-Open-IAM root folder containing the tool distribution. For each component model of the system `Outputs` can be specified. When an output is specified for a forward model the values of that output are written to a file (*output_name.txt*) in the `Output Directory`. For a stochastic model (LHS or parametric study analysis) the outputs are included in the results file (*LHS_results.txt* or *parstudy_results.txt*) as well as a file for a statistical summary of the input parameters and output observations (*LHS_statistics.txt* or *parstudy_statistics.txt*). A copy of the input control file is also written to the `Output Directory` folder. Through the GUI, this input file can be loaded back in to rerun the simulation.

After a simulation is run, the post processing section of the GUI can be used to generate plots of the results and run sensitivity analysis. When the post processing page is first opened it asks for a folder specification. This folder is the output folder of the results you want to analyze. Navigate to that output folder using the **Browse** button.

2.4.1 Plotting

User can access post-processing capabilities of GUI by clicking on the **Post Processing** button on the main page. The **Post Processor** window will appear. After a folder containing the results of the simulation is selected different options for the simulation results appear that are already set for plotting. There are several types of plots that can be created depending on what type of simulation was run and what components were specified. The simplest plot is a `Time Series` plot where the output is plotted against time, multiple realizations will be plotted as separate lines. Specify a title to give the plot and a file name along with making a selection of what output to plot. Pressing the plot button will generate the plot, it will be saved with the filename given to the output directory for the results. If a simulation was run with multiple realizations a `Time Series Stats` plot or a `Time Series and Stats` plot will be options in the `Plot Type` menu. A `Time Series Stats` plot will shade the quadrants of the results along with plotting the mean and median results, but will not plot the individual realizations. A `Time Series and Stats` plot will overlay the realizations on the stats plots of the shaded quadrants. If AtmosphericROM component was included in the simulation, map-view plots of the plume for a single realization or probabilistic ensemble can be generated.

2.4.2 Sensitivity Analysis

If the simulation results are from a LHS simulation the `Processing` menu will have options for several types of sensitivity analysis. Note that while a sensitivity analysis can be run on simulations with a small number of realizations, the results will most likely be inaccurate. If the sensitivity coefficients do not sum to one, or if they vary largely through time, the number of realizations might need to be increased. Generally, 500 to 1000 realizations are needed for a sensitivity analysis. However, this might change depending on the complexity of the simulation. Each type of sensitivity analysis will produce plots and/or text file output in the output directory.

`Correlation Coefficients` option produces a plot matrix of either `Pearson` or `Spearman` correlation coefficients. Any system model observation can be excluded from the analysis if needed, although no exclusions need to be made.

`Sensitivity Coefficients` option calculates the sensitivity coefficients for each selected output to all inputs. Selecting multiple outputs will run the sensitivity coefficient calculation multiple times. The capture point is the index for point in time at which the sensitivity coefficient are to be calculated. The analysis produces a bar chart.

`Multiple Sensitivity Coefficients` option calculates the impact of input parameters on multiple outputs. Multiple outputs should be selected here. The capture point is the index for point in time at which the sensitivity coefficient are to be calculated. The analysis will produce a bar chart.

`Time Series Sensitivity` option will produce a line graph illustrating how the impact from input parameters changes over time with respect to an output value. Selecting multiple output values will run the analysis multiple times. The capture point determines the time at which the sensitivity coefficients are compared and then ordered based on the comparison.

2.5 Analysis Options in Control File

The NRAP-Open-IAM uses the Model Analysis ToolKit (MATK) [8] for the basis of its probabilistic framework. More information about MATK can be found here: http://dharp.github.io/matk/. The MATK code repository can be found here: https://github.com/dharp/matk.

Parameter input and output interactions can be explored using the *Analysis* section of the control file. Correlation coefficients can be calculated using the `CorrelationCoeff` keyword. Parameter sensitivity coefficients for any output simulation value can be calculated using a Random-Balanced-Design Fourier Amplitude Sensitivity Test (RBD-Fast) technique. The control file keywords `SensitivityCoeff`, `MultiSensitivities`, `TimeSeriesSensitivity` can be used to access different sensitivity coefficient outputs. See *ControlFile_ex8.yaml* for details on using the analysis section.

The Sensitivity Analysis is done with the `SALib` package [11]. For more information on the RBD-Fast technique see [30] and [27]. While not accessible through the control files, a scripting interface is provided to a Sobol sensitivity analysis [29].

This section will be expanded in the future.

2.6 Units

Data passed between models need to have consistent units. Here is a list of units used by the NRAP-Open-IAM.

- Pressure is assumed to be in units of Pascals (Pa).
- Time is assumed to be in days.
- Distance, width, length, height, depth are assumed to be in units of meters (m).
- Flow rates are assumed to be in units of kilograms per second (kg/s).
- Mass is assume to be in units of kilograms (kg).
- Viscosities are assumed to be in units of Pascal seconds ($Pa{\cdot}s$).
- Permeability is assumed to be in units of meters squared (m^2).

CHAPTER

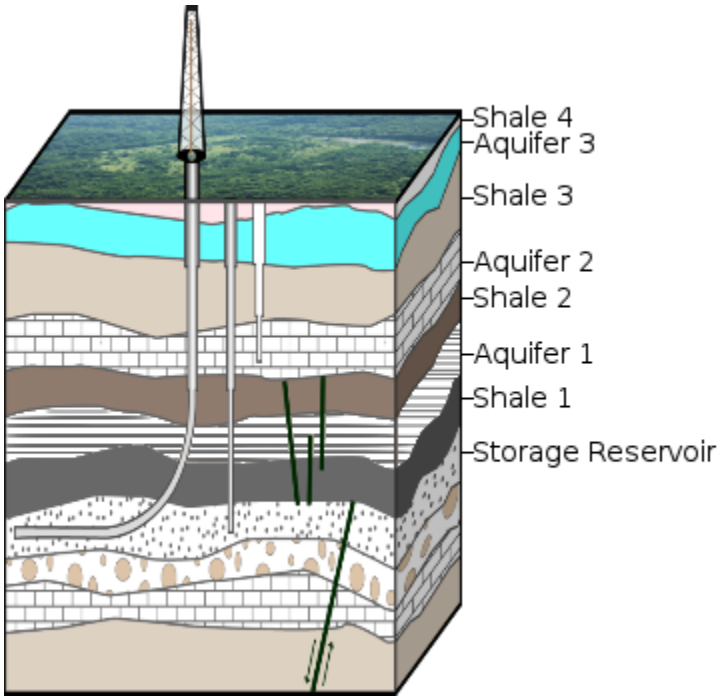
THREE

COMPONENTS DESCRIPTION

This section of the document will describe each of the component models available for use in the NRAP-Open-IAM. For each component model all parameters that can be specified are described along with units and acceptable ranges. Description of the outputs that can be returned by each component is also provided.

3.1 Stratigraphy Component

The Stratigraphy component is a component containing parameters describing the structure of the storage reservoir system. The stratigraphy component allows the number of shale (or aquitard) layers to be set, thus, setting the total number of layers in the system. Each shale or aquifer layer can take on the default thickness for that layer type or be assigned a user defined value with `shale#Thickness` or `aquifer#Thickness` keywords where # is replaced by an index of the layer (e.g., `shale1Thickness`). Layers are numbered from the bottom upward: shale 1 is the layer above the storage reservoir, and, with N shale layers total, shale N is the surface layer.



The description of the component's parameters is provided below.

- **numberOfShaleLayers** [-] (3 to 30) - number of shale layers in the system (default: 3). The shale units must be separated by an aquifer.

- **shaleThickness** [m] (1 to 1600) - thickness of shale layers (default 250). Thickness of shale layer 1, for example, can be defined by shale1Thickness; otherwise, shale layers for which the thickness is not defined will be assigned a default thickness.
- **aquiferThickness** [m] (1 to 1600) - thickness of aquifers (default: 100). Thickness of aquifer 1, for example, can be defined by aquifer1Thickness; otherwise, aquifers for which the thickness is not defined will be assigned a default thickness.
- **reservoirThickness** [m] (1 to 1600) - thickness of reservoir (default: 50)
- **datumPressure** [Pa] (80,000 to 300,000) - pressure at the top of the system (default: 101,325)
- **depth** [m] (5 to 30,000) - depth to the top of reservoir (default: 950).

3.2 Simple Reservoir Component

The Simple Reservoir component model is a semi-analytical model for the reservoir. It is focused on flow across relatively large distances and does not take into account discrete features of the flow paths such as fractures, cracks, etc. The model is based on work of Nordbotten et al., [5]. Further reading can be found in [22], [4], [23], [21].

In the NRAP-Open-IAM control file, the type name for the Simple Reservoir component is `SimpleReservoir`. The description of the component's parameters is provided below:

- **logResPerm** [$\log_{10} m^2$] (-14 to -9) - logarithm of reservoir permeability (default: -12)
- **reservoirPorosity** [-] (0.01 to 1) - porosity of reservoir (default: 0.3)
- **brineDensity** [kg/m^3] (900 to 1500) - density of brine phase (default: 1000)
- **CO2Density** [kg/m^3] (100 to 1500) - density of CO_2 phase (default: 479)
- **brineViscosity** [$Pa{\cdot}s$] (1.0e-4 to 5.0e-3) - viscosity of brine phase (default: 2.535e-3)
- **CO2Viscosity** [$Pa{\cdot}s$] (1.0e-6 to 1.0e-4) - viscosity of CO_2 phase (default: 3.95e-5)
- **brineResSaturation** [-] (0 to 0.7) - residual saturation of brine phase (default: 0.1)
- **compressibility** [Pa^{-1}] (5.0e-11 to 1.0e-9) - compressibility of brine and CO_2 phases (assumed to be the same for both phases) (default: 5.1e-11)
- **injRate** [m^3/s] (1.0e-3 to 10) - CO_2 injection rate (default: 0.1)
- **numberOfShaleLayers** [-] (3 to 30) - number of shale layers in the system (default: 3); *linked to Stratigraphy*. The shale units must be separated by an aquifer.
- **shaleThickness** [m] (1 to 1600) - thickness of shale layers (default 250); *linked to Stratigraphy*. Thickness of shale layer 1, for example, can be defined by shale1Thickness; otherwise, shale layers for which the thickness is not defined will be assigned a default thickness.
- **aquiferThickness** [m] (1 to 1600) - thickness of aquifers (default: 100); *linked to Stratigraphy*. Thickness of aquifer 1, for example, can be defined by aquifer1Thickness; otherwise, aquifers for which the thickness is not defined will be assigned a default thickness.
- **reservoirThickness** [m] (1 to 1600) - thickness of reservoir (default: 50); *linked to Stratigraphy*
- **datumPressure** [Pa] (80,000 to 300,000) - pressure at the top of the system (default: 101,325); *linked to Stratigraphy*.

Possible observations from the Simple Reservoir component are:

- **pressure** [Pa] - pressure at top of the reservoir at the user defined location(s)
- **CO2saturation** [-] - CO_2 saturation at the top of the reservoir at the user defined location(s)

- **mass_CO2_reservoir** [kg] - mass of the CO_2 in the reservoir.

3.3 Analytical Reservoir Component

The Analytical Reservoir component model is a semi-analytical model for the reservoir. It is focused on flow across relatively large distances and does not take into account discrete features of the flow paths such as fractures, cracks, etc. The model is based on work of Nordbotten et al., [5]. Further reading can be found in [21], [2].

In the NRAP-Open-IAM control file, the type name for the analytical reservoir component is `AnalyticalReservoir`. The description of the component's parameters is provided below:

- **logResPerm** [$\log_{10} m^2$] (-15.3 to -12) - logarithm of reservoir permeability (default: -13.69897)
- **reservoirPorosity** [-] (0.1 to 0.3) - porosity of reservoir (default: 0.15)
- **reservoirRadius** [m] (500 to 100,000) - distance between injection well and outer reservoir boundary (default: 500)
- **brineDensity** [kg/m^3] (965 to 1195) - density of brine phase (default: 1045)
- **CO2Density** [kg/m^3] (450 to 976) - density of CO_2 phase (default: 479)
- **brineViscosity** [$Pa{\cdot}s$] (2.3e-4 to 15.9e-4) - viscosity of brine phase (default: 2.535e-4)
- **CO2Viscosity** [$Pa{\cdot}s$] (0.455e-6 to 1.043e-4) - viscosity of CO_2 phase (default: 3.95e-5)
- **brineResSaturation** [-] (0 to 0.25) - residual saturation of brine phase (default: 0)
- **brineCompressibility** [Pa^{-1}] (3.63e-12 to 2.31e-11) - brine compressibility (default: 4.5e-12 = 3.1e-8 1/psi)
- **injRate** [m^3/s] (0.0024 to 3.776) - CO_2 injection rate (default: 0.01)
- **numberOfShaleLayers** [-] (3 to 30) - number of shale layers in the system (default: 3); *linked to Stratigraphy*. The shale units must be separated by an aquifer.
- **shaleThickness** [m] (1 to 1600) - thickness of shale layers (default: 250); *linked to Stratigraphy*. Thickness of shale layer 1, for example, can be defined by shale1Thickness; otherwise, shale layers for which the thickness is not defined will be assigned a default thickness.
- **aquiferThickness** [m] (1 to 1600) - thickness of aquifers (default: 100); *linked to Stratigraphy*. Thickness of aquifer 1, for example, can be defined by aquifer1Thickness; otherwise, aquifers for which the thickness is not defined will be assigned a default thickness.
- **reservoirThickness** [m] (15 to 500) - thickness of reservoir (default: 50); *linked to Stratigraphy*. Reservoir bottom depth is determined as shaleThickness*numberOfShaleLayers+aquiferThickness*(numberOfShaleLayers-1) +reservoirThickness if shaleThickness and aquiferThickness parameters are the same for all shale and aquifer layers respectively.
- **datumPressure** [Pa] (80,000 to 300,000) - pressure at the top of the system (default: 101,325); *linked to Stratigraphy*.

Possible observations from the Analytical Reservoir component are:

- **pressure** [Pa] - pressure at top of the reservoir at the user defined location(s)
- **pressureAve** [Pa] - pressure vertically averaged at the user defined location(s)
- **CO2saturation** [-] - CO_2 saturation vertically averaged at the user defined location(s)
- **mass_CO2_reservoir** [kg] - (injected total) mass of the CO_2 in the reservoir.

3.4 Lookup Table Reservoir Component

The Lookup Table Reservoir component model is a reduced order model based on interpolation of data from a set of lookup tables. The lookup tables are based on the full-physics scale simulations. Each lookup table is determined by a particular set of M input model parameters which define a signature of the given set of lookup tables.

In the NRAP-Open-IAM control file, the type name for the Lookup Table Reservoir component is `LookupTableReservoir`. The component's parameters depend on the M input model parameters used to create lookup tables data. The minimum and maximum values of lookup table parameters determine boundaries of component parameters. Moreover, the component parameters values as a set can only be one of the combination of values that went into one of the lookup table linked to the component.

In the NRAP-Open-IAM control file a `FileDirectory` keyword must be specified. It indicates the directory where files with the simulation data for the lookup tables are located. A `TimeFile` keyword is a name of the .csv file that stores the time points (in years) at which the results in the tables are provided. If `TimeFile` is not specified then, by default, the name of the file with time data is assumed to be *time_points.csv*. The time file must be located in the directory specified by `FileDirectory`.

A `ParametersFilename` keyword can also be specified. It defines the names and values of lookup table parameters that were used to create the given set of lookup tables. Additionally, it lists the names of the *.csv* files containing simulation data for each of the lookup table in the set. By default, the name of the file with parameters data is assumed to be named *parameters_and_filenames.csv*. The parameters file should be in a comma separated values format. The first M entries in the first row of the file are the names of the lookup table parameters which were varied for different realizations; the (M+1)st entry is a word *filename*. Each subsequent row of the parameters file contains the M values of the lookup table parameters followed by the name of file (lookup table) with the corresponding realization data. The provided filename must match with one of the files in the `FileDirectory`.

The user should make sure that the information provided in `ParametersFilename` file on parameters and simulation data files is accurate and complete. In general, a given parameter of the Lookup Table Reservoir component can have any possible name. At the same time the (possibly random) names specified by user in the `ParametersFilename` file should be the same names that the user would use in the control file for the description of the Lookup Table Reservoir component parameters. Due to the way the lookup tables are produced, each parameter of the reservoir component can only take on certain deterministic values. The possible values of a given parameter should be listed after the `values:` keyword followed by the list in square brackets ('['). The weights for each parameter can be specified with the `weights:` keyword followed by the list of weights for each value in square brackets. The weights should sum to 1, otherwise, they will be normalized. If no weights are provided all values are assumed to be equally likely to occur.

There exists an option to sample the data from the lookup tables without direct reference to any of the parameters used for creating the tables. User can use an auxiliary parameter `index` added to the Lookup Table Reservoir component to sample data from a particular lookup table file based on its index in the file *parameters_and_filenames.csv*. This option allows to use lookup tables in the scenarios where the total number of lookup table data files is less than the number of all possible combinations of the lookup table parameters.

Simulation data files (listed in `ParametersFilename` file) in a comma separated values format contain the reservoir simulation data, e.g., pressure and CO_2 saturation, varying over time. The data is used to build the Lookup Table Reservoir component output. Each realization file begins with a header line that is ignored by the code. Each subsequent row of the file represents a particular spatial location. The first and the second columns are the x- and y-coordinates of the location, respectively. The subsequent columns contain reservoir simulation data at the location defined in the first two columns. The names of the columns should represent the data in them and have the form *base.obs.nm_#* where *base.obs.nm* is the name of observation as used in the system model and # is an index of the time point at which the given observation is provided. The indexing of the reservoir simulation data should always start with 1 not with 0. For example, the pressure data at the first time point (even if this time point is 0) should always be indexed as *pressure_1*. Further, if the column contains pressure data at the second time point, its name should be *pressure_2*, and so on. If the column contains saturation data at the 12th time point, its name should be *CO2saturation_12*. The order of the columns in the lookup table except the first two x and y columns is arbitrary. If some reservoir simulation data does not vary in time then the column name should indicate it: in any case its name should not contain underscore symbol

_ followed by number (time index). For example, column with name #temperature# would indicate that the provided temperature data is constant in time.

The Lookup Table Reservoir component produces the output using interpolation in space and time within the spatio-temporal domain defined by the lookup tables simulation model setup. Observations from the Lookup Table Reservoir component are:

- **pressure** [Pa] - pressure at top of the reservoir at the wellbore location(s)
- **CO2saturation** [-] - CO_2 saturation at the top of the reservoir at the wellbore location(s).

Observations *pressure* and *CO2saturation* are mandatory for the Lookup Table Reservoir component which means that the linked lookup tables should contain the necessary data to produce them. In addition, the component can return any other type of observations provided in the lookup tables.

3.5 Multisegmented Wellbore Component

The Multisegmented Wellbore component estimates the leakage rates of brine and CO_2 along wells in the presence of overlying aquifers or thief zones. The model is based on work of Nordbotten et al., [23]. Further reading can be found in [21].

The model is focused on flow across relatively large distances and does not take into account discrete features of the flow paths such as fractures, cracks, etc. It assumes that leakage is occurring in the annulus between the outside of the casing and borehole. This area is assigned an "effective" permeability of the flow path. The permeability is applied over a length along the well that corresponds to the thickness of a shale formation. Each well is characterized by an effective permeability assigned to each segment of the well that crosses an individual formation. For example, if a well crosses N permeable formations, then it is characterized by N different permeability values. The model utilizes the one-dimensional multiphase version of Darcy's law to represent flow along a leaky well.

In the NRAP-Open-IAM control file, the type name for the Multisegmented Wellbore component is `MultisegmentedWellbore`. The description of the component's parameters are provided below. Names of the component parameters coincide with those used by `model` method of the `MultisegmentedWellbore` class.

- **logWellPerm** [$\log_{10} m^2$] (-101 to -9) - logarithm of well permeability along shale layer (default: -13). Logarithm of well permeability along shale 3, for example, can be defined by logWell3Perm. Permeability of the well along the shale layers not defined by user will be assigned a default value.
- **logAquPerm** [$\log_{10} m^2$] (-17 to -9) - logarithm of aquifer permeability (default: -12). Logarithm of aquifer 1 permeability, for example, can be defined by logAqu1Perm. Aquifer permeability not defined by user will be assigned a default value.
- **brineDensity** [kg/m^3] (900 to 1500) - density of brine phase (default: 1000)
- **CO2Density** [kg/m^3] (100 to 1000) - density of CO_2 phase (default: 479)
- **brineViscosity** [$Pa{\cdot}s$] (1.0e-4 to 5.0e-3) - viscosity of brine phase (default: 2.535e-3)
- **CO2Viscosity** [$Pa{\cdot}s$] (1.0e-6 to 1.0e-4) - viscosity of CO_2 phase (default: 3.95e-5)
- **aquBrineResSaturation** [-] (0 to 0.99) - residual saturation of brine phase in each aquifer (default: 0.0). For example, the residual brine saturation of aquifer2 can be defined by aqu2BrineResSaturation; otherwise, aquifer layers for which the residual brine saturation is not defined will be assigned a default value.
- **compressibility** [Pa^{-1}] (1.0e-13 to 1.0e-8) - compressibility of brine and CO_2 phases (assumed to be the same for both phases) (default: 5.1e-11)
- **wellRadius** [m] (0.01 to 0.5) - radius of leaking well (default: 0.05)
- **numberOfShaleLayers** [-] (3 to 30) - number of shale layers in the system (default: 3); *linked to Stratigraphy*. The shale units must be separated by an aquifer.

- **shaleThickness** [m] (1 to 3000) - thickness of shale layers (default: 250); *linked to Stratigraphy*. Thickness of shale layer 1, for example, can be defined by shale1Thickness; otherwise, shale layers for which the thickness is not defined will be assigned a default thickness.
- **aquiferThickness** [m] (1 to 1600) - thickness of aquifers (default: 100); *linked to Stratigraphy*. Thickness of aquifer 1, for example, can be defined by aquifer1Thickness; otherwise, aquifers for which the thickness is not defined will be assigned a default thickness.
- **reservoirThickness** [m] (1 to 1600) - thickness of reservoir (default: 30); *linked to Stratigraphy*. Reservoir bottom depth is determined as shaleThickness*numberOfShaleLayers+aquiferThickness*(numberOfShaleLayers-1) +reservoirThickness if shaleThickness and aquiferThickness parameters are the same for all shale and aquifer layers respectively.
- **datumPressure** [Pa] (80,000 to 300,000) - pressure at the top of the system (default: 101,325); *linked to Stratigraphy*

The possible outputs from the Multisegmented Wellbore component are leakage rates of CO_2 and brine to each of the aquifers in the system and atmosphere. The names of the observations are of the form:

- **CO2_aquifer1**, **CO2_aquifer2**,..., **CO2_atm** [kg/s] - CO_2 leakage rates
- **brine_aquifer1**, **brine_aquifer2**,..., **brine_atm** [kg/s] - brine leakage rates
- **mass_CO2_aquifer1**, **mass_CO2_aquifer2**,..., **mass_CO2_aquiferN** [kg] - mass of the CO_2 leaked into the aquifer.

3.6 Cemented Wellbore Component

The Cemented Wellbore component model is based on a multiphase well leakage model implemented in the NRAP-IAM-CS, [9]. The model is built off detailed full-physics Finite Element Heat and Mass (FEHM) simulations, [38]. The FEHM simulations are three-dimensional (3-D), multiphase solutions of heat and mass transfer of water and supercritical, liquid, and gas CO_2. After the simulations are completed, the surrogate model is built based on the key input parameters and corresponding output parameters. The approximate (surrogate) model is represented by polynomials in terms of input parameters that then can be sampled to estimate leakage rate for wells. Early development work can be found in [14].

When using the control file interface with more than 3 shale layers, the `ThiefZone` keyword can be used to specify the thief zone aquifer and the `LeakTo` keyword can be specified to name the upper aquifer. These values will default to *aquifer1* and *aquifer2* respectively.

Component model input definitions:

- **logWellPerm** [$\log_{10} m^2$] (-13.95 to -10.1) - logarithm of wellbore permeability (default: -13)
- **logThiefPerm** [$\log_{10} m^2$] (-13.9991 to -12.00035) - logarithm of thief zone permeability (default: -12.2)
- **wellRadius** [m] (0.025 to 0.25) - radius of the wellbore (default: 0.05)
- **initPressure** [Pa] (1.0e+5 to 5.0e+7) - initial pressure at the base of the wellbore (default: 2.0e+7 Pa, or 20 MPa); *from linked component*
- **wellDepth** [m] (960 to 3196.8) - depth in meters from ground surface to top of reservoir (default: 1500); *linked to Stratigraphy*
- **depthRatio** [-] (0.30044 to 0.69985) - fraction of well depth to the center of the thief zone from the top of the reservoir (default: 0.5); *linked to Stratigraphy*.

Temporal inputs of the Cemented Wellbore component are not provided directly to the component model method but rather are calculated from the current and several past values of pressure and CO_2 saturation. The calculated temporal

inputs are then checked against the boundary assumptions of the underlying reduced order model. The Cemented Wellbore component model temporal inputs are:

- **deltaP** [Pa] (105891.5 to 9326181.69) - difference between the current and initial pressure at the wellbore
- **pressurePrime** [Pa/s] (-6675.03 to 2986.7) - first pressure derivative
- **pressureDPrime** [Pa/s^2] (-111.265, 10.806) - second pressure derivative
- **saturation** [-] (0.001 to 1.0) - CO_2 saturation at the wellbore
- **saturationPrime** [$1/s$] (-4.290e-7 to 1.117e-3) - first CO_2 saturation derivative
- **saturationDPrime** [$1/s^2$] (-6.923e-6 to 1.176e-6) - second CO_2 saturation derivative.

The possible outputs from the Cemented Wellbore component are leakage rates of CO_2 and brine to aquifer, thief zone and atmosphere. The names of the observations are of the form:

- **CO2_aquifer1**, **CO2_aquifer2**, **CO2_atm** [kg/s] - CO_2 leakage rates
- **brine_aquifer1**, **brine_aquifer2**, **brine_atm** [kg/s] - brine leakage rates
- **mass_CO2_aquifer1**, **mass_CO2_aquifer2** [kg] - mass of CO_2 leaked into aquifers.

3.7 Open Wellbore Component

The Open Wellbore model is a lookup table reduced order model based on the drift-flux approach, see [25]. This model treats the leakage of CO_2 up an open wellbore or up an open (i.e., uncemented) casing/tubing. The lookup table is populated using T2Well/ECO2N Ver. 1.0 [24], which treats the non-isothermal flow of CO_2 and brine up an open wellbore, allows for the phase transition of CO_2 from supercritical to gaseous, with Joule-Thompson cooling, and considers exsolution of CO_2 from the brine phase.

By default, when used within the user interface the Open Wellbore is connected to the upper aquifer (e.g., aquifer 2 if there are 2 aquifers in the system). For user-defined scenarios the `LeakTo` keyword can be used to specify either the name of the aquifer (e.g., *aquifer1*) CO_2 leaks to or *atmosphere* for leakage to the atmosphere. The default value is *aquifer#* where # is an index of the uppermost aquifer.

Component model input definitions:

- **logReservoirTransmissivity** [$\log_{10}\ m^3/s$] (-11.27 to -8.40) - reservoir transmissivity (default: -9.83)
- **logAquiferTransmissivity** [$\log_{10}\ m^3/s$] (-11.27 to -8.40) - reservoir transmissivity (default: -9.83)
- **brineSalinity** [-] (0 to 0.2) - brine salinity (mass fraction) (default: 0.1)
- **wellRadius** [m] (0.025 to 0.25) - radius of the wellbore (default: 0.05)
- **wellTop** [m] (0 to 500) - depth of well top (default: 500); *linked to Stratigraphy*
- **reservoirDepth** [m] (1000 to 4000) - depth of reservoir (well base) (default: 2000); *linked to Stratigraphy*

The possible outputs from the Open Wellbore component are leakage rates of CO_2 and brine to aquifer and atmosphere. The names of the observations are of the form:

- **CO2_aquifer** and **CO2_atm** [kg/s] - CO_2 leakage rates
- **brine_aquifer** and **brine_atm** [kg/s] - brine leakage rates.

3.8 Generalized Flow Rate Component

The Generalized Flow Rate component model is a model representing wide range of carbon dioxide (CO_2) and brine leakage flow rates and created based on the results of multiple wellbore simulations. The generalized models facilitate the implementation of flow rates in an uncertainty quantification (UQ) framework since the relevant leakage rate and time parameters can be generated randomly. The basic shape for these models were constructed from the results of numerical wellbore simulations based on pressure and saturation profiles derived from the Kimberlina reservoir model [32] coupled with wellbore permeability to yield CO_2 and complimentary brine leakage functions. More details covering derivation and application of the model can be found in [20].

In the IAM control file, the type name for the Generalized Flow Rate component is `GeneralizedFlowRate`. The description of the possible component's parameters are provided below.

- **numberOfShaleLayers** [-] (3 to 30) - number of shale layers in the system (default: 3); *linked to Stratigraphy*. The shale units must be separated by an aquifer.
- **logPeakCO2Rate** [$\log_{10}\ kg/s$] (-inf to 5) - logarithm of the largest CO_2 flow rate (default: -5)
- **timePeakCO2Rate** [years] (0 to 1000) - time to reach the largest CO_2 flow rate from initial time (default: 5)
- **durationPeakCO2Rate** [years] (0 to 1000) - length of time period during which CO_2 flow rate was the largest (default: 10)
- **durationPeakZeroCO2Rate** [years] (0 to 1000) - length of time period during which CO_2 flow rate decreased from the largest rate to zero (default: 100)
- **logInitBrineRate** [$\log_{10}\ kg/s$] (-inf to 5) - logarithm of the initial brine flow rate (default: -10)
- **logFinalBrineRate** [$\log_{10}\ kg/s$] (-inf to 5) - logarithm of the final brine flow rate (default: -11.5). Ratio of initial brine rate over final brine rate is recommended to be between 0.2 and 0.3
- **durationInitBrineRate** [years] (0 to 1000) - length of initial brine flow rate time period (default: 2)
- **durationInitFinalBrineRate** [years] (0 to 1000) - length of time period during which brine flow rate decreased from initial to final rate (default: 10)
- **mitigationTime** [years] (0 to inf) - time at which the leakage was remediated (default: 10000)

The possible outputs from the Generalized Flow Rate component are leakage rates of CO_2 and brine to the aquifer specified by user. The names of the observations are of the form:

- **CO2_aquifer#** [kg/s] - CO_2 leakage rates where # is an aquifer index
- **brine_aquifer#** [kg/s] - brine leakage rates
- **mass_CO2_aquifer#** [kg] - mass of CO_2 leaked into the specified aquifer.

3.9 Seal Horizon Component

The Seal Horizon component model simulates the flow of CO_2 through a low permeability but fractured rock horizon (a "seal" formation) overlying the storage reservoir into which CO_2 is injected.

The rock horizon is represented by a number of "cells" arranged (conceptually) in an arbitrary shape grid. A two-phase, relative permeability approach is used with Darcy's law for one-dimensional (1D) flow computations of CO_2 through the horizon in the vertical direction. The code also allows the simulation of time-dependent processes that can influence such flow.

The model is based on an earlier code, NSealR, created with GoldSim, and described in [18]. A stand-alone version of this code in Python is also available on the NETL EDX system, described as Seal ROM.

In the NRAP-Open-IAM control file, the type name for the component is SealHorizon. The following is a list of the component parameters, including the parameter names, units, accepted value range and the default value.

Reference parameters for each cell:

- **area** [m^2] (1 to 2.6e+5) - area of the cell (default: 10000.0)
- **thickness** [m] (5 to 1000) - thickness of the cell (vertically) (default: 100)
- **baseDepth** [m] (800 to 9500) - depth to the base of seal (default: 1100)
- **permeability** [m^2] (1.0e-22 to 1.0e-15) - cell equivalent initial permeability (default: 1.0e-18)
- **entryPressure** [Pa] (100 to 2.0e+6) - entry threshold pressure that controls flow into rock (default: 5000)

Distribution parameters for thickness of the seal layer

- **aveThickness** [m] (10 to 1000) - mean of the truncated normal distribution for thickness (default: 100)
- **stdDevThickness** [m] (0 to 500) - standard deviation of the thickness distribution (default: 0)
- **minThickness** [m] (5 to 1000) - minimum thickness; this value truncates the distribution and limits lower values (default: 75)
- **maxThickness** [m] (10 to 1000) - maximum thickness; this value truncates the distribution and limits higher values (default: 125)

Note: The setup of the four distribution parameters above is not yet implemented in the control file interface or GUI of NRAP-Open-IAM and available only in the script interface.

Distribution parameters for permeability of the seal layer:

- **avePermeability** [m^2] (1.0e-22 to 1.0e-16) - mean total vertical permeability of a lognormal distribution; equivalent value for fractured rock (default: 2.5e-16)
- **stdDevPermeability** [m^2] (0 to 1.0e-17) - standard deviation of the total vertical permeability distribution (default: 0.0)
- **minPermeability** [m^2] (1.0e-24 to 1.0e-17) - minimum total vertical permeability; this value truncates (censors) the vertical random distribution and limits lower values (default: 1.0e-18)
- **maxPermeability** [m^2] (1.0e-21 to 1.0e-12) - maximum total vertical permeability; this value truncates (censors) the random distribution and limits higher values (default: 1.0e-15)

Note: The setup of the four distribution parameters above is not yet implemented in the control file interface or GUI of NRAP-Open-IAM and available only in the script interface.

- **heterFactor** [-] (1.0e-2 to 100) - increase factor of the permeability of cells selected for heterogeneity, if the heterogeneity approach is used (default: 0.5).

Reference parameters for all cells:

- **aveBaseDepth** [m] (800 to 9500) - average depth to base of cell/reservoir top; interpolation depth (default: 1100)
- **aveBasePressure** [Pa] (1.0e+6 to 6.0e+7) - average pressure at seal base during injection (default: 3.3e+7)
- **aveTemperature** [$^\circ C$] (31 to 180) - average temperature of seal (default: 50)
- **salinity** [ppm] (0 to 80000) - average salinity of seal (default: 1.5e+4)
- **staticDepth** [m] (800 to 9500) - reference depth for computing static pressure at top of seal (default: 1000)
- **staticPressure** [Pa] (1.0e+6 to 6.0e+7) - pressure at static reference depth for computing pressure at the cell top (default: 1.0e+7).

Fluid (conditions) parameters:

- **brineDensity** [kg/m^3] (880 to 1080) - density of brine phase (default: 1004)

- **CO2Density** [kg/m^3] (93 to 1050) - density of CO_2 phase (default: 597.8)
- **brineViscosity** [$Pa{\cdot}s$] (1.5e-4 to 1.6e-3) - viscosity of brine phase (default: 5.634e-4)
- **CO2Viscosity** [$Pa{\cdot}s$] (1.8e-5 to 1.4e-4) - viscosity of CO_2 phase (default: 4.452e-5)
- **CO2Solubility** [mol/kg] (0 to 2) - solubility of CO_2 phase in brine (default: 0.035).

Two-phase model parameters for LET model:

- **wetting1** [-] (0.5 to 5) - wetting phase parameter L (default: 1)
- **wetting2** [-] (0.1 to 30) - wetting phase parameter E (default: 10)
- **wetting3** [-] (0 to 3) - wetting phase parameter T (default: 1.25)
- **nonwet1** [-] (0.5 to 5) - nonwetting phase parameter L (default: 1.05)
- **nonwet2** [-] (0.1 to 30) - nonwetting phase parameter E (default: 10)
- **nonwet3** [-] (0 to 3) - nonwetting phase parameter T (default: 1.25)
- **capillary1** [-] (0.01 to 5) - LET-model parameter L for capillary pressure (default: 0.2)
- **capillary2** [-] (0.01 to 30) - LET-model parameter E for capillary pressure (default: 2.8)
- **capillary3** [-] (0.01 to 3) - LET-model parameter T for capillary pressure (default: 0.43)
- **maxCapillary** [Pa] (100 to 2.0e+8) - maximum capillary pressure for model (default: 1.0e+7)

Note: Parameters wetting1, wetting2, wetting3, nonwet1, nonwet2, nonwet3, capillary1, capillary2, capillary3, and maxCapillary are used only if parameter relativeModel is set to LET.

Parameters for BC model:

- **lambda** [-] (0 to 5) - lambda parameter in Brooks-Corey model (default: 2.5)

Note: Parameter lambda is used only if parameter relativeModel is set to BC.

Additional parameters for two-phase flow:

- **brineResSaturation** [-] (0.01 to 0.35) - residual brine saturation (default: 0.15)
- **CO2ResSaturation** [-] (0 to 0.35) - residual CO_2 saturation (default: 0)
- **relativeModel** [-] (LET or BC) - relative permeability model (default: LET)
- **permRatio** [-] (0 to 1.5) - ratio of nonwetting to wetting permeability (default: 0.6).

Time-model and rock type parameters:

- **influenceModel** [-] (integer: 0, 1, 2) - time-dependent permeability model (default: 0); deterministic parameter, i.e. cannot be set to be random. Model type used to compute the influence factor of the fluid flow on permeability for time-dependent response:
  - 0: No influence factor used.
  - **1: Use a time-dependent model based on exposure time to CO2.** Parameters rateEffect and totalEffect control the initial time delay and the maximum extent of effect.
  - **2: Use a multivariant model that considers reactivity, clayType,** clayContent and carbonateContent values together with rateEffect and totalEffect parameters to establish the magnitude of the influence factor.
- **influence** [-] (0 to 1) - initial permeability influence factor (default: 1)
- **rateEffect** [-] (0.01 to 0.65) - time variance parameter; this parameter controls the initial time delay in the permeability effect of the model (default: 0.1)

- **totalEffect** [-] (0.01 to 200) - Time variance parameter; this parameter defines the total change in permeability of the model (as a factor) (default: 0.1)
- **reactivity** [-] (0 to 10) - reactivity of time model; factor controls the magnitude of permeability change (default: 8)
- **clayType** [-] (smectite, illite, or chlorite) - predominate clay mineral content in the seal horizon, defined as one of following categories:
  - Smectite (high swelling material)
  - Illite (moderate swelling material)
  - Chlorite (low swelling material) (default: smectite)
- **carbonateContent** [%] (0 to 100) - carbonate content in seal layer rock (default: 8)
- **clayContent** [%] (0 to 100) - clay mineral content in seal layer rock (default: 60).

Note: Parameters rateEffect and totalEffect are used only when parameter influenceModel is set to 1 or 2. These parameters control the initial time delay and the maximum extent of effect.

Note: Parameters reactivity, clayType, carbonateContent, and clayContent are used only when parameter influenceModel is set to 2.

The possible outputs from the Seal Horizon component are leakage rates of CO_2 and brine to aquifer through seal layer. The names of the observations are of the form:

- **CO2_aquifer**, **brine_aquifer** [kg/s] - CO_2 and brine leakage rates to aquifer through seal layer (individual cells) into overlying aquifer
- **mass_CO2_aquifer**, **mass_brine_aquifer** [kg] - mass of the CO_2 and brine leaked through seal layer (individual cells) into overlying aquifer
- **CO2_aquifer_total**, **brine_aquifer_total** [kg/s] - cumulative (for all cells) CO_2 and brine leakage rates to aquifer through seal layer into overlying aquifer
- **mass_CO2_aquifer_total**, **mass_brine_aquifer_total** [kg] - cumulative (for all cells) mass of the CO_2 and brine leaked through seal layer into overlying aquifer.

3.10 Fault Flow Component

The Fault Flow component model simulates the flow of carbon dioxide along a low permeability fault from an injection horizon (into which carbon dioxide is injected) up to a freshwater aquifer. The theoretical base is predicated on one-dimension (1D), steady-state, two-phase flow of CO_2 through a saturated discontinuity (parallel plates) under CO_2 supercritical conditions. The flow in the current implementation uses the near-surface CO_2 supercritical point to be the upper point of flow. The surrounding rock matrix is considered relatively impermeable.

In the NRAP-Open-IAM control file, the type name for the Fault Flow component is `FaultFlow`. The description of the component's parameters is provided below:

Fault core setup parameters:

- **strike** [°] (0 to 360) - direction of fault: trend of fault strike taken clockwise from north (default: 30)
- **dip** [°] (10 to 90) - inclination of fault plane from strike, using right-hand rule from strike (default: 70)
- **length** [m] (0 to 10,000) - length of fault trace at surface from start point (default: 100)
- **xStart** [m] (-5.0e+07 to 5.0e+07) - x-coordinate of the fault start point taken as the left point on fault trace (default: 500)

- **yStart** [m] (-5.0e+07 to 5.0e+07) - y-coordinate of the fault start point taken as the left point on fault trace (default: 500)
- **nSegments** [-] (1 to 100) - number of separate fault divisions of the fault (default: 4)
- **faultProbability** [%] (0 to 100) - probability of fault existence (default: 100)

Fault aperture setup parameters:

- **aperture** [m] (0 to 0.05) - effective aperture of fault (default: 2.5e-6)
- **SGR** [-] (0 to 100) - shale gouge ratio for fault (default: 0)
- **stateVariable** [-] (0 to 1) - correction factor for near-surface flow (default: 1)

For variability of fault properties and orientation setup one can use the following eight distribution parameters.

Note: The setup of the eight distribution parameters below is not yet implemented in the control file interface or GUI of NRAP-Open-IAM and available only in the script interface.

Strike distribution parameters:

- **aveStrike** [°] (0 to 360) - average direction of fault: average trend of fault strike taken clockwise from north (default: 90); also default value for no variation in strike
- **spreadStrike** [°] (0 to 180) - spread in strike orientation (range of 2-sigma around average) (default: 0)

Dip distribution parameters:

- **aveDip** [°] (10 to 90) - average inclination of fault plane from strike, using right-hand rule from strike (default: 90)
- **stdDevDip** [°] (0 to 90) - standard deviation of angle of dip (default: 0)

Aperture distribution parameters:

- **aveAperture** [m] (0 to 1.01e-1) - average effective aperture of fault (default: 1.0e-2)
- **stdDevAperture** [m] (0 to 2.0e-2) - standard deviation of effective aperture (default: 0.0)
- **minAperture** [m] (0 to 1.0e-3) - minimum aperture (default: 1.0e-7)
- **maxAperture** [m] (0 to 5.0e-2) - maximum aperture (default: 2.0e-2)

Field parameters:

- **aquiferDepth** [m] (200 to 2,000) - depth to base of deepest aquifer along/above fault (default: 240)
- **aquiferTemperature** [$°C$] (15 to 180) - temperature of brine of deepest aquifer at base (default: 22)
- **aquiferPressure** [Pa] (1.0e+6 to 6.0e+8) - pressure at base of aquifer (default: 1.42E+07)
- **injectDepth** [m] (860 to 20,000) - reference depth positive below grade to top of injection horizon (default: 1880)
- **injectTemperature** [$°C$] (31 to 180) - average temperature of brine at injection depth in reservoir (default: 95)
- **fieldPressure** [Pa] (1.0e+5 to 6.0e+7) - initial pressure at injection depth before injection starts (default: 1.9140e+07)
- **injectPressure** [Pa] (7.0e+6 to 6.0e+8) - average pressure at base during injection period for interpolation of viscosity and density (default: 2.9290E+07)
- **finalPressure** [Pa] (1.0e+5 to 6.0e+7) - final average pressure at injection depth for interpolation of viscosity and density (default: 1.9140e+07)
- **injectX** [m] (-5.0e+07 to 5.0e+07) - x-coordinate of the location of injection well (default: 0)
- **injectY** [m] (-5.0e+07 to 5.0e+07) - y-coordinate of the location of injection well (default: 0)

- **injectEndTime [years] (0 to 10000) - time when injection stops** (default: 50)

Reservoir conditions parameters:

- **salinity** [ppm] (0 to 80000) - salinity of the brine (default: 0). The value is used to compute density and viscosity of the brine
- **CO2Density** [kg/m^3] (93 to 1050) - average density of CO_2 phase for fault (default: 673.84). The value is used if interpolation is not conducted by code
- **CO2Viscosity** [$Pa{\cdot}s$] (1.8e-05 to 1.4e-04) - viscosity of CO_2 phase for fault (default: 5.5173e-05). The value is used if interpolation is not conducted by code
- **brineDensity** [kg/m^3] (880 to 1080) - density of brine phase for fault (default: 974.895). The value is used if interpolation is not conducted by code
- **brineViscosity** [$Pa{\cdot}s$] (1.5e-04 to 1.6e-03) - viscosity of brine phase for fault (default: 3.0491e-04). The value is used if interpolation is not conducted by code
- **CO2Solubility** [mol/kg] (0 to 2) - solubility of CO_2 phase in brine for fault (default: 0.035). The value is used if interpolation is not conducted by code

Aquifer conditions parameters:

- **aquiferCO2Density** [kg/m^3] (93 to 1050) - density of CO_2 phase in the aquifer (default: 886.44)
- **aquiferCO2Viscosity** [$Pa{\cdot}s$] (1.1e-05 to 1.4e-04) - viscosity of CO_2 phase in the aquifer (default: 8.8010e-05)
- **aquiferBrineDensity** [kg/m^3] (880 to 1080) - density of brine phase in the aquifer (default: 1004.10)
- **aquiferBrineViscosity** [$Pa{\cdot}s$] (1.5e-04 to 1.6e-03) - viscosity of brine phase in the aquifer (default: 3.0221e-04)

Relative flow parameters:

- **brineResSaturation** [-] (0.01 to 0.35) - residual wetting brine saturation used in two-phase model (default: 0.15)
- **CO2ResSaturation** [-] (0 to 0.35) - residual nonwetting CO_2 saturation used in two-phase model (default: 0.0)
- **relativeModel** [-] (LET or BC) - relative permeability model (default: LET)
- **permRatio** [-] (0 to 1.5) - ratio of maximum nonwetting permeability to the maximum wetting permeability (default: 0.6)
- **entryPressure** [Pa] (100 to 2.0e+6) - entry/threshold/bubbling pressure that controls flow into rock (default: 5000)

Two-phase model parameters for LET model:

- **wetting1** [-] (0.5 to 5) - wetting phase parameter L (default: 1)
- **wetting2** [-] (1 to 30) - wetting phase parameter E (default: 10)
- **wetting3** [-] (0 to 3) - wetting phase parameter T (default: 1.25)
- **nonwet1** [-] (0.5 to 5) - nonwetting phase parameter L (default: 1.05)
- **nonwet2** [-] (1 to 30) - nonwetting phase parameter E (default: 10)
- **nonwet3** [-] (0 to 3) - nonwetting phase parameter T (default: 1.25)
- **capillary1** [-] (0.01 to 5) - LET-model parameter L for capillary pressure (default: 0.2)
- **capillary2** [-] (0.01 to 30) - LET-model parameter E for capillary pressure (default: 2.8)
- **capillary3** [-] (0.01 to 3) - LET-model parameter T for capillary pressure (default: 0.43)
- **maxCapillary** [Pa] (100 to 2.0e+8) - maximum capillary pressure for model (default: 1.0e+7)

Note: Parameters wetting1, wetting2, wetting3, nonwet1, nonwet2, nonwet3, capillary1, capillary2, capillary3, and maxCapillary are used only if parameter relativeModel is set to LET.

BC model parameters:

- **lambda** [-] (0 to 5) - lambda term in Brooks-Corey model (default: 2.5)

Note: Parameter lambda is used only if parameter relativeModel is set to BC.

Stress parameters:

- **maxHorizontal** [Pa] (0 to 5.0e+7) - secondary maximum horizontal principal stress at top of injection horizon (default: 3.0e+7)
- **minHorizontal** [Pa] (0 to 5.0e+7) - secondary minimum horizontal principal stress at top of injection interval (default: 2.0e+7)
- **maxTrend** [$^\circ$] (0 to 180) - strike of secondary maximum horizontal stress clockwise from north (default: 55)

The possible outputs from the Fault Flow component are leakage rates of CO_2 and brine to aquifer through fault. The names of the observations are of the form:

- **CO2_aquifer**, **brine_aquifer** [kg/s] - CO_2 and brine leakage rates to aquifer through fault (individual segments) into overlying aquifer
- **mass_CO2_aquifer**, **mass_brine_aquifer** [kg] - mass of the CO_2 and brine through fault (individual segments) to overlying aquifer
- **CO2_aquifer_total**, **brine_aquifer_total** [kg/s] - cumulative CO_2 and brine leakage rates to aquifer through fault into overlying aquifer
- **mass_CO2_aquifer_total**, **mass_brine_aquifer_total** [kg] - cumulative mass of the CO_2 and brine through fault (individual cells) to overlying aquifer.

Observations with names CO2_aquifer, brine_aquifer, mass_CO2_aquifer and mass_brine_aquifer are provided as arrays of values of length equal to the number of fault segments. To output observations corresponding to a particular fault segment (e.g., segment 1) one can add observations with names CO2_aquifer_segm# where # is an index of a segment of interest (e.g., CO2_aquifer_segm1) to the output of the Fault Flow component.

3.11 Carbonate Aquifer Component

The Carbonate Aquifer component model is a reduced-order model that can be used to predict the impact that carbon dioxide (CO_2) and brine leaks from a CO_2 storage reservoir might have on overlying aquifers. The model predicts the size of "impact plumes" according to nine water quality metrics, see [1], [6], [16].

Although the Carbonate Aquifer model was developed using site-specific data from the Edwards aquifer, the model accepts aquifer characteristics as variable inputs and, therefore, may have more broad applicability. Careful consideration should be given to the hydrogeochemical character of the aquifer before using this model at a new site. Guidelines and examples are presented in [15].

The size of "impact plumes" are calculated using two alternative definitions of "impact" which should be selected by user: 1) changes that cause an exceedance of a drinking water standard or maximum contaminant level (MCL); and 2) changes that are above and beyond "natural background variability" in the aquifer, [17].

Component model input definitions:

- **ithresh** [-] (1 or 2) - threshold, either 1: MCL or 2: No-impact (default: 2)
- **rmin** [m] (0 to 100) - maximum distance between leaks for them to be considered one leak (default: 15)
- **perm_var** [$\log_{10} m^4$] (0.017 to 1.89) - logarithm of permeability variance (default: 0.9535)

- **corr_len** [m] (1 to 3.95) - correlation length (default: 2.475)
- **aniso** [-] (1.1 to 49.1) - anisotropy factor: ratio of horizontal to vertical permeability (default: 25.1)
- **mean_perm** [$\log_{10} m^2$] (-13.8 to -10.3) - logarithm of mean permeability (default: -12.05)
- **hyd_grad** [-] (2.88e-4 to 1.89e-2) - horizontal hydraulic gradient (default: 9.59e-03)
- **calcite_ssa** [m^2/g] (0 to 1.0e-2) - calcite surface area (default: 5.5e-03)
- **organic_carbon** [-] (0 to 1.0e-2) - organic carbon volume fraction (default: 5.5e-03)
- **benzene_kd** [$\log_{10}$ K_oc] (1.49 to 1.73) - benzene distribution coefficient (default: 1.61)
- **benzene_decay** [$\log_{10}$ day] (0.15 to 2.84) - benzene decay constant (default: 0.595)
- **nap_kd** [$\log_{10}$ K_oc] (2.78 to 3.18) - naphthalene distribution coefficient (default: 2.98)
- **nap_decay** [$\log_{10}$ day] (-0.85 to 2.04) - naphthalene decay constant (default: 0.595)
- **phenol_kd** [$\log_{10}$ K_oc] (1.21 to 1.48) - phenol distribution coefficient (default: 1.35)
- **phenol_decay** [$\log_{10}$ day] (-1.22 to 2.06) - phenol decay constant (default: 0.42)
- **cl** [$\log_{10}$ molality] (0.1 to 6.025) - brine salinity (default: 0.776)
- **logf** [-] (0 or 1) - type of transform of output plume volume; 0: linear, 1: log (default: 0)
- **aqu_thick** [m] (100 to 500) - aquifer thickness (default: 300); *linked to Stratigraphy*

Component model dynamic inputs:

- **brine_rate** [kg/s] (0 to 0.075) - brine rate
- **brine_mass** [kg] (0 to 2.0e+8) - cumulative brine mass
- **co2_rate** [kg/s] (0 to 0.5) - CO_2 rate
- **co2_mass** [kg] (0 to 2.0e+9) - cumulative CO_2 mass.

Possible observations from the Carbonate Aquifer component are:

- **pH_volume** [m^3] - volume of aquifer below pH threshold
- **Flux** [kg/s] - CO_2 leakage rate to atmosphere
- **dx** [m] - length of impacted aquifer volume in x-direction
- **dy** [m] - width of impacted aquifer volume in y-direction
- **TDS_volume** [m^3] - volume of aquifer above TDS threshold in mg/L
- **As_volume** [m^3] - volume of aquifer above arsenic threshold in $\mu g/L$
- **Pb_volume** [m^3] - volume of aquifer above lead threshold in $\mu g/L$
- **Cd_volume** [m^3] - volume of aquifer above cadmium threshold in $\mu g/L$
- **Ba_volume** [m^3] - volume of aquifer above barium threshold in $\mu g/L$
- **Benzene_volume** [m^3] - volume of aquifer above benzene threshold
- **Naphthalene_volume** [m^3] - volume of aquifer above naphthalene threshold
- **Phenol_volume** [m^3] - volume of aquifer above phenol threshold.

3.12 Deep Alluvium Aquifer Component

The Deep Alluvium Aquifer component model is a reduced order model which can be used to predict the changes in diluted groundwater chemistry if CO_2 and brine were to leak into a deep alluvium aquifer similar to the one located below the Kimberlina site, in the Southern San Joaquin Valley, California. The protocol allows uncertainty and variability in aquifer heterogeneity, fluid transport, and potential CO_2 and brine leakage rates from abandoned or damaged oil and gas wells to be collectively evaluated to assess potential changes in groundwater pH, total dissolved solids (TDS), and changes in the aquifer pressure resulting from leakage.

Although the Deep Alluvium Aquifer model was developed using site-specific data from the LLNL's Kimberlina Model (version 1.2), the model accepts aquifer characteristics as variable inputs and, therefore, may have broader applicability. Careful consideration should be given to the hydrogeochemical character of the aquifer before using this model at a new site.

Model was created using the `py-earth` Python package [28]. Simulation data used to build this model was created by Mansoor et al. [19]. In the NRAP-Open-IAM control file, the type name for the Deep Alluvium Aquifer component is `DeepAlluviumAquifer`.

Component model input definitions:

- **logK_sand1** [$\log_{10} m^2$] (-12.92 to -10.92) - permeability of layer 1 at depth between 10 and 546 m (default: -11.92)
- **logK_sand2** [$\log_{10} m^2$] (-12.72 to -10.72) - permeability of layer 2 at depth between 546 and 1225 m (default: -11.72)
- **logK_sand3** [$\log_{10} m^2$] (-12.7 to -10.7) - permeability of layer 3 at depth between 1225 and 1411 m (default: -11.70)
- **logK_caprock** [$\log_{10} m^2$] (-16.699 to -14.699) - permeability of caprock at depth between 0 and 10 m (default: -15.70)
- **correlationLengthX** [m] (200 to 2000) - correlation length in x-direction (default: 1098.99)
- **correlationLengthZ** [m] (10 to 150) - correlation length in z-direction (default: 79.81)
- **sandFraction** [-] (0.7 to 0.9) - sand volume fraction (default: 0.8)
- **groundwater_gradient** [-] (0.001000 to 0.001667) - regional groundwater gradient (dh/dx=change in hydraulic head/distance) (default: 0.001333)
- **leak_depth** [m] (424.36 to 1341.48) - depth of leakage interval (default: 885.51).

Component model dynamic inputs:

- **brine_rate** [kg/s] (0 to 0.017) - brine rate (default: 0.0003)
- **brine_mass** [kg] (238.14419 to 8689604.29) - cumulative brine mass (default: 84722.74=10**4.928)
- **co2_rate** [kg/s] (0 to 0.385) - CO_2 rate (default: 0.045)
- **co2_mass** [kg] (1.002 to 1.621e+9) - cumulative CO_2 mass (default: 1.636e+7=10**7.214).

Observations from the Deep Alluvium Aquifer component are:

- **TDS_volume** [m^3] - volume of plume above baseline TDS change in mg/L (change in TDS > 100 mg/L)
- **TDS_dx** [m] - length of plume above baseline TDS change in mg/L (change in TDS > 100 mg/L)
- **TDS_dy** [m] - width of plume above baseline TDS change in mg/L (change in TDS > 100 mg/L)
- **TDS_dz** [m] - height of plume above baseline TDS change in mg/L (change in TDS > 100 mg/L)
- **Pressure_volume** [m^3] - volume of plume above baseline pressure change in Pa (change in pressure > 500 Pa)

- **Pressure_dx** [m] - length of plume above baseline pressure change in Pa (change in pressure > 500 Pa)
- **Pressure_dy** [m] - width of plume above baseline pressure change in Pa (change in pressure > 500 Pa)
- **Pressure_dz** [m] - height of plume above baseline pressure change in Pa (change in pressure > 500 Pa)
- **pH_volume** [m^3] - volume of plume below pH threshold (pH < 6.75)
- **pH_dx** [m] - length of plume below pH threshold (pH < 6.75)
- **pH_dy** [m] - width of plume below pH threshold (pH < 6.75)
- **pH_dz** [m] - height of plume below pH threshold (pH < 6.75).

3.13 FutureGen2 Aquifer Component

The FutureGen 2.0 Aquifer component model is a reduced order model that can be used to predict the impact that carbon dioxide (CO_2) and brine leakage from the CO_2 storage reservoir at the FutureGen 2.0 site might have on overlying aquifers or monitoring units. The model predicts the size of "impact plumes" according to four metrics: pH, total dissolved solids (TDS), pressure and dissolved CO_2.

The FutureGen 2.0 Aquifer model is a regression model fitted to the results of STOMP-CO2E-R multiphase flow and reactive transport simulations of CO_2 and brine leakage using the `py-earth` Python package ([28]). The `py-earth` package is a Python implementation of the Multivariate Adaptive Regression Splines algorithm ([7]), in the style of `scikit-learn` ([26]), a library of machine-learning methods.

The aquifer simulations used to train the FutureGen 2.0 Aquifer component model were based on modeling done for monitoring program design at the FutureGen 2.0 site ([31]), as well as porosity and permeability values from the ELAN logs and core samples taken from the characterization well. Isothermal simulations were performed for training the aquifer component model.

In the NRAP-Open-IAM control file, the type name for the FutureGen 2.0 Aquifer component is `FutureGen2Aquifer`. The description of the possible component's parameters are provided below:

- **aqu_thick** [m] (30 to 90) - thickness of unit (default: 33.2); *linked to Stratigraphy*
- **depth** [m] (100 to 700) - depth to bottom of unit (default: 590.1); *linked to Stratigraphy*
- **por** [-] (0.02 to 0.2) - porosity of unit (default: 0.118)
- **log_permh** [$\log_{10} m^2$] (-14 to -11) - horizontal permeability (default: -13.39)
- **log_aniso** [$\log_{10}$] (0 to 3) - anisotropy ratio (default: 0.3)
- **rel_vol_frac_calcite** [-] (0 to 1) - relative volume fraction of calcite in solid phase (default: 0.01).

Component model dynamic inputs:

- **brine_rate** [kg/s] (0 to 31.622) - brine rate
- **brine_mass** [kg] (0 to 6.985e+10) - cumulative brine mass
- **co2_rate** [kg/s] (0 to 31.622) - CO_2 rate
- **co2_mass** [kg] (0 to 6.985e+10) - cumulative CO_2 mass.

Observations from the FutureGen 2.0 Aquifer component are:

- **Pressure_volume** [m^3] - volume of plume where relative change in pressure > 0.065%
- **Pressure_dx** [m] - length of plume where relative change in pressure > 0.065%
- **Pressure_dy** [m] - width of plume where relative change in pressure > 0.065%
- **Pressure_dz** [m] - height of plume where relative change in pressure > 0.065%

- **pH_volume** [m^3] - volume of plume where absolute change in pH > 0.2
- **pH_dx** [m] - length of plume where absolute change in pH > 0.2
- **pH_dy** [m] - width of plume where absolute change in pH > 0.2
- **pH_dz** [m] - height of plume where absolute change in pH > 0.2
- **TDS_volume** [m^3] - volume of plume where relative change in TDS > 10%
- **TDS_dx** [m] - length of plume where relative change in TDS > 10%
- **TDS_dy** [m] - width of plume where relative change in TDS > 10%
- **TDS_dz** [m] - height of plume where relative change in TDS > 10%
- **Dissolved_CO2_volume** [m^3] - volume of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dx** [m] - length of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dy** [m] - width of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dz** [m] - height of plume where relative change in dissolved CO_2 concentration > 20%

3.14 FutureGen2 AZMI Component

The FutureGen 2.0 Above Zone Monitoring Interval (AZMI) component model is a reduced order model that can be used to predict the impact that carbon dioxide (CO_2) and brine leakage from the CO_2 storage reservoir at the FutureGen 2.0 site might have on overlying aquifers or monitoring units. The model predicts the size of "impact plumes" according to five metrics: pH, total dissolved solids (TDS), pressure, dissolved CO_2 and temperature.

The FutureGen 2.0 AZMI model is a regression model fitted to the results of STOMP-CO2E-R multiphase flow and reactive transport simulations of CO_2 and brine leakage using the `py-earth` Python package ([28]). The `py-earth` package is a Python implementation of the Multivariate Adaptive Regression Splines algorithm ([7]), in the style of `scikit-learn` ([26]), a library of machine-learning methods.

The aquifer simulations used to train the FutureGen 2.0 AZMI component model were based on modeling done for monitoring program design at the FutureGen 2.0 site ([31]), as well as porosity and permeability values from the ELAN logs and core samples taken from the characterization well. Nonisothermal simulations were performed for training the AZMI component model.

In the NRAP-Open-IAM control file, the type name for the FutureGen 2.0 AZMI component is `FutureGen2AZMI`. The description of the possible component's parameters are provided below:

- **aqu_thick** [m] (30 to 90) - thickness of unit (default: 33.2); *linked to Stratigraphy*
- **depth** [m] (700 to 1600) - depth to bottom of unit (default: 1043.9); *linked to Stratigraphy*
- **por** [-] (0.02 to 0.2) - porosity of unit (default: 0.118)
- **log_permh** [$\log_{10}$ m^2] (-14 to -11) - horizontal permeability (default: -13.39)
- **log_aniso** [$\log_{10}$] (0 to 3) - anisotropy ratio (default: 0.3)
- **rel_vol_frac_calcite** [-] (0 to 1) - relative volume fraction of calcite in solid phase (default: 0.01).

Component model dynamic inputs:

- **brine_rate** [kg/s] (0 to 31.622) - brine rate
- **brine_mass** [kg] (0 to 6.985e+10) - cumulative brine mass
- **co2_rate** [kg/s] (0 to 31.622) - CO_2 rate
- **co2_mass** [kg] (0 to 6.985e+10) - cumulative CO_2 mass.

Observations from the FutureGen 2.0 AZMI component are:

- **Pressure_volume** [m^3] - volume of plume where relative change in pressure > 0.065%
- **Pressure_dx** [m] - length of plume where relative change in pressure > 0.065%
- **Pressure_dy** [m] - width of plume where relative change in pressure > 0.065%
- **Pressure_dz** [m] - height of plume where relative change in pressure > 0.065%
- **pH_volume** [m^3] - volume of plume where absolute change in pH > 0.2
- **pH_dx** [m] - length of plume where absolute change in pH > 0.2
- **pH_dy** [m] - width of plume where absolute change in pH > 0.2
- **pH_dz** [m] - height of plume where absolute change in pH > 0.2
- **TDS_volume** [m^3] - volume of plume where relative change in TDS > 10%
- **TDS_dx** [m] - length of plume where relative change in TDS > 10%
- **TDS_dy** [m] - width of plume where relative change in TDS > 10%
- **TDS_dz** [m] - height of plume where relative change in TDS > 10%
- **Dissolved_CO2_volume** [m^3] - volume of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dx** [m] - length of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dy** [m] - width of plume where relative change in dissolved CO_2 concentration > 20%
- **Dissolved_CO2_dz** [m] - height of plume where relative change in dissolved CO_2 concentration > 20%
- **Temperature_volume** [m^3] - volume of plume where relative change in temperature > 0.03%
- **Temperature_dx** [m] - length of plume where relative change in temperature > 0.03%
- **Temperature_dy** [m] - width of plume where relative change in temperature > 0.03%
- **Temperature_dz** [m] - height of plume where relative change in temperature > 0.03%

3.15 Generic Aquifer Component

The Generic Aquifer component model is a surrogate model that can be used to predict the leakage of carbon dioxide (CO_2) and brine from a CO_2 storage reservoir. The model predicts the mass fraction of CO_2 and salt on a 100x10 radial grid surrounding the leaky well and outputs these as gridded observations. The model also predicts the volume and dimensions of aquifer where pore water concentrations exceed specified threshold values of dissolved CO_2 and salt.

The Generic Aquifer model is a machine learning regression model fitted to the results of STOMP-CO2E-R multiphase flow and reactive transport simulations of CO_2 and brine leakage using Tensorflow 2.4. 50,000 nonisothermal multiphase flow simulations were used to train the Generic Aquifer component model. Input parameters were varied using Latin Hypercube Sampling across wide ranges.

In the NRAP-Open-IAM control file, the type name for the Generic Aquifer component is `GenericAquifer`. The description of the component's parameters are provided below:

- **aqu_thick** [m] (25 to 250) - thickness of unit (default: 33.2); *linked to Stratigraphy*
- **top_depth** [m] (100 to 4100) - depth to the top of the aquifer (default: 590.1); *linked to Stratigraphy*
- **por** [-] (0.02 to 0.25) - porosity of unit (default: 0.118)
- **log_permh** [$\log_{10} m^2$] (-14 to -10) - horizontal permeability (default: -13.39)
- **log_aniso** [-] (0 to 3) - anisotropy ratio Kh/Kv (default: 0.3)

- **aquifer_salinity** [-] (0.0 to 0.015) - salt mass fraction in aquifer water (default: 0.005)
- **reservoir_salinity** [-] (0.015 to 0.05) - salt mass fraction in leak water (default: 0.03)
- **dissolved_salt_threshold** [-] (0.0 to 1.0) - threshold for salt mass fraction (default: 0.02)
- **dissolved_co2_threshold** [-] (0.0 to 1.0) - threshold for CO2 mass fraction (default: 0.01)

Component model dynamic inputs:

- **brine_mass** [kg] (0 to 6.985e+10) - cumulative brine mass
- **co2_mass** [kg] (0 to 6.985e+10) - cumulative CO_2 mass.

Observations from the Generic Aquifer component are:

- **Dissolved_salt_volume** [m^3] - volume of plume where relative change in salt mass fraction > dissolved_salt_threshold
- **Dissolved_salt_dr** [m] - radius of plume where relative change in salt mass fraction > dissolved_salt_threshold
- **Dissolved_salt_dz** [m] - height of plume where relative change in salt mass fraction > dissolved_salt_threshold
- **Dissolved_CO2_volume** [m^3] - volume of plume where dissolved CO_2 mass fraction > dissolved_co2_threshold
- **Dissolved_CO2_dr** [m] - radius of plume where dissolved CO_2 mass fraction > dissolved_co2_threshold
- **Dissolved_CO2_dz** [m] - height of plume where dissolved CO_2 mass fraction > dissolved_co2_threshold

Gridded observations from the Generic Aquifer component are:

- **Dissolved_CO2_mass_fraction** [-] - mass fraction of CO_2 in aquifer pore water on a 100x10 radial grid surrounding the leaky well
- **Dissolved_salt_mass_fraction** [-] - mass fraction of salt in aquifer pore water on a 100x10 radial grid surrounding the leaky well

3.16 Atmospheric Model Component

The Atmospheric model is meant to be used for performing scoping studies for CO_2 dispersion after leakage out of the ground. The employed method is an extension of the nomograph approach of Britter and McQuaid (1988) [3] developed for estimating dense gas plume length from a single or multiple leakage sources. The method is very fast and, therefore, amenable to general system-level geologic carbon sequestration (GCS) risk assessment. The method is conservative: it assumes the wind could be from any direction and handles multiple sources by a simple superposition approach [37]. A user's manual for the standalone model is available at [36].

The model is intended to be used for large CO_2 leakage rates (e.g., leakage from an open wellbore). It may not be suitable for very small leakage rate, as, in general, small release rates (e.g., less than 1.0e-5 kg/s) do not form a dense gas release due to ambient mixing. The inputs to the model are leakage rate(s) from leaky well(s), location(s) of leaky well(s), ambient conditions (wind speed), and receptor locations (home or business locations where people are present). The outputs from the model are flags at receptors indicating whether the CO_2 concentration at the location exceeds a pre-defined critical value, and the critical downwind distance from the sources.

Within the control file interface, receptor locations can be specified with the `receptors` keyword argument assigned a full path (including a name) to a csv file containing x- and y-coordinates of the receptors. Alternatively, the `x_receptor` and `y_receptor` keywords can be assigned a list of x- and y-coordinates of the receptors, respectively. In the NRAP-Open-IAM control file, the type name for the Atmospheric model component is `AtmosphericROM`.

Component model input definitions:

- **T_amb** [$°C$] (5 to 40) - ambient temperature (default: 15)
- **P_amb** [atmosphere] (0.7 to 1.08)- ambient pressure (default: 1)

- **V_wind** [m/s] (1.e-10 to 20)- wind velocity (default: 5)
- **C0_critical** [-] (0.002 to 0.1) - critical concentration (default: 0.01)
- **T_source** [$^{\circ}C$] (5 to 50) - released CO_2 temperature (default: 15)
- **x_receptor** [m] - x-coordinate of receptor
- **y_receptor** [m] - y-coordinate of receptor

Possible observations from the Atmospheric Model component are:

- **outflag_r###** [-] - count of critical distances receptor is within from original leak points; here, ### is a receptor number starting at 000
- **num_sources** [-] - number of sources. The possible maximum is a number of leakage points; could be less as leakage sources can potentially coalesce.
- **x_new_s###** [m] - x-coordinate of leakage source; here ### is a source number starting at 000
- **y_new_s###** [m] - y-coordinate of leakage source
- **critical_distance_s###** [m] - critical downwind distance from each source.

3.17 Plume Stability Component

The Plume Stability component model produces quantitative metrics of the area, change in area over time, mobility and spreading [10]. Plume mobility is the effective centroid velocity including the speed and direction of movement. Plume spreading is the effective longitudinal dispersion of the plume along its direction of maximum elongation. This direction is returned by the model as well. The mobility and spreading metrics are comprehensive in that they can effectively handle and account for complex continuous and discontinuous plumes and intra-plume migration. The metrics are calculated using 2D-scalar attribute field values as inputs. The model can read in field values formatted in the NRAP-Open-IAM dataset format. In order to process 3D scalar field data for the model, it is recommended to collapse the 3D data to 2D using a maximization approach as described in [10].

In the NRAP-Open-IAM control file, the type name for the Plume Stability component is `PlumeStability`. The data files providing input for the Plume Stability component need to satisfy the same requirements imposed on the data files used as input for the Lookup Table Reservoir component. In particular, for control file setup of the Plume Stability component the following three keywords have the same meaning:

- `FileDirectory` is a directory where files with the simulation data for the component are located, and which contains files described below;
- `TimeFile` keyword specifies a name of the .csv file that stores the time points (in years) at which the results in the data files are provided;
- `ParametersFilename` keyword contains a name of the .csv file containing the names and values of the parameters used to create the given set of data files; in addition, it lists the names of the .csv files in the folder `FileDirectory` containing simulation data for each of the data file in the set.

The additional keywords of the component's control file interface are:

- `Variables` is a list of observations names provided in the data files and for which some (or all) metrics will be calculated;
- `Thresholds` is a dictionary of pairs (observation name, value) providing threshold value above which the change in the observation value should be taken into account for the calculation of the plume stability metrics.

The only component model input parameter is `index` which indicates the index of the data file from the list in the last column of `ParametersFilename` to be used to produce plume stability metrics. The minimum and maximum value of the parameter is defined by the indices of data files provided in the list.

Possible observations from the Plume Stability component are

- **{obs}_areas** - area of the plume above the predefined threshold
- **{obs}_areas** - change in the area of the plume above the predefined threshold
- **{obs}_mobility** - velocity of centroid of the plume above the predefined threshold
- **{obs}_mobility_angles** - angles/direction at which the centroid of the plume above the predefined threshold is changing
- **{obs}_spreading** - longitudinal dispersion of the plume above the predefined threshold along its direction of maximum elongation
- **{obs}_spreading_angles** - angles/direction at which the dispersion of the plume occurs.

Above, {obs} determines the name of observation for which the plume stability metrics are to be calculated and for which the data is provided in the data files used as input for the component, e.g. pressure, CO2saturation, etc.

3.18 Chemical Well Sealing Component

The Chemical Well Sealing component is based on the model described in [12]. It predicts whether a fracture at the cement caprock interface, upon exposure to CO_2, would self-seal or not due to calcite precipitation. The model couples two-phase flow of supercritical CO_2 and brine through fractures, advective and diffusive transport along the fracture, diffusive transport within the cement, and chemical reactions between cement and carbonated brine. If the fracture is predicted to self-seal, the time required for sealing is also computed. The original model is described in [33], [35], and [13] and was calibrated using experimental data presented in [33], [35], and [34].

Component model input definitions:

- **fractureAperture** $[m]$ (1.0e-5 to 2.0e-3) - aperture of the fractured leakage path (default: 2.0e-5). Any input aperture that is lower than 10 micron (lower bound) is set to 10 micron.
- **fractureLength** $[m]$ (10.0 to 400.0) - length of the fractured leakage path (default: 20)
- **maxOverpressure** $[Pa]$ (1.0e+6 to 1.5e+7) - maximum overpressure the base of the fracture is expected to experience (default: 5.0e+6).

The output from the Chemical Well Sealing component informs about the sealing ability of the fractured leakage pathway. In case the fracture seals, the component would also report sealing time.

- **seal_flag** [-] - flag informing whether a fracture would seal (1) or not (0) due to calcite precipitation
- **seal_time** $[s]$ - predicted time for sealing a fracture by calcite recipitation. If fracture doesn't seal this variable is set to 0.0.

CHAPTER

FOUR

COMPONENT COMPARISON

This section of the documentation provides the comparison tables for the wellbore component models available in NRAP-Open-IAM.

Table 4.1 provides comparison of the models parameters.

Table 4.1: Comparison of wellbore components in NRAP-Open-IAM

Input variable	Cemented wellbore ROM	Multisegmented wellbore ROM	Open wellbore ROM
logWellPerm (well Permeability)	-13.95 to -10.1	-17 to -9	Open tubing or casing
logAquPerm or logThiefPerm (aquifer or thief zone permeability)	-13.995 to -12	-14 to -9	log of aquifer and reservoir transmissivity: -11.27 to -8.39
wellRadius (radius of the leaky well)	0.025 to 0.25	0.01 to 0.5	0.025 to 0.25
Brine and CO_2 properties	Included in the ROM simulations	Calculated as a function of depth. Pressure gradient: 9792 Pa/m. Temperature gradient: 25 C/km.	Mass fraction of salt: 0 to 0.2. Temperature gradient: 25 C/km. Temperature at surface: 15 degrees Celcius.
Number of shale layers	3	3 to 30	1
reservoirDepth and wellDepth (depth of the reservoir, well)	960 to 3200	No limitation	1000 to 4000
shaleThickness, aquiferThickness, reservoirThickness (thickness of shale, aquifer or reservoir)	reservoir: 51.2 m, thief zone: 22.4 m, aquifer: 29.2 m, upper caprock layer: 11.2 m	1 to 1600 m	Well Top: 0 to 500 m
brineResSaturation (residual brine saturation)	0.001	Used as tuning parameter to allow CO_2 to accumulate in intermediate aquifers	Not needed
deltaP (increase in pressure due to injection)	0.1 to 9.3 MPa	No limitations	0 to 20 MPa
Energy transport consideration	Nonisothermal	Isothermal	Nonisothermal
Governing wellbore equation employed	Two phase Darcy equation	Two phase Darcy equation	Drift flux
Type of ROM	numerical	analytical	numerical

continues on next page

Table 4.1 – continued from previous page

Input variable	Cemented wellbore ROM	Multisegmented wellbore ROM	Open wellbore ROM
Reference	D. R. Harp, R. Pawar, J. W. Carey, C. W. Gable, Reduced order models of transient CO_2 and brine leakage along abandoned wellbores from geologic carbon sequestration reservoirs, Int. J. Greenhouse Gas Control, 45 (2016), pp. 150-162	S. Baek, D. H. Bacon, N. J. Huerta, NRAP-Open-IAM Multisegmented Wellbore Reduced-Order Model, 2021, PNNL-32364	L. H. Pan, S. W. Webb, C. M. Oldenburg, Analytical solution for two-phase flow in a wellbore using the drift-flux model. Adv. Water Resour. 34 (2011), pp. 1656-1665

Table 4.2 describes limitations of each model.

Table 4.2: Limitations of the wellbore components in NRAP-Open-IAM

Cemented wellbore ROM	Multisegmented wellbore ROM	Open wellbore ROM
Limited flexibility in specifying layer thicknesses	Deviations from full physics simulations due to analytical nature of the model	The ROM was derived from short-time simulations. Simulations were terminated after 1,000-time steps or 100 hours, whichever came first. It should not be used for long term predictions if leakage rate is high and would result in significant mass loss from reservoir.
Limited flexibility in specifying the number of thief zones (only 1 thief zone supported)	Large shale thicknesses, "Large wellbore segment length for shale (or cap rock) layers may lead to errors due to the nature of the analytical approach employed. Less than 100 m for each segment is recommended with the current model. Although a particular combination of model parameters can relax the degree of the error or enlarge the applicable length of the segment, the quality of the performance is not guaranteed with large segment lengths."	

continues on next page

Table 4.2 – continued from previous page

Cemented wellbore ROM	Multisegmented wellbore ROM	Open wellbore ROM
Limitations on total reservoir pressure change. Reservoir pressure changes greater than 9.3 MPa are outside the bounds of the model. Pressure changes in saline aquifers are typically below this range. However, pressure changes can be larger than this range in other formations that are more limited in extent (e.g., depleted gas fields)	No leakage of CO_2 in intermediate aquifers, "The analytical model does not consider the lateral leakage into intermediate aquifers, resulting in zero accumulation of CO_2 in intermediate aquifers. All the CO_2 is transported to the topmost aquifer, yielding an overestimation of the amount of CO_2 leaking into the topmost aquifer. Residual brine saturation can be used as a proxy for lateral leakage into intermediate aquifers. Users can calibrate this parameter to yield a desirable CO_2 leakage rate/mass into the thief layers (intermediate aquifers). The parameter would have to be recalibrated if any of the other input parameters, like reservoir pressure, well permeability, etc., are changed."	
Limitations of the first and second derivative of pressure and saturation changes		

CHAPTER

FIVE

USE CASES

In the folder *examples/Control_Files* there are a number of example control files distributed with the NRAP-Open-IAM tool. The description of the files is provided in the Table 5.1.

Table 5.1: Control file examples distributed with NRAP-Open-IAM

File name	Included components	Comments
ControlFile_ex1.yaml	Simple reservoir, cemented wellbore	Forward simulation. The saturation and pressure output produced by simple reservoir model is used as input for cemented wellbore model. The example produces three plots. The first two plots is of the CO_2 leakage rates into the intermediate aquifer (aquifer 1) and the shallow aquifer (aquifer 2). The third plot is of the pressure in the reservoir at the wellbore locations.
ControlFile_ex2.yaml	Simple reservoir, multisegmented wellbore	Latin hypercube sampling, 30 realizations. A fixed seed can be specified for the sampling setup: symbol # before the seed has commented it out. This example shows an alternative way to specify wellbore locations inside the wellbore component specification with the `Locations` keyword.
ControlFile_ex3.yaml	Simple reservoir, multisegmented wellbore, carbonate aquifer	Latin hypercube sampling, 30 realizations. Example illustrates use of known and random wellbore locations.
ControlFile_ex4.yaml	Simple reservoir, open wellbore, carbonate aquifer	Latin hypercube sampling, 30 realizations. Example demonstrates several plotting options: `TimeSeries`, `TimeSeriesStats`, and `TimeSeriesAndStats`. For analysis of the large number of realizations a user might find it more helpful to plot the time series statistics rather than the data for each realization using `TimeSeriesStats` plotting option. `TimeSeriesAndStats` plots the simulated values and the related statistics. The `subplot` keyword can be used to present some of the results in subplots.
ControlFile_ex5.yaml	Simple reservoir, cemented wellbore	Example is used to demonstrate parameter study analysis.

continues on next page

Table 5.1 – continued from previous page

File name	Included components	Comments
ControlFile_ex6.yaml	Lookup table based reservoir	Latin hypercube sampling, 10 realizations. To run this example, the additional *Kimberlina* data set have to be downloaded and unzipped into the *source/components/reservoir/lookuptables/Kimb_54_sims* folder. The data files can be downloaded from the same EDX directory where the NRAP-Open-IAM was downloaded or from https://gitlab.com/NRAP/Kimberlina_data. The data set comes from simulation work done by Wainwright et. al. [32].
ControlFile_ex7a.yaml	Multisegmented wellbore	Latin hypercube sampling, 30 realizations. Example illustrates the use of dynamic input to drive a wellbore model without attaching a reservoir model. This functionality can be used to quickly evaluate behavior of a single component model with a fixed input or interactions between several component models without constructing a full systems model. In the example the dynamic input is provided as a list of pressure and CO_2 saturation data at the simulation time points.
ControlFile_ex7b.yaml	Multisegmented wellbore	Latin hypercube sampling, 30 realizations. Example illustrates the use of dynamic input to drive a wellbore model without attaching a reservoir model. In the example the dynamic input is provided as a path to the file containing pressure and CO_2 saturation data at the simulation time points.
ControlFile_ex8.yaml	Simple reservoir, open wellbore, carbonate aquifer	Latin hypercube sampling, 1000 realizations. Example demonstrates the use of the `Analysis` section to compute correlation and sensitivity coefficients and create visualizations of the analysis results. Each subsection of the `Analysis` section shows all available options for the user to control (required inputs are marked as such).
ControlFile_ex9.yaml	Simple reservoir, open wellbore, atmospheric ROM	Latin hypercube sampling, 30 realizations. The AtmosphericROM model simulates CO_2 dispersion in the atmosphere as a dense gas leak. Example illustrates two plotting options available only for the AtmosphericROM model. `AtmPlumeSingle` keyword can be used to plot the critical distance from leakage points for a single realization. For multiple Monte-Carlo simulations probability of being within a critical distance can be estimated and plotted using `AtmPlumeEnsemble` keyword. Both types of plots produce a map-view of the release area for each time step. It is recommended that *{time_index}* modifier is provided to the `savefig` keyword argument so that an image for each time-step plot produced can be saved in a separate file.
ControlFile_ex10.yaml	Lookup table based reservoir, cemented wellbore, deep alluvium aquifer	Latin hypercube sampling, 30 realizations. Example illustrates a setup connecting lookup table based reservoir, wellbore and aquifer impact components.

continues on next page

Table 5.1 – continued from previous page

File name	Included components	Comments
ControlFile_ex11.yaml	Simple reservoir, multisegmented wellbore, carbonate aquifer	Forward simulation. The saturation/pressure output produced by simple reservoir model is used to drive leakage from five multisegmented wellbore models separated into two groups according to their properties. Two carbonate aquifer components are linked to both groups of wellbores and estimate the impact from the leakage of CO_2 and brine into the aquifers 1 and 2.
ControlFile_ex12.yaml	Generalized flow rate	Forward simulation. Example simulates brine and CO_2 leakage rates to the deepest aquifer (aquifer 1) illustrating the use of the generalized flow rate component. The component does not require linking to other components.
ControlFile_ex13.yaml	Generalized flow rate, carbonate aquifer	Forward simulation. Example computes the leakage rates of brine and CO_2 to aquifers 1 and 2 utilizing the generalized flow rate component, and calculates the associated impact with the help of carbonate aquifer component.
ControlFile_ex14.yaml	Lookup table based reservoir, multisegmented wellbore, FutureGen2 aquifer	Latin hypercube sampling, 50 realizations. Example illustrates a setup connecting lookup table based reservoir, multisegmented wellbore and aquifer impact components.
ControlFile_ex15.yaml	Lookup table based reservoir, multisegmented wellbore, FutureGen2 AZMI	Latin hypercube sampling, 100 realizations. Example illustrates a setup connecting lookup table based reservoir, multisegmented wellbore and aquifer impact components.
ControlFile_ex16.yaml	Plume stability	Example is used to demonstrate parameter study analysis for plume stability component.
ControlFile_ex17.yaml	Fault flow	Example demonstrates forward simulation for fault flow component.
ControlFile_ex18.yaml	Lookup table based reservoir, fault flow	Latin hypercube sampling, 10 realizations. To run this example, the additional *Kimberlina* data set have to be downloaded and unzipped into the *source/components/reservoir/lookuptables/Kimb_54_sims* folder. The data files can be downloaded from the same EDX directory where the NRAP-Open-IAM was downloaded or from https://gitlab.com/NRAP/Kimberlina_data. The data set comes from simulation work done by Wainwright et. al. [32].
ControlFile_ex19.yaml	Lookup table based reservoir, seal horizon	Latin hypercube sampling, 5 realizations. To run this example, the additional *Kimberlina* data set have to be downloaded and unzipped into the *source/components/reservoir/lookuptables/Kimb_54_sims* folder. The data files can be downloaded from the same EDX directory where the NRAP-Open-IAM was downloaded or from https://gitlab.com/NRAP/Kimberlina_data. The data set comes from simulation work done by Wainwright et. al. [32].
ControlFile_ex20.yaml	Analytical reservoir	Latin hypercube sampling, 10 realizations. Example illustrates use of analytical reservoir component.
ControlFile_ex21.yaml	Lookup table based reservoir, multisegmented wellbore, deep alluvium aquifer (ML)	Forward simulation. Example illustrates use of deep alluvium aquifer component (ML).
ControlFile_ex22.yaml	Chemical well sealing component	Forward simulation. Example illustrates setup of the chemical well sealing component.

continues on next page

Table 5.1 – continued from previous page

File name	Included components	Comments
ControlFile_ex23.yaml	Lookup table based reservoir, seal horizon	Forward simulation. To run this example, the additional *Kimberlina* data set have to be downloaded and unzipped into the *source/components/reservoir/lookuptables/Kimb_54_sims* folder. The data files can be downloaded from the same EDX directory where the NRAP-Open-IAM was downloaded or from https://gitlab.com/NRAP/Kimberlina_data. The data set comes from simulation work done by Wainwright et. al. [32].
ControlFile_ex24.yaml	Lookup table based reservoir, multisegmented wellbore, generic aquifer	Forward simulation. Example illustrates a setup connecting lookup table based reservoir, multisegmented wellbore and aquifer impact components. This example requires the additional FutureGen 2.0 data set that can be downloaded from the following source: https://edx.netl.doe.gov/dataset/futuregen-2-0-1008-simulation-reservoir-lookup-table
ControlFile_ex25.yaml	Multisegmented wellbore, generic aquifer	Latin hypercube sampling, 10 realizations. Example illustrates the use of dynamic input to drive a wellbore component providing input for aquifer impact component.
ControlFile_ex26.yaml	Lookup table based reservoir, multisegmented wellbore, FutureGen2 aquifer	Forward simulation. Example illustrates a setup connecting lookup table based reservoir linked to 3d data, multisegmented wellbore and aquifer impact components.
ControlFile_ex27.yaml	Lookup table based reservoir, multisegmented wellbore	Forward simulation. Example illustrates a setup connecting lookup table based reservoir and multisegmented wellbore components. Reservoir component is linked to lookup tables with additional temperature metric.
ControlFile_ex28.yaml	Lookup table based reservoir, multisegmented wellbore	Forward simulation. Example illustrates a setup connecting lookup table based reservoir and multisegmented wellbore components. Reservoir component is linked to lookup tables with additional data metric.
ControlFile_ex29.yaml	Lookup table based reservoir, multisegmented wellbore	Forward simulation. Example illustrates use of known and random wellbore locations in 3d domain.

Beyond control files the described scenarios can be implemented with a help of a Python script. Example scripts can be found in the *examples/scripts* folder.

BIBLIOGRAPHY

[1] D. H. Bacon, Z. Dai, and L. Zheng. Geochemical impacts of carbon dioxide, brine, trace metal and organic leakage into an unconfined, oxidizing limestone aquifer. *Energy Procedia*, 63:4684–4707, 2014. doi:10.1016/j.egypro.2014.11.502.

[2] S. Baek, D. Bacon, and N Huerta. NRAP-Open-IAM Analytical Reservoir Model. Development and Testing. Technical Report, Pacific Northwest National Laboratory, Richland, Washington, 2021. PNNL-31418.

[3] R. E. Britter and J. D. McQuaid. *Workbook on the dispersion of dense gases*. Contract Research Report 17 Health and Safety Executive, Sheffield, UK, 1988.

[4] M. A. Celia, J. M. Nordbotten, S. Bachu, M. Dobossy, and B. Court. Risk of leakage versus depth of injection in geological storage. *Energy Procedia*, 1(1):2573–2580, 2009. Greenhouse Gas Control Technologies 9 Proceedings of the 9th International Conference on Greenhouse Gas Control Technologies (GHGT-9), 16-20 November 2008, Washington DC, USA. doi:10.1016/j.egypro.2009.02.022.

[5] M. A. Celia, J. M. Nordbotten, B. Court, M. Dobossy, and S. Bachu. Field-scale application of a semi-analytical model for estimation of CO2 and brine leakage along old wells. *International Journal of Greenhouse Gas Control*, 5(2):257–269, 2011.

[6] Z. Dai, E. Keating, D. Bacon, H. Viswanathan, P. Stauffer, A. Jordan, and R. Pawar. Probabilistic evaluation of shallow groundwater resources at a hypothetical carbon sequestration site. *Scientific Reports*, 4:4006, 2014. URL: http://www.ncbi.nlm.nih.gov/pubmed/24844225, doi:10.1038/srep04006.

[7] Jerome H Friedman. Multivariate adaptive regression splines. *The Annals of Statistics*, 19(1):1–67, 1991.

[8] D. R. Harp. Model analysis toolkit (MATK). URL: http://matk.lanl.gov.

[9] D. R. Harp, R. Pawar, J. W. Carey, and C. W. Gable. Reduced order models of transient CO2 and brine leakage along abandoned wellbores from geologic carbon sequestration reservoirs. *International Journal of Greenhouse Gas Control*, 45:150–162, 2016. URL: http://www.sciencedirect.com/science/article/pii/S1750583615301493, doi:10.1016/j.ijggc.2015.12.001.

[10] Dylan Harp, Tsubasa Onishi, Shaoping Chu, Bailian Chen, and Rajesh Pawar. Development of quantitative metrics of plume migration at geologic CO2 storage sites. *Greenhouse Gases: Science and Technology*, 9(4):687–702, 2019. URL: https://onlinelibrary.wiley.com/doi/full/10.1002/ghg.1903.

[11] J. Herman and W. Usher. SALib: an open-source python library for sensitivitiy analysis. *Journal of Open Source Software*, 2(9):97, 2017. URL: https://github.com/SALib/SALib, doi:10.21105/joss.00097.

[12] Jaisree Iyer, Xiao Chen, and Susan A. Carroll. Impact of chemical and mechanical processes on leakage from damaged wells in CO2 storage sites. *Environmental Science & Technology*, 54(2):1196–1203, 2020. doi:10.1021/acs.est.9b05039.

[13] Jaisree Iyer, Stuart D.C. Walsh, Yue Hao, and Susan A. Carroll. Incorporating reaction-rate dependence in reaction-front models of wellbore-cement/carbonated-brine systems. *International Journal of Greenhouse Gas Control*, 59:160–171, 2017. doi:https://doi.org/10.1016/j.ijggc.2017.01.019.

[14] A. B. Jordan, P. H. Stauffer, D. Harp, J. W. Carey, and R. J. Pawar. A response surface model to predict CO2 and brine leakage along cemented wellbores. *International Journal of Greenhouse Gas Control*, 33:27–39, 2015. doi:10.1016/j.ijggc.2014.12.002.

[15] E. Keating, D. Bacon, S. Carroll, K. Mansoor, Y. Sun, L. Zheng, D. Harp, and Z. Dai. Applicability of aquifer impact models to support decisions at CO2 sequestration sites. *International Journal of Greenhouse Gas Control*, 52:319–330, 2016. doi:10.1016/j.ijggc.2016.07.001.

[16] E. H. Keating, D. H. Harp, Z. Dai, and R. J. Pawar. Reduced order models for assessing CO2 impacts in shallow unconfined aquifers. *International Journal of Greenhouse Gas Control*, 46:187–196, 2016. doi:10.1016/j.ijggc.2016.01.008.

[17] G. V. Last, C. J. Murray, and Y. Bott. Derivation of groundwater threshold values for analysis of impacts predicted at potential carbon sequestration sites. *International Journal of Greenhouse Gas Control*, 49:138–148, 2016. doi:10.1016/j.ijggc.2016.03.004.

[18] E. Lindner. NSealR—A User's Guide, third-generation. Technical Report, National Energy Technology Laboratory, Morgantown, WV, 2015.

[19] K. Mansoor, T. A. Buscheck, X. Yang, S. A. Carroll, and X. Chen. LLNL Kimberlina 1.2 NUFT Simulations, June 2018. URL: https://edx.netl.doe.gov/dataset/llnl-kimberlina-1-2-nuft-simulations-june-2018.

[20] K. Mansoor, Y. Sun, and Carroll S. Development of a general form CO2 and brine flux input model. NRAP Technical Report Series, Lawrence Livermore National Laboratory, 2014.

[21] J. M. Nordbotten and M. A. Celia. *Geological storage of CO2: modeling approaches for large-scale simulation*. John Wiley & Sons, 2011. doi:10.1002/9781118137086.

[22] J. M. Nordbotten, M. A. Celia, S. Bachu, and H. K. Dahle. Semianalytical solution for CO2 leakage through an abandoned well. *Environmental Science & Technology*, 39(2):602–611, 2005. doi:10.1021/es035338i.

[23] J. M. Nordbotten, D. Kavetski, M. A. Celia, and S. Bachu. Model for CO2 leakage including multiple geological layers and multiple leaky wells. *Environmental Science & Technology*, 43(3):743–749, 2009. doi:10.1021/es801135v.

[24] L. H. Pan and C. M. Oldenburg. T2Well - an integrated wellbore-reservoir simulator. *Computers & Geosciences*, 65:46–55, 2014. doi:10.1016/j.cageo.2013.06.005.

[25] L. H. Pan, S. W. Webb, and C. M. Oldenburg. Analytical solution for two-phase flow in a wellbore using the drift-flux model. *Advances in Water Resources*, 34(12):1656–1665, 2011. doi:10.1016/j.advwatres.2011.08.009.

[26] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

[27] E. Plischke. An effective algorithm for computing global sensitivity indices (EASI). *Reliability Engineering & System Safety*, 95(4):354–360, 2010. URL: http://www.sciencedirect.com/science/article/pii/S0951832009002579, doi:10.1016/j.ress.2009.11.005.

[28] J. Rudy. Py-earth. 2013. URL: https://contrib.scikit-learn.org/py-earth.

[29] I.M. Sobol' and S. Kucherenko. Derivative based global sensitivity measures and their link with global sensitivity indices. *Mathematics and Computers in Simulation*, 79(10):3009–3017, 2009. URL: http://www.sciencedirect.com/science/article/pii/S0378475409000354, doi:10.1016/j.matcom.2009.01.023.

[30] J.-Y. Tissot and C. Prieur. Bias correction for the estimation of sensitivity indices based on random balance designs. *Reliability Engineering & System Safety*, 107:205–213, 2012. SAMO 2010. URL: http://www.sciencedirect.com/science/article/pii/S0951832012001159, doi:10.1016/j.ress.2012.06.010.

[31] Vince R Vermeul, James E Amonette, Chris E Strickland, Mark D Williams, and Alain Bonneville. An overview of the monitoring program design for the FutureGen 2.0 CO2 storage site. *International Journal of Greenhouse Gas Control*, 51:193–206, 2016.

[32] H. Wainwright, S. Finsterle, Q. Zhou, and J. Birkholzer. Modeling the performance of large-scale CO2 storage systems: a comparison of different sensitivity analysis methods. Technical Report, U.S. Department of Energy, National Energy Technology Laboratory, Morgantown, WV, 2012.

[33] Stuart D.C. Walsh, Wyatt L. Du Frane, Harris E. Mason, and Susan A. Carroll. Permeability of wellbore-cement fractures following degradation by carbonated brine. *Rock Mechanics and Rock Engineering*, 46(3):455–464, 2013. doi:https://doi.org/10.1007/s00603-012-0336-9.

[34] Stuart D.C. Walsh, Harris E. Mason, Wyatt L. Du Frane, and Susan A. Carroll. Experimental calibration of a numerical model describing the alteration of cement/caprock interfaces by carbonated brine. *International Journal of Greenhouse Gas Control*, 22:176–188, 2014. doi:https://doi.org/10.1016/j.ijggc.2014.01.004.

[35] Stuart D.C. Walsh, Harris E. Mason, Wyatt L. Du Frane, and Susan A. Carroll. Mechanical and hydraulic coupling in cement–caprock interfaces exposed to carbonated brine. *International Journal of Greenhouse Gas Control*, 25:109–120, 2014. doi:https://doi.org/10.1016/j.ijggc.2014.04.001.

[36] Y. Zhang and C. Oldenburg. *Multiple Source Leakage Reduced-Order Model (MSLR) Tool User's Manual, Version: 2016.11-1.0.1*. U.S. Department of Energy, National Energy Technology Laboratory, Morgantown, WV, 2016. NRAP Technical Report Series NRAP-TRS-III-016-2016. doi:10.18141/1592689.

[37] Y. Zhang, C. M. Oldenburg, and L. Pan. Fast estimation of dense gas dispersion from multiple continuous CO2 surface leakage sources for risk assessment. *International Journal of Greenhouse Gas Control*, 49:323–329, 2016. URL: http://www.sciencedirect.com/science/article/pii/S1750583616301074, doi:10.1016/j.ijggc.2016.03.002.

[38] G. Zyvoloski. FEHM: a control volume finite element code for simulating subsurface multi-phase multi-fluid heat and mass transfer. Technical Report, Los Alamos National Laboratory, Los Alamos, NM, 2007. URL: https://fehm.lanl.gov/pdfs/FEHM_LAUR-07-3359.pdf.

PYTHON MODULE INDEX

O