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Software Requirements for a Consequence Management Sample Data Simulator for Training and Drills

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Introduction and Executive Summary

This document describes the requirements for a software tool that will enable FRMAC to simulate large sets of sample result data that is based realistically on simulated radionuclide deposition grids from NARAC. The user of this tool would be scientists involved in exercise and drill planning or part of the simulation cell of an exercise controller team. A key requirement is that this tool must be able to be run with a reasonable amount of training and job aids by any person within the Assessment, Laboratory Analysis, or Monitoring and Sampling divisions of the FRMAC to support any level of exercise from the small IPX to the national level full scale exercise. This tool should be relatively lean and stand-alone so that the user can run it in the field with limited IT resources. This document will describe the desired architecture, design characteristics, order of operations, and algorithms that can be given to a software development team to assist them in project scoping, costing, and eventually, development.

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CM Sample Simulation Process

In support of Consequence Management drills and exercises, simulated samples and sample results are needed in bulk. This data must be injected into existing operational databases such as RAMS and RadResponder to support exercises and drills. Samples and their results must be tied to the exercise scenario and master simulation models so users have a realistic data set that can be used to practice technical data evaluation techniques and the generation of data products. Currently, generating this data set is an extremely labor intensive, error prone, and expert-driven process that only a few people in the CM community can accomplish. The goal of this simulator is to make the simulation process more accessible to the CM community and significantly reduce the manpower needed to produce realistic, objective-driven data sets for drills and exercises. This way, CM planners can focus on practicing the operations and science during drills.

To integrate the simulation of laboratory samples into the overall exercise design, the simulation of laboratory sample results for samples collected during play may also need to be extended to include the simulation of field teams collecting laboratory samples. This way, data can be made more dense as if there were more participants in the exercise. For exercises where field team activities (e.g. sample collection) will be simulated, planners start the simulation process by leveraging scenario-designed outcomes and data needs to determine where pre-staged samples should be "collected" – ideally using a graphical interface to select sample locations on a map. These sample locations are then used to generate simulated laboratory results for the samples "collected" at each location (Fig. 1). Alternatively, exercises may deploy actual field teams to collect samples. For these exercises, the simulation tool must be able to read in the sampling time, location, and sample types from the operational database (RAMS or RadResponder) and generate laboratory sample results in near real-time so that the simulated results can be injected in place of the laboratory analysis of the actual (blank) samples collected.

The sample result simulation process can be broken down into logical steps. The initial planning and deposition modeling step involves the import of the master simulation models from NARAC so that deposition activity can be probed given a time and location. The next steps involve choosing sampling locations, sample types, radionuclide mixtures, and analysis methods. The user then chooses the conversion factors from the probed values to the radioactivity found in each sample type (i.e. transfer factors). Once the radioactivity in the sample is known, the expected result uncertainty is generated as well as the best estimate of the laboratory measurement sensitivity (Minimum Detectable Activity and Critical Level) given assumptions about the laboratory method capabilities. To provide an additional layer of realism, the impacts of sampling bias, sampling uncertainty, and measurement uncertainty can be simulated and factored in to the simulated results. This way, analytical results will not exactly match the probed values but will have some natural statistical fluctuation to give data users a realistic picture of what they would expect in a real response (e.g. adding the "fuzziness" to the data). The final stage of the simulation process is the generation of data import formats compatible with the operational database systems for injection during exercise play. Many of these formats are already defined but flexibility and adaptability here is key to ensure this system has longevity in the CM toolbox. To support training and exercise play for the Quality Assurance team in Lab Analysis, a functionality can be developed to generate the simulated laboratory reports and data packages for QA review. This module can also be used to inject pre-planned transcription errors between the electronic results and simulated reports or other potential error modes to support QA training, as needed.

Figure 1 shows the steps in each stage for each simulation mode. The remainder of this document will be dedicated to describing how the simulator should work and what it should look like to meet the objectives.

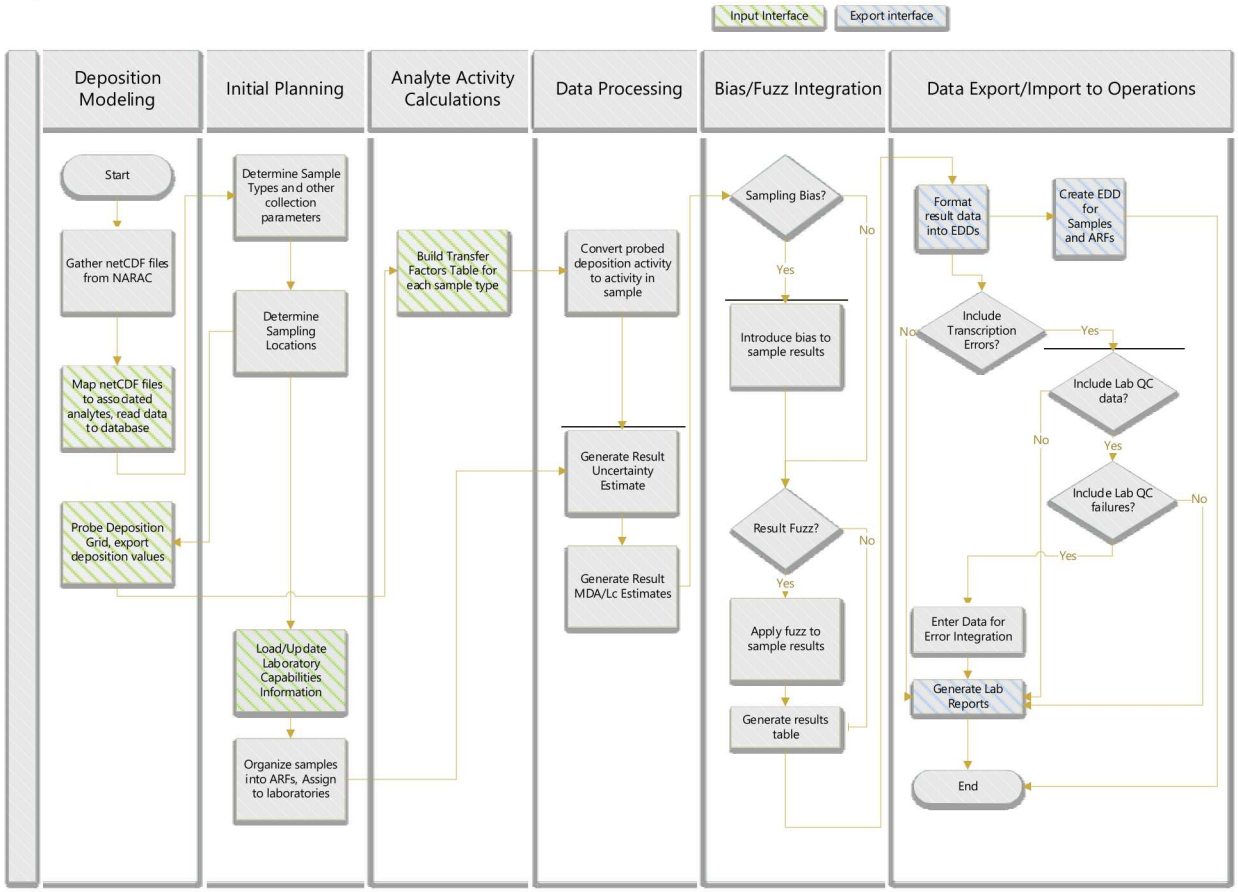


Figure 1: Sample result simulation process

Modular Design Concept

The simulator will consist of several semi-independent modules unified under a single UI. This will allow users to generate data with each module that will feed the next or provide utility outside the simulator itself. The modules are as follows:

- The Source Term Module will allow the user to map several input files from NARAC to analytes so the simulator will know where to draw inject deposition data from.
- The Sampling Location Selection Module is an optional module that can be used to visually generate a table of sampling locations and sample types that will feed the Probing Module which will generate a table of locations and known "true" deposition activities for each analyte. There may need to be a second version of this module built in the future to retrieve sample location information from the operational database to support near real-time simulation of laboratory sample results from samples collected by real teams during an exercise. This can be done through existing API where applicable. In phase I of development, however, the system must allow for the import of this real-time data in this step through an import format. This separate mode or even separate module is described as the Sample Location Import Module.
- The Probing Module will perform the interpolation of the NETCDF file(s) in space and output the probed deposition values at each sampling location.
- The Transfer/Matrix Module will translate the deposition activity to the expected activity in each sample type chosen in the Sampling Location Selection Module.
- The Sample Control Module is used to organize the samples into Analysis Request Forms and to assign them to laboratories. In this module, users will organize samples into analytical groups and assign them to "Analysis Request Forms" or ARFs.
- The Lab Simulation Module will generate the expected sample analytical results, uncertainties, and limits of detection for each analyte in each sample based on user-provided information about the laboratory capabilities.
- The Data Export Module is where the user can configure how data will be exported. Users will have the option to toggle result bias and/or fuzz (randomness) at this step. This module will allow the user to display a map with the NARAC contours used in the simulation with sampling locations for the various sample types indicated. The electronic data deliverable (EDD) format for RadResponder and associated lab reports for each simulated ARF will be available for download.

Figure 2 below describes how all the modules lace together in the simulator framework.

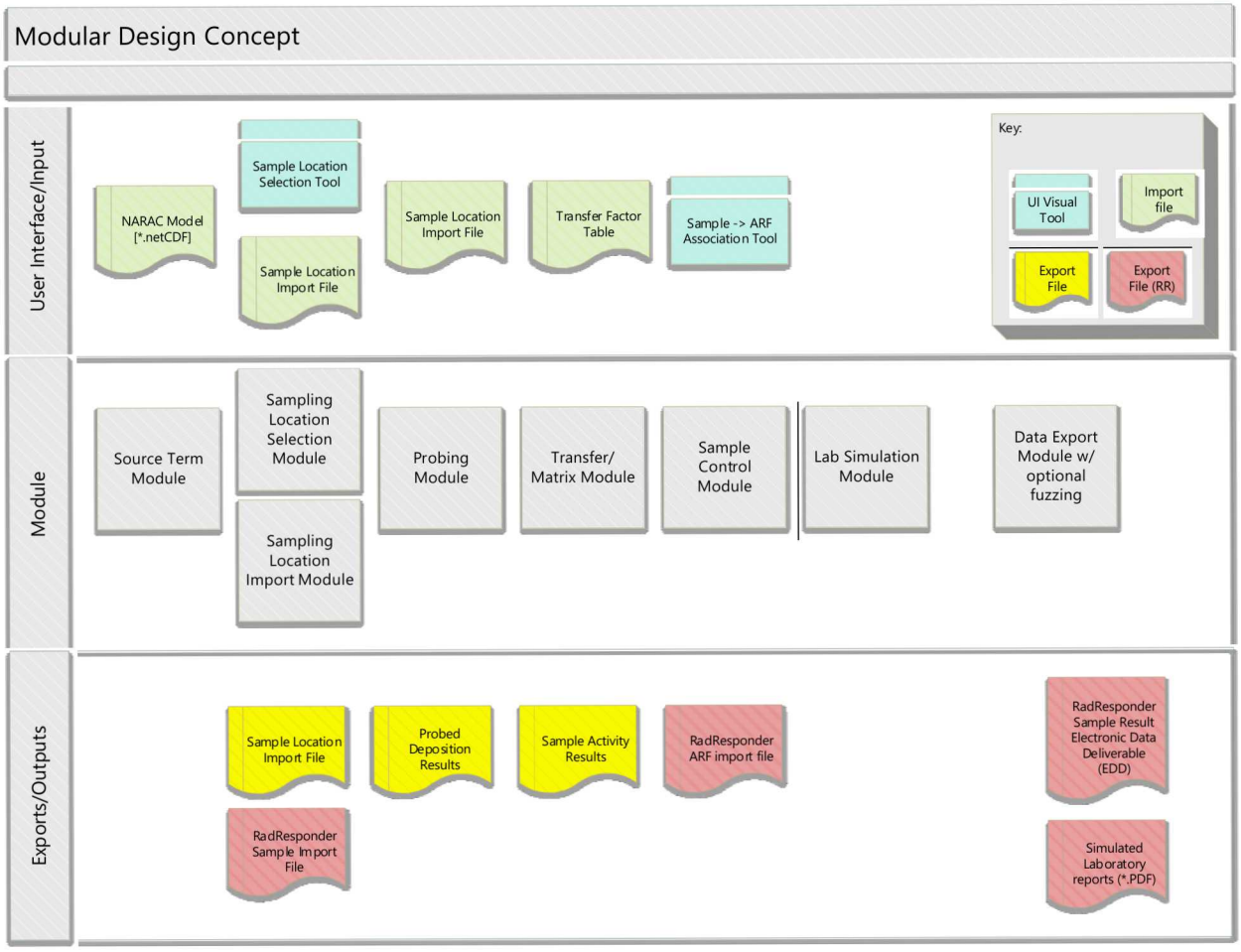


Figure 2: Modular Design Concept describing inputs and outputs

Source Term Module

The purpose of the source term module is to read in deposition grid files (*.NETCDF) file format from NARAC simulation runs to a local database for future probing. This simulator software will NOT replace the need to run NARAC to estimate release deposition geospatially. These file(s) are a necessary input to this simulator and this simulator will not be able to be run without them. This simulator will allow multiple *.NETCDF files to be imported and used in a simulation.

In addition to the NARAC inputs, the simulator will need the user to import a file or fill out a table in the UI that describes what analytes will be simulated, what fraction of the total deposition activity each analyte represents, and which *.NETCDF file will the deposition activity come from for the analyte. This will allow for the most flexibility in simulating deposition via NARAC. The simulator will ignore any data contained in the .NETCDF files that are not mapped to analytes included in the mixture file. Figure 3 below visually describes the relationship between the mixture table and the NETCDF files.

Analyte	Fraction to Total Deposition	Reference Deposition Filename
Cs-137	0.25	Mixture_Total.NETCDF
Sr-90	0.75	Mixture_Total.NETCDF
Y-90	0.75	Mixture_Total.NETCDF
Gross Beta	1	GrossBeta_Total.NETCDF

Mixture_Total.NETCDF

GrossBeta_Total.NETCDF

Figure 3: Analyte-to-NETCDF mapping example

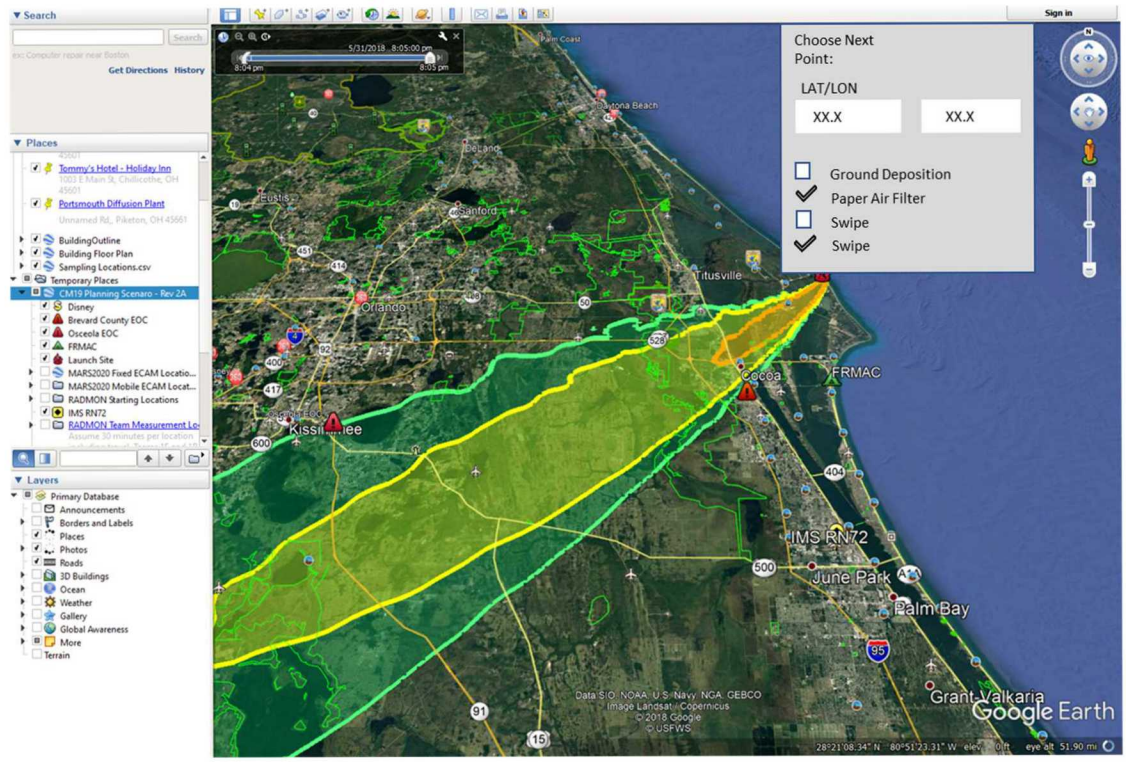
Designing the source term module in this way should allow for the flexibility in scenario simulation. For example, exercise planners may choose to have a single NETCDF file defined for all analytes summed together in a total deposited activity. Alternatively, separate files may be run for individual radionuclides. Having the flexibility to map each analyte to an individual file allows for either scenario to be used in the simulation.

Sampling Location Selection Module

The sample location selection module will be used to visually choose sampling locations for a simulated field team to generate the Probing Module input file. In general, the tool will first ask the user for the following input:

1. Field Team Name
2. Sampling campaign start date/time
3. Average time between sampling points
4. What sample types will be collected and how many of each
5. What sample sizes will be collected for each type?
6. Is the sample a "background" sample
7. Additional information (sample type dependent, see Mockup)

This "input card" is mocked up in Appendix I. The user will save the "card" and then be asked if they wish to create another or continue to the sampling location selection step. Next, the user will be presented a map view that shows the NARAC contour as an overlay. The user will select the first sampling point. At each sampling point, the user will be presented with a control that shows all the sample types collected at that point. The user will be presented the option to deselect the sample types they do not want to collect at that point or choose to move to the next point and create all the sample types. Then, in a stepwise fashion, the user will select each subsequent sampling point or select "complete sampling plan" which will end the field team's sampling campaign. Next, the user will be asked if they wish to plan another team to begin the process again. This process is repeated until all the sampling campaigns (one for each field team card defined) have been completed. Figure 4 represents a mock-up of what this UI may look like.



Sampling Points

Field Team Name	Latitude	Longitude	DateTime				
RADMON 1E	28.5331	-80.5929	10/21/2019 10:00	Ground Deposition	Paper Air Filter	Swipe	Swipe
RADMON 1E	28.5332	-80.5943	10/21/2019 10:30	Ground Deposition	Paper Air Filter	Swipe	Swipe
RADMON 1E	...	...	10/21/2019 11:00	Ground Deposition	Paper Air Filter	Swipe	Swipe

Complete Sampling Campaign

Figure 4: Mock-up of sampling location selection module

This module can be bypassed if the user already has a list of field team names, sampling points, sample types in the format the Probing Module requires by running the Sampling Location Import Module instead.

Sampling Location Import Module

Alternative to selecting sampling points, choosing field teams, sample matrices, date/times, etc. in the UI, the simulator will be able to read in a file and perhaps eventually use an API to gather all the necessary information from an operational data management system such as RadResponder to feed to the probing module. The location import module will take a file with the following .CSV format as input.

{Collection Date/time, Sample Type, Sample ID, , Field Team Name, Latitude, Longitude, Is Background?, **ARF Name* }

** Optional field*

This information is all that is needed to proceed with the rest of the simulator. Note that the optional ARF name field can be used to bypass the sample control module later in the simulation or the user can choose to leave this blank and associate samples with an ARF in the sample control module. If an ARF is

provided, the user must be aware of the analysis methods and analytes chosen for the sample and ensure they match what was set up in the source term module of the simulation.

Probing Module

The Probing Module will read in a sampling point input file that describes the field team, the sampling locations, the datetime of the sampling event, and the sample types collected at each point. This module will draw from the data collected in the sample location selection module or the sample location import module. The purpose of this module is to probe the NETCDF file in time and space to find the closest deposition value for each sampling location.

In this first iteration of the simulator, no corrections for ingrowth/decay/weathering will be done by this simulator. The user will need to handle radionuclide decay, ingrowth, and weathering by including these in the NARAC runs. The NETCDF file may contain different evaluation times within a single file which will account for these phenomena. The simulator will simply choose the evaluation time in the applicable NETCDF that is nearest to the collection date/time prior to the spatial interpolation step.

At each location in space defined in the sampling location file, the system will interpolate the applicable *.NETCDF files in the spatial dimensions for each analyte to determine the deposition (activity per unit area) for each location. A bilinear interpolation algorithm will need to be employed so that probe results match existing tools in CMweb. This algorithm involves calculating the weighted average value for the probe that considers the distance to the four nearest NETCDF nodes as the weighting factor. An easy to follow reference for this method can be found here:

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

Transfer/Matrix Module

The transfer/matrix module will read in the output of the Probing Module which is the analyte-specific deposition at each location in space and time and which sample types were collected at each and translate the deposition activity to the expected activity in each sample matrix collected. This is done by using the transfer factor matrix that is either loaded in from default and modified as needed or built from scratch for the simulation. In the context of this simulator, the transfer factor is the value by which the deposition activity (in uCi/m2) for an analyte in a sample is multiplied by to get the expected radioactivity concentration in the sample (uCi/{sample size units}).

There are several different matrix-dependent methods that are used to generate the transfer factor. Much of the mathematics involved in determining the transfer factor will happen outside the simulator and the result of which will simply be placed in the transfer factor matrix. The following sections will describe each sample type and some considerations for each. The transfer factors are stored in a table mocked up in table 1.

Air Filter

In general, air is collected on two types of media, paper to capture the particulate mass and cartridges to collect the noble and volatile species. These samples are traditionally collected in pairs when collected together only when noble gases or other volatile compounds such as iodine are expected. If these are not expected, only paper filters are used to collect the particulate matter. A release can be characterized as a plume phase and a deposition phase. During the plume phase, contaminants exist in

the air while they deposit on the ground. During the deposition phase, air contaminants are in the form of resuspended material from the ground. The NARAC run may include integrated air concentration for times during the plume phase. Considering samples collected during the plume phase adds a layer of complexity that is unnecessary in the first phase of this simulator.

Only air samples collected in the deposition phase will be simulated by the phase I simulator. In simulations and for air DRL calculations, a resuspension factor is used for samples collected after contaminant deposition. By default, this value is taken to be 1e-6 times the deposited activity but can be larger for earlier times in the event and for different source material. This resuspension factor has units of inverse meters and multiplies with the deposition activity to yield a concentration of uCi/m3. When cartridges are used, the relative collection yield can be considered for each and fractionated across the filters. An example is particulate vs. Gaseous iodine. Using the transfer factor table, the user must be able to enter values in for each to account for this effect.

The system will have some default transfer factors built-in for the novice user but will allow a more advanced user to tweak the values as needed to support the objectives of the exercise and to match what simulation parameters will be assumed.

Feed

Users will enter the fraction of the deposited activity expected to be found in the feed. This of course depends on if the feed is a crop or a stored and covered feed silo. Each of these types will need to be simulated separately since the transfer factors will likely be much different. Feed will be collected by mass and assumptions as to which how much of the area will be sampled during collection will need to be made to come up with the conversion of uCi/area to uCi/mass.

Food

Food is handled very similarly to feed in that assumptions as to how much of the radioisotopes of concern have been deposited on the food and how much area each sample will represent will need to be factored in to get the conversion from uCi/area to uCi/mass. Largely different foods will likely need to be modeled separately as their transfer factors will be much different. For example, a crop of oranges will have a much different transfer factor than for beef from potentially contaminated feed-fed cattle.

Ground Deposition

Ground deposition is the most straightforward of the sample types and is simply equal to the deposited activity assuming the collection efficiency is 100%. Bias in the collection efficiency for ground deposition samples can be simulated by changing the transfer factor for this sample type.

In-Situ Spectra

In-Situ spectra will need to leverage tools outside this simulator to fully simulate. This simulator however, will be used to generate the gamma spectroscopy simulation source term in a specific format. Traditionally, all gamma-emitting radionuclides will have a transfer factor of 1 when In-Situ spectra are to be simulated much like the ground deposition sample. Non-gamma emitting radionuclides, or those that would not be detected by field equipment can be blocked out by using a zero transfer factor.

Milk

Milk is handled much like food and the transfer factor will be determined using tools in Turbo FRMAC.

Other

The other-type sample is used as a catch-all for samples that do not fall into any other category. The transfer factor will be manually entered for the type of sample being modeled. Users will need to take note as to what units other-type samples will be using so that they consistently handle this type in subsequent modules.

Soil

Soils are collected instead of ground deposition samples when bulk radioactivity deeper in the soil is needed. In this simulator, soils are handled identically to ground deposition using an assumed sample collection area. Allowing the user to tweak the values in this table will allow them to add in factors relating to the weathering into the soil to get a more accurate simulation.

Swipe

Swipes are handled exactly like ground deposition samples and the factor is 1 when the collection efficiency is 100%. Bias in the collection efficiency for ground deposition samples can be simulated by changing the transfer factor for this sample type.

Vegetation

Vegetation is handled similarly to food in this simulator.

Water

Water is handled similarly to food in this simulator with the exception that the concentration units for water have a dimension of volume rather than mass.

Table 1: Example transfer factors table, for gross alpha and gross beta, I indicates the transfer factor and Y is the yield.

Analyte	**Paper Air sample**	**Charcoal Air**	**Ground Deposition**	**Drinking Water**	**…**	**Beta Yield** Y_β	**Alpha Yield** Y_α
Analysis Unit	**uCi/m3**	**uCi/mL**	**uCi/m2**	**pCi/L**			
Cs-137	1e-7	1e-3	1	0.23		.12	…
I-131	1e-5	1e-6	1	0.01		0.1	…
Sr-90	0	0	1	1		…	…
Gross Alpha	$\sum_i (I * Y_\alpha)_i$						
Gross Beta	$\sum_i (I * Y_\beta)_i$						

Note: See Appendix II for the full table format

The output of this module will be the total radioactivity in the sample and the export table will have the following format:

{*sampleID, analyte, team name, lat, lon, datetime, Sample Type, uCi/[sample size unit]sample for each analyte, Analysis Unit*}

Sample Control Module

The Sample control module will allow the user to organize the simulated samples into groups that will be analyzed together. These are called "Analysis Request Forms" or ARFs. It is important because samples need to be assigned to a laboratory and that laboratory must be told how to analyze the samples. First, the user will map each analyte defined in the Source Term Module to a specific analysis method. The available analysis methods in RAMS and Rad Responder may change over time so the simulator must begin with what exist in the systems today but allow users to add more as needed or optionally sync with an API.

Once the Analyte to method map is created, the user will see a table of all the samples that will display, at minimum, the sample ID, the Field Team, the collection date/time, and the sample type. The UI should allow the user to sort and filter the list then select multiple samples and associate them with an Analysis Request Form which will be named by the user using a format of ARF-#### or any free text entry to allow for flexibility. By default each ARF will request all analytes be reported. The user will either choose to continue or may wish to deselect some of the analytes for some of the ARFs. This will allow for flexibility when the user wishes to leave out some of the analytes on some of the ARFs. Each ARF will then be mapped to a laboratory. When RadResponder is being used, the laboratory name must match one that exists in the RR database, so users will need to take care to match things appropriately. If the lab does not exist yet, the user will need to pause work in this module and move to the Lab Module to create one. Also, if an analyte is being assigned to a lab that does not exist in its analyte-method parameters table, the user should be warned that they will need to add this data for the simulator to progress.

Once samples are attached to the first ARF, the samples will be removed from the queue and the user will then be able to create another ARF and attach other samples. This process continues until all samples have been associated with ARFs. The output of this module has a format described in Appendix II. As an added feature, users should be able to attach samples to multiple ARFs if needed. Users should be presented with an option at the end of this module to choose samples to attach to another ARF even if they have already been assigned to one previously. This will allow for flexibility and will match how this step is done in RadResponder and RAMS.

When users are simulating results for samples and ARFs created during exercise play, the users will need to make sure the matching ARF name is included as an optional field in the Sample Location Import Module and carry on the simulation from that point, skipping this step.

Special note for In-Situ spectra simulation

In-Situ spectra will not be grouped under an Analysis Request form but will always be grouped together by default. The data export format for In-Situ will be special and be exported at the end of this module if the user has toggled on this data type. The format the In-Situ spectra simulator data will take is a hybrid tab/comma delimited text file described as follows:

{ ID/Loc (tab) Det. Height cm (tab) Lat deg N (tab) Long deg E (tab) Elevation meters (tab) Date/time (tab) Real time sec (tab) Nuclide, activity uCi/m2, age (tab) Nuclide, activity uCi/m2, age (tab) Nuclide, activity uCi/m2, age (tab) … }

The file must be plain text that is tab delimited for each metadata field and comma separated within the Nuclide/Activity and age field. This way, any number of combined nuclides can be exported and each row in the export will represent a single spectral file that will be simulated in GADRAS.

Example (2 rows):

Sample 123 \t 100.0 \t 35 \t 253.4 \t 1620 \t 05-Mar-2019 07:32:36 \t 900 \t Cs-137, 10uCi{age=10d} \t Cs-134, 1uCi{age=10d}

Sample 124 \t 100.3 \t 35 \t 253.4 \t 1620 \t 05-Mar-2019 07:32:36 \t 900 \t Cs-137, 1.6uCi{age=10d} \t Cs-134, 0.18uCi{age=10d}

Note: \t represents a tab character as the delimiter between data elements

This exported file will then be used in a GADRAS add-in that will bulk generate inject files for in-situ measurements based on the probed deposition activities. See Appendix 5 for more details.

Alternatively, the user may wish to simulate the results of In-Situ measurements and bypass the generation of spectra altogether. The results of In-Situ measurement results can be simulated directly similarly to gamma spectroscopy sample results by defining a "laboratory" and specifying analysis defaults that will yield the correct results. This "laboratory" created in the lab simulation module will have parameters specified for the "Gamma Spectroscopy" analysis method.

Lab Simulation Module

The Lab Simulation Module will be the engine for which measurement detection limits and uncertainties are estimated given a set of assumptions about a laboratory's capability. A library of default laboratories will be available to the user with the option to create and store a new one. For each analysis method (defaults and user created) the user will need to fill in key information that will allow the simulator to calculate an estimate of the measurement uncertainty and the measurement critical level for the sample when the analyte is present in the sample at the simulated value. This is essentially back-calculating the detector response given the activity in the sample and depends on factors such as the instrument background, the count time, the detection efficiency, radiative yield factors, etc.

For each lab, a "card" will need to be filled in that specify the default parameters that will be used in the calculations that follow. The tables below describe what parameters need to be set for each laboratory. Table 2 defines the name of the laboratory and some other general information and toggles for the data produced by the simulated lab.

Table 2: General Laboratory Information

Laboratory Name:	Alpha-numeric open text field – note: for proper RR integration, this must match the lab name in RR verbatim
Generate Hardcopy Reports?	Yes/No – yes toggles on additional information card specified in Appendix III
Analyst Name:	Open text (default =John Doe) -greyed out if "generate reports" = no
Reviewer Name:	Open text (default = Jane Doe) -greyed out if "generate reports" = no
Analyst Signature	150 pixel by 750 pixel signature .PNG file (default given) -greyed if "generate reports" = no

Reviewer Signature	150 pixel by 750 pixel signature .PNG file (default given) -greyed if “generate reports” = no
Coverage Factor	1 or 2 (defaults to 1)
Include fuzz?	Yes/no
Include Bias?	Yes/no *this toggles on a bias field in the laboratory analyte-method parameters table

Table 3 specifies the analysis method-specific parameters needed for the calculations. Each of these variables are described in the equations below. For each lab, users can activate analysis methods and enter in the information for each in a table. Over time, analysis methodologies will change in RadResponder so the system should allow for power users to define new ones. To start, the analysis methods available to users should be:

- Alpha Spectroscopy
- Gamma Spectroscopy
- Gas Proportional Counting
- ICP-MS
- Liquid Scintillation Counting
- Radon Compensating Alpha/Beta
- Other

The system should allow for the definition of tables 3 and 4 for each sample matrix and sub-type. The system should also have a place where users can take note of the assumptions made for each analysis method. An open comment field would suffice.

The system should have the ability to store a library of table 3 and table 4 parameters the users can call into a laboratory they are creating. The stored defaults should contain notes on the assumptions made for each so users can determine which are applicable to the simulation they are running. Users should be able to call in specific analysis methods into the tables they are building from this defaults library.

Table 3: Laboratory method parameters

Sample Matrix:	Ground Deposition		
Notes:	350g sample in bag flattened out on detector	5 g sub aliquot, fusion digestion and sequential extraction chem.	…
Parameter	**Gamma Spectroscopy**	**Alpha Spectroscopy**	**…**
T_L	6000	60000	
K_y	1.0	0.80	
$\mathrm{K_u}$	1.0	1.0	
T_e	86400 (24hr)	6.04e5 (7d)	
T_b	60000	120000	
$\sigma_{sys}\%$	8%	5%	

Table 4 specifies the analyte and method specific parameters needed for the calculations. For a detailed description of each, see the equations below. A generic table containing many analytes can be defined for the laboratory. Should a simulation contain analytes that are not included in the activated lab's card, the system should warn the user and indicate which analytes are missing and should be added to the labs card by the user before proceeding.

Table 4: Laboratory analyte-method parameters

Sample Matrix:	Ground Deposition						
Analyte	**Analysis Method**	Comment	$\varepsilon(E_i)$	R_b (cps)	y_i	$T_{1/2}$ (s)	Bias (frac)
Cs-137	Gamma Spectroscopy	Assumes Cs-137.Ba-137m in seq. eq.; 30% coax HPGE well shielded	0.0123	1.25	0.85	9.5e8	0
Ba-140	Gamma Spectroscopy	30% coax HPGE well shielded	0.01	3.2	0.24	1.1e6	0
Am-241	Gamma Spectroscopy	30% coax HPGE well shielded	0.0001	15.2	0.35	1.36e10	.12
Am-241	Alpha Spectroscopy	Vac chamber PIPS detector	0.23	0.0001	0.98	1.36e10	-0.25
Sr-90	Gas Proportional Counting	2.5" GPC chamber, dried salt method	0.35	1.25	1.0	9.1e8	0
Gross Alpha	Liquid Scintillation Counting	Packard tricarb LSC with UGXR cocktail	0.98	1.2	1.0	N/A	.30
Gross Beta	Liquid Scintillation Counting	Packard tricarb LSC with UGXR cocktail	0.86	3.6	1.0	N/A	-.15
…							

General measurement model

In general, the measurement model used for radionuclide concentration, C is found in the equation below. In the context of the simulator, the value of C is simply the probed deposition value multiplied by the applicable transfer factor.

$$C = \frac{S_i - S_b}{V \cdot \varepsilon(E_i) \cdot y_i \cdot T_L \cdot K_w \cdot K_y \cdot K_u} \quad (1)$$

Where C is the radioactivity concentration measured in the sample

S_i is the raw number of counts observed for analyte, i

S_b is the raw number of background counts observed for analyte, i in the same counting period T_L when the background count rate for that analyte is R_b in units of counts per second. Note that the count time for the measurement of background will be denoted as T_b in subsequent equations.

$$S_b = (R_b * T_L) \quad (2)$$

V is the sample size in units of mass or in volume

$\varepsilon(E_i)$ is the detection efficiency for the analyte, I at the measured energy E (if applicable)

y_i is the radiative yield of the radionuclide

T_L is the live count time of the measurement in seconds

K_w is the correction factor for decay for the time elapsed between the sample collection date/time and the measurement time $(T_c - T_s) = T_e$

$$K_w = \exp\left[\frac{ln(2) \cdot T_e}{T_{1/2}}\right] \quad (3)$$

K_y is the radiochemical yield recovery (if applicable)

K_u is the unit correction factor from Bq to the activity units of C.

The model above is a combination of method parameters $(T_L, K_y, \mathrm{K_u}, T_c)$ sample parameters (C, V, K_w, T_s) and analyte parameters $(y_i, E_i, T_{1/2})$. In general, a library of method parameters is maintained for the laboratory in the simulator, the sample parameters are inherited from the sampling location selection module, and the analyte parameters are entered by the user (See tables 3 and 4 above). One exception is the elapsed time T_e for simplicity's sake, a general time elapsed will be stored as a method parameter. Mobile laboratories will have shorter T_e than fixed labs. Methods with more radiochemical prep will have larger T_e than direct assay methods. The detection efficiency and background count rate $(\varepsilon(E_i), R_b)$ are a function of both the analyte and the analysis method. A separate lab-specific table is needed to identify those factors.

Estimating Detection Limit (Critical Level) and MDA (Minimum Detectable Activity)

Using the laboratory data above, an estimate of the measurement critical level can be done using the following equation.

$$L_c = \frac{1.645\sqrt{\left(\frac{R_b}{T_s}\right) + \left(\frac{R_b}{T_b}\right)}}{\left[V \cdot \varepsilon(E_i) \cdot y_i \cdot T_L \cdot K_w \cdot K_y \cdot K_u\right]} \tag{4}$$

For simplicity's sake it follows that the measurement MDA is as follows:

$$MDA = \frac{2.71}{\left[V \cdot \varepsilon(E_i) \cdot y_i \cdot T_L \cdot K_w \cdot K_y \cdot K_u\right]} + 2 * L_c \tag{5}$$

Estimating the measurement uncertainty

In general, a measurement's total propagated uncertainty is a function of the strength of the signal itself combined in quadrature with other sources of error. Each of the components of the activity equation (Eq 1) have uncertainties associated with them. Rearranging equation 1 for the expected sample count rate yields the following equation:

$$S_i = C * [V \cdot \varepsilon(E_i) \cdot y_i \cdot T_L \cdot K_w \cdot K_y \cdot K_u] + S_b \tag{6}$$

It follows then that the expected counting uncertainty is simply:

$$\sigma_s = \sqrt{S_i} \tag{7}$$

Next, the uncertainty in all the other factors that go into the measurement can be estimated as $\sigma_{sys}\%$ which is stored as a method parameter. Combining these in quadrature yields the measurement uncertainty, σ_m

$$\sigma_m = C * \sqrt{\left(\frac{\sigma_s}{S_i}\right)^2 + \left(\sigma_{sys}\%\right)^2} \tag{8}$$

Lab Qualifier Determination

The lab qualifier is a flag applied to the data which allows the lab to mark suspect or rejected results. In general, this field is used to quickly compare a result to its detection limit. For this simulator, the Lab Qualifier is determined using the logic below:

```
If: [Result] < [Lc];
Lab Qualifier = "Less Than Lc"
If: [Result] > [Lc] and [Result] < [MDA];
Lab Qualifier = "Estimated"
```
(9)

```
If: [Result] > [MDA];
Lab Qualifier = "Approved"
```

Electronic Data Deliverable Results mapping

The simulated data is calculated for each analyte and mapped to an Electronic Data Deliverable (EDD) and a hardcopy report (if toggled on). The details of this data export step are described in a section below along with Appendix II and III. Table 5 maps the EDD field to the appropriate equation number above.

Table 5: EDD field to equation mapping

Column	Equation Reference or Field
Result Date	[Sample Collection Date/Time]
Reported By	[Laboratory Analyst Name]
ID/Barcode	[Sample ID]
QC Batch #	*Null*
Analysis Request Name	[ARF Name]
Laboratory Name	[Laboratory Name]
Analysis Methodology	[Analysis Method]
Nuclide Type	[Analyte]
Result	[Probed Deposition Activity] * [Transfer Factor] *{fuzz factor} (see Eq. 1)
Result Unit	[Analysis Unit] from transfer factor table
Uncertainty/Error	Eq. 8
Coverage Factor	[Coverage Factor] from lab card
MDA/MDC	Eq. 5
Measured Critical Level	Eq. 4
Quantity as Analyzed	[Sample Size]
Quantity Unit	[Sample Size Unit]
Wet or Dry?	Wet
Lab Qualifier	Eq. 9
Comment	*null*
Upload Type	New

Data Export Module

The data Export module will arrange the data in several formats compatible with Rad Responder and RAMS platforms (with minimal human intervention). Samples, their Analysis Request Forms, and the results will be in import files ready to inject into these systems for drills and exercises. The requirements for the export formats are found in Appendix II.

If toggled on, the simulator will generate a .PDF hardcopy report to go along with the EDD files for samples and results. The requirements and details for this hardcopy report can be found in Appendix III.

Bias/Fuzz Integration

As an option to toggle on/off in the simulator, bias or "fuzz" to the results can be added in with some simple approximations. The user should choose this in the Lab Simulation module (see Table 2).

Bias is the shifting of results one way or the other away from the "true" value. This can be a static percentage multiplier applied to each analyte. Bias factors are defined as an optional field on the lab card.

To integrate "fuzz" or randomness around the "true" value, the user would toggle on/off in the Lab Card. The calculated result, C and its 1-σ measurement uncertainty σ_m have been calculated using the probed plume value and various assumptions about a labs methodology. One could expect any value C' (the measured radioactivity concentration) from a normal distribution centered about C (the true radioactivity concentration) with a distribution width at 1-sigma equal to σ_m. Thus, to add a bit of "fuzz" or realistic variation to the result, the reported activity concentration value can be randomly sampled from a Gaussian distribution with a center about the known value, C and a width of σ_m. To avoid the employment of more complex numerical methods, a Box-Muller transform provides enough accuracy for the purposes of this simulator. This transform takes two distributions of uniformly distributed random numbers from 0 to 1 and transforms them into one distribution of normally distributed numbers centered about 0 with a standard deviation of 1. The generation of the uniformly distributed random numbers can be done using any standard available method built into the programming language. This estimated distribution is then scale-location transformed using the calculated mean C and the standard deviation σ_m.

$$C' = C + \sigma_m * \sqrt{-2 * Ln(U_1)} * \cos(2\pi U_2) \tag{10}$$

Where U_1 and U_2 are random numbers sampled uniformly between 0 and 1

Appendix I: Sample Point Generator Input Card

Enter Field Team Name

RADMON 1E

Enter starting DateTime

10/21/2019 10:00

Enter time between sampling points (min)

30

Select Sample Types

Sample Type	# of each
Ground Deposition	1
Paper Air Filter	1
Cartridge Air Filter	0
Swipe	2
Water	0
Feed	0
Food	0
Milk	
Soil	
Vegetation	0
Other	0
Spectra	1

Select Sample Sizes

Sample Type	Size	Unit
Ground Deposition	0.01	m^2
Paper Air Filter	20	m^3
Cartridge Air Filter		
Swipe	100	cm^2
Water		
Feed		
Food		
Milk		
Soil		
Vegetation		
Other		
Spectra	600	sec

Is Background?	Category 1	Category 1
	Potable Non-Potable	Water Type
	Milk Type	Milk Feed

Appendix II: I/O Formats

NARAC NETCDF file

The NETCDF file is a standard file format used by NARAC to export deposition grid results. In general, the file gives the user the deposited activity for each grid cell on a 2D map. An example NETCDF has been provided by NARAC so that the programmers of the simulator have an idea of what will need to be imported to the system. The attached file: smoothedBin0.nc.pdf is a copy of the file in a PDF format that can be referenced by page number.

A few facts about the example file are listed below:

- The file contains four hourly average air concentration plots in a concentration grid of 140 x 140 graded (not uniform) grid cells)
- The release point is 39.7675, 116.027778 (near the Dashi River in China)
- The corresponding CMweb run is located here (contact Lydia Tai for access to it)
    - Lydia I. Tai, CHP; NARAC Operations; 925-422-0475; tai2@llnl.gov

A few facts about the NETCDF file in general are listed below:

- The grid cells are defined by an (x,y) coordinate at the midpoint of each cell
- Grid cells may or may not be the same size within a file
- All coordinates are in a UTM coordinate format

Sections of the NETCDF file: Contact NARAC for more specific details of each section

- Page 1: Dimensions
- Page 1-2: Variables
- Page 2-4: Global attributes
- Page 4 – end: Data
    - 140 rows by 140 comma separated columns
    - Gr1 = x – coordinates of midpoints of the grid cells
    - Gr2 – y-coordinates of the midpoints of the grid cells
    - Zt = height of the top of the grid
    - Num_reg = number of bins, (4 in the example)
    - Peak_conc = the grid cell with the highest concentration at each of the times (4 times in the example)
    - Plume_eta = plume arrival time in seconds

- Plume_edt = plume departure time, in seconds
- Concen = quantity of material per unit volume
- Area_cell = area of each grid cell
- Cgridx = gridpoint x-coordinates
- Cgridy = gridpoint y-coordinates
- Zgij = matrix of surface elevation for each grid cell

A copy of the example file in a readable PDF format is here:

smoothedBin0.nc.pdf

Sample Location Import File

The sample location import file is a .CSV with the following format:

{Collection Date/time, Sample Type, Sample ID, Field Team Name, Latitude, Longitude, Is Background?, **ARF Name* }

** Optional field*

Probed Deposition Results

{Collection Date/time, Sample Type, Sample ID, Field Team Name, Latitude, Longitude, Analyte, Deposition Value (uCi/m2) }

RadResponder Sample Import Template

RadResponder provides users a detailed sample import template in Excel. This file has a separate tab for each sample type and specific fields identified for each that can be read in a bulk wise fashion in Rad Responder. This simulator must be able to export results in this format so that minimal human data manipulation is required prior to RR import. Detailed specifications on how this import file is structured is available in Rad Responder and attached in this document for reference. A description of how the sample information from the simulator will map into the proper format is described in the mapping table below. Each field will either be "Simulator Generated" or calculated by the simulator, "User entered" or input by the user in one of the modules of the simulator, or left null. Items marked "next phase" are to be considered in future simulator development.

RadResponder Sample Import Field Mapping

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
All Sheets General Information	Collection Date	Date	Yes	Format MM-DD-YYYY HH:mm	yes	
	Collected By	Text	No	Last Name, First Name OR First Name Last Name		
	Field Team	Text	No	Refer to list in 'Allowed Values'		yes
	Facility	Text	No	Refer to list in 'Allowed Values'		
	Sampling Location	Text	No	Refer to list in 'Allowed Values.' Not required if coordinates are provided.		
	Latitude	Numeric	Yes	Street Address is not required if coordinates are provided	yes	
	Longitude	Numeric	Yes	Longitude is required if latitude is provided	yes	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Street	Text	No	Coordinates are not required is street address is provided		
	City	Text	No	Required if Street is provided		
	State	Text	No	Required if Street is provided		
	Zip Code	Text	No	Required if Street is provided		
	Indoor?	Text	No	Either 'yes' or 'no' value is valid	next phase	
	Building/Structure	Text	No	Only applicable if location is indoor.	next phase	
	Floor/Section	Text	No	Only applicable if location is indoor.	next phase	
	Room #	Text	No	Only applicable if location is indoor.	next phase	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Direction	Text	No	Only applicable if location is indoor. Refer to list in 'Allowed Values'.	next phase	
	Surface	Text	No	Only applicable if location is indoor.	next phase	
	Material	Text	No	Only applicable if location is indoor.	next phase	
	Indoor Comment	Text	No	Only applicable if location is indoor.	next phase	
	ID/Barcode	Alphanumeric	Yes	Must be unique to event	yes	
	Sample Description	Text	No	Free text field to specify a description for the sample.		
	Contact Dose Rate	Text	No	Required if dose rate unit is provided	next phase	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Contact Dose Rate Unit	Text	No	Refer to list in 'Allowed Values'	next phase	
	Contact Dose Rate Radiation Type	Text	No	Refer to list in 'Allowed Values'	next phase	
	Contact Dose Meter Serial Number	Text	No	Free text field to specify the meter serial number.	next phase	
	Contact Dose Meter Property Number	Text	No	Free text field to specify the meter property number.	next phase	
	Contact Dose Probe Serial Number	Text	No	Free text field to specify the probe serial number.	next phase	
	Contact Dose Probe Property Number	Text	No	Free text field to specify the probe property number.	next phase	
	Contact Dose Height	Decimal	No		next phase	
	Contact Dose Height Unit	Text	No	Refer to list in 'Allowed Values'	next phase	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Contact Dose Window Open/Closed	Text	No	Either 'open' or 'closed' value is valid	next phase	
	Contact Dose Orientation	Text	No	Refer to list in 'Allowed Values'	next phase	
	Contact Dose Rate Comment	Text	No	Free text field to specify a description for the contact dose rate.	next phase	
	Background?	Text	No	Either 'yes' or 'no' value is valid		yes
	Contamination Check - Completed Timestamp	Date	No	Local Time. Required if other contamination check fields are provided.	yes, end of sampling campaign	
	Contamination Check - Completed By	Text	No	Required if other contamination check fields are provided. Free text field to specify who completed the	yes, "simulated"	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
				contamination check		
	Contamination Check - Is Clean?	Text	No	Either 'yes' or 'no'. Required if other contamination check fields are provided.	yes, "yes"	
Feed, Food, Other, Soil & Vegetation	Volume	Numeric	No	Either Volume OR Mass must be provided for Feed, Food, Other & Vegetation		yes
	Volume Unit	Text	No	Refer to list in 'Allowed Values'		yes
	Mass	Numeric	No	Either Volume OR Mass can be provided, not both.		yes
	Mass Unit	Text	No	Refer to list in 'Allowed Values'		yes

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
Air	Cartridge Number	Alphanumeric	Yes	Must be unique to event	yes, Sample ID/Barcode for this type	
	Cartridge Description	Text	No	Free text field to specify a description for the cartridge.		
	Filter Number	Alphanumeric	Yes	Must be unique to event	yes, Sample ID/Barcode for this type	
	Filter Description	Text		Free text field to specify a description for the filter.		
	Air Pump Serial Number	Alphanumeric	No	Free text field to specify the air pump serial number.		
	Air Pump Property Number	Alphanumeric	No	Free text field to specify the air pump property number.		
	Cartridge Media	Text	No	Refer to list in 'Allowed Values'		
	Filter Media	Text	No	Refer to list in 'Allowed Values'		

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Flow Type	Numeric	Yes	Refer to list in 'Allowed Values'	yes, "total volume"	
	Date On	Date & Time	No	If Flow Rate is set to 'Start Stop' Date On is required.		
	Date Off	Date & Time	No	If Flow Rate is set to 'Start Stop' Date Off is required.		
	Start Flow	Numeric	No	If Flow Rate is set to 'Start Stop' Start Flow is required.		
	Stop Flow	Numeric	No	If Flow Rate is set to 'Start Stop' Stop Flow is required.		
	Flow Unit	Text	No	Refer to list in 'Allowed Values'		
	Volume	Numeric	No	If Flow Rate is set to 'Total Volume' Volume is required.		yes

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Volume Unit	Text	No	Refer to list in 'Allowed Values'		yes
Ground Deposition	Depth	Numeric	No		yes "2"	
	Depth Unit	Text	No	Refer to list in 'Allowed Values'	yes "centimeter"	
	Surface Area	Numeric	Yes		yes "100"	
	Area Unit	Text	Yes	Refer to list in 'Allowed Values'	yes "Square Centimeters"	
Milk	Milk Type	Text	No	Refer to list in 'Allowed Values'		yes
	Milk Feed	Text	No	Refer to list in 'Allowed Values'		yes* may need special transfer factor
	Milking Date	Date	No	Format MM-DD-YYYY		
	Herd Population	Numeric	No			
	Preservative	Text	No	Refer to list in 'Allowed Values'		

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Volume	Numeric	Yes	Either Volume OR Mass can be provided, not both.		yes
	Volume Unit	Text	Yes	Refer to list in 'Allowed Values'		yes
	Mass	Numeric	No	Either Volume OR Mass can be provided, not both.		yes
	Mass Unit	Text	No	Refer to list in 'Allowed Values'		yes
Swipe	Surface Area	Numeric	No		yes "100"	
	Area Unit	Text	No	Refer to list in 'Allowed Values'	yes "Square Centimeters"	
Water	Water Type	Text	Yes	Refer to list in 'Allowed Values'		yes * may need special transfer factor
	Potable	Text	Yes	valid entries are 'yes' or 'no'		yes

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Preservative	Text	Yes	Refer to list in 'Allowed Values'		
	Volume	Numeric	Yes	Either Volume OR Mass can be provided, not both.		yes
	Volume Unit	Text	Yes	Refer to list in 'Allowed Values'		yes
	Mass	Numeric	No	Either Volume OR Mass can be provided, not both.		yes
	Mass Unit	Text	No	Refer to list in 'Allowed Values'		yes
In Situ						
	ID/Barcode type	Auto generated or Custom	yes		yes, "custom"	
	ID/Barcode	alphanumeric	yes		yes, [sampleID]	
	Spectroscopic Instrument	lookup from equipment table				
	Background?	yes				yes
	Data File	file upload			yes* (from GADRAS)	

Sample Upload Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User entered**
	Configuration File	file upload			yes* (from GADRAS)	
	Time Entry Mode	Enter Start & Stop Time			yes "Enter Dwell Time"	
	Start Time	Datetime				
	Stop Time	Datetime				
	Dwell Time (seconds)	numeric				yes
	Live Time (seconds)	numeric			yes* (from GADRAS)	
	Dead Time (seconds)	numeric			yes* (from GADRAS)	
	Height	numeric			yes "1"	
	Height Unit	Centimeter			yes "meter"	
	Distance From Source	numeric				
	Distance from Source Unit	centimeter				
	Comment	text				

Since RadResponder is currently under development to support bulk import of spectroscopic data, a preliminary schema is defined here and has been given to the RR developers for future implementation.

Transfer Factors Table

The transfer factors table will be a variable length .CSV file with the following format:

Analyte	**Ground Deposition**	**Paper Air Filter**	**Cartridge Air Filter**	**Swipe**	**Water**	**Feed**	**Food**	**Milk**	**Soil**	**Vegetation**	**Other**	**Spectra**	**Beta Yield** Y_β	**Alpha Yield** Y_α
[unit]	**uCi/m2**	**uCi/mL**	**uCi/m3**	**pCi**	**…**									

Cs-137	1e-7	1e-3	1	0.23									.12	…
I-131	1e-5	1e-6	1	0.01									0.1	…
Sr-90	0	0	1	1									…	…
Gross Alpha	$\sum_i (I * Y_\alpha)_i$													
Gross Beta	$\sum_i (I * Y_\beta)_i$													

The columns will correspond to the available sample types and the last two columns will be the beta yield and alpha yield of the analytes. The second row of the .CSV will have an analyte of [unit] and the units will be specified for each sample type. Then the analytes' transfer factors (I) will fill in the table. If gross alpha and Gross Beta are entered as analytes, and the user does not specify a value, the system will calculate them based on the equations above.

Sample Activity Results

This file will be a .CSV with the following format:

{sampleID, analyte, team name, lat, lon, datetime, Sample Type, uCi/sample for each analyte}

RadResponder ARF import file

The import of ARFs to RadResponder is done through a two-part excel import file. A copy of the data dictionary for the import file is below:

Analysis Request Data Dictionary

Sheet	Column	Data Type	Required?	Comment	Simulator Generated	User Entered
Analysis Request	Name	Text	Yes	Unique to Event.	[ARF Name]	
	Laboratory	Text	No	Refer to list in 'Allowed Values'.	[Laboratory Name]	
	Mixture	Text	No	Refer to list in 'Allowed Values'.		Yes, must match with one in RadResponder

Analysis Request Data Dictionary

Sheet	Column	Data Type	Required?	Comment	Simulator Generated	User Entered
	Event Analysis Poc Name	Text	No	Last Name, First Name OR First Name Last Name	(null)	
	Event Analysis Poc Phone	Text	No		(null)	
	Event Analysis Poc Email	Text	No		(null)	
	Event Analysis Poc Fax	Text	No		(null)	
	Event Analysis Poc Street 1	Text	No		(null)	
	Event Analysis Poc Street 2	Text	No		(null)	
	Event Analysis Poc City	Text	No		(null)	
	Event Analysis Poc State	Text	No	Refer to list in 'Allowed Values'.	(null)	
	Laboratory Comment	Text	No		(null)	
	Sample Management Comment	Text	No		(null)	
	Ship To Poc Name	Text	No		(null)	
	Ship To Poc Phone	Text	No		(null)	
	Ship To Poc Email	Text	No		(null)	
	Ship To Poc Fax	Text	No		(null)	
	Ship To Street 1	Text	No		(null)	

Analysis Request Data Dictionary						
Sheet	**Column**	**Data Type**	**Required?**	**Comment**	Simulator Generated	User Entered
	Ship To Street 2	Text	No		(null)	
	Ship To City	Text	No		(null)	
	Ship To State	Text	No	Refer to list in 'Allowed Values'.	(null)	
	Ship To Zip	Text	No		(null)	
Analysis Request Sample	Analysis Request Name	Text	Yes	Refer to list in 'Allowed Values'.	[ARF Name]	
	Sample Id/Barcode	Text	Yes	Refer to list in 'Allowed Values'.	[Sample ID]	
	Nuclide Type	Text	Yes	Refer to list in 'Allowed Values'.	[Analyte]	
	Critical Level	Decimal	No		(Null) - RR infers this from the mixture linked in ARF definition sheet	
	Critical Level Unit	Text	No	Refer to list in 'Allowed Values'.	(Null) - RR infers this from the mixture linked in ARF definition sheet	
	Analysis Method	Text	No	Refer to list in 'Allowed Values'.	[Analysis Method]	

Rad Responder Sample Result Electronic Data Deliverable (EDD) Import field mapping

Rad Responder includes a general sample results import template in Excel to allow users to bulk import sample results. The table below describes how this simulator will generate this file for each ARF that is being simulated.

Analytical Result Upload Data Dictionary					
Column	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User Entered**
Result Date	Date Time	Yes	Local Time	[Sample Date/Time]	
Reported By	Text	Yes	Last Name, First Name OR First Name Last Name	{Jane Doe}	
ID/Barcode	Text	Yes	Must match existing sample or spectra number for the event	[Sample ID]	
QC Batch #	Text	No	Unique identifier for the batch, also known as Lab/LIMS #		
Analysis Request Name	Text	No	Must match existing analysis request for the event	[ARF Name]	
Laboratory Name	Text	No	Must match existing laboratory in RadResponder.	[Laboratory Name]	
Analysis Methodology	Text	Yes	Must match existing analysis method in RadResponder.	[Analysis Method]	
Nuclide Type	Text	Yes	Must match existing nuclide types in RadResponder.	[Analyte]	
Result	Decimal	Yes	The following formats are valid x.xx, <x.xx, >x.xx or <MDA	[Result]	

Analytical Result Upload Data Dictionary					
Column	**Data Type**	**Required?**	**Comment**	**Simulator Generated**	**User Entered**
Result Unit	Text	Yes	Must match a measurement unit in RadResponder	[Result Unit]	
Uncertainty/Error	Decimal	No		[Result Uncertainty]	
Coverage Factor	Decimal	No			{Coverage Factor}
MDA/MDC	Decimal	No		[MDA]	
Measured Critical Level	Decimal	No		[LC]	
Quantity as Analyzed	Decimal	No		[Sample Size]	
Quantity Unit	Text	No	Must match EITHER volume or weight unit in RadResponder	[Sample Size Unit]	
Wet or Dry?	Text	No	Either 'Wet' or 'Dry' value is valid	Wet	
Lab Qualifier	Text	No	Refer to options in 'Lab Qualifiers' tab	{Calculated *See Note}	
Comment	Text	No	Any comments about the result		
Upload Type	Text	No	Valid entries are 'No Change', 'New', 'Update' and 'Append'. If updating a record a combination of sample number, nuclide type and analysis method are used to link results.	New	

* Calculating Lab Qualifier:

If [Result] < Lc, Lab Qualifier = “Less Than Lc”

If [Result] > Lc and [Result] < [MDA], Lab Qualifier = “Estimated”

If [Result] > [MDA], Lab Qualifier = “Approved”

Appendix III: Lab Reports Template

The simulator will generate simulated laboratory hardcopy reports that can be uploaded to RadResponder alongside the results to give the FRMAC QA Specialist some reports to look at. Within the laboratory there will be several reporting options that are able to be toggled on and off to control what data gets reported, what internal laboratory QC samples get reported, and what "QA issues" may be included in the reports. QA issues include discrepancies between the reported value and the electronic data, QA sample failures, and missing samples from the report.

The analysis report will include at a minimum, a case narrative and the unknown sample reports. If toggled, the QA reports will be reported at the end. The whole report will be in a single .PDF file. An answer key highlighting all the failures or the fields that are typo' d on the EDD results will be highlighted. The naming convention for the PDF will be the following:

[ARF Name]_HardcopyResults_{key}.pdf.

The simulator will only generate the extra {key} file if any failures are toggled on.

Case Narrative	• This is the first page of the report
Unknown Sample Report	• One page per analysis method, per sample, per ARF • Analysis Results contain all the analytes reported for the analysis method • Results are pulled in from the simulated electronic results • Discrepancies are randomly placed in the electronic (EDD) file, the hardcopy report is always correct. • When typos are turned on, a special "Answer key" report is printed with the fields highlighted where there are typos on the EDD file.
Lab control Sample Report	• When toggled on, one report per analysis method per ARF • Count time matches the count time of the analysis method used in the generation of results • Analysis table contains a row for each analyte reported for the analysis method. • Passing bias is calculated as random number between -0.25 and 0.25 • When toggled on, failing bias is randomly chosen to be between { -0.75 and -0.25} OR {0.25 and 0.75}
Method Blank Report	• When toggled on, one report per analysis method per ARF • Analysis table contains a row for each analyte reported for the analysis method. • Count time matches the count time of the analysis method used in the generation of results • The average Lc or MDA (whichever was toggled on for the laboratory) for all the samples on the ARF gets placed on the ARF's MB report.

	• {20%fuzz}=a gaussian fuzz factor centered about the value with a 20% 1-sigma standard deviation. Use Box Muller Approximation. • Pass/Fail toggle determines which equation is used in calculation of the result

Laboratory hardcopy report toggle form:

This table will be included in the laboratory section and will define what the hardcopy results will look like for each ARF sent to the laboratory.

Include Hardcopy Report in simulation?	Yes/No
Include Typos on Electronic Data?	Yes/No
How many Typos/ARF? Note: Typos will be randomly distributed amongst all data in the EDD for an ARF, on the hardcopy key, the values that were changed will be highlighted.	Number from 1 to 10
Report Coverage Factor? Note: this governs how data is reported in the EDD as well	1 or 2
Report Lc or MDA?	Lc or MDA
Report Lab Control Sample with each method?	Yes/no
Report failed LCS analyte on each analysis method? Note: this will force an LCS failure (a bias outside of +/- 0.25) on one analyte per analysis method randomly distributed amongst all analytes reported for that method	Yes/no
Report Method Blank Sample with each method?	Yes/no
Report failed MB analyte on each analysis method? Note: this will force an MB failure (a result that far exceeds the reported average Lc value) on one analyte per analysis method randomly distributed amongst all analytes reported for that method	Yes/no

Case Narrative

[Laboratory Name]			
Analyzed By:	[Signature 1]	**Reviewed By:**	[Signature 2]
Case Narrative			
Customer Request ID	:	[Analysis Request Name]	

A batch of {count of samples} were received by the laboratory and processed according to a standard operating procedure in accordance with the requirements stated in the Analysis Request Form.

A continuous chain of custody for the samples was maintained and documented on the original Analysis Request Form which will be submitted at a future time. This Level I data package contains a Case Narrative, the analytical reports for the unknown samples, and any applicable QC samples (if reported). In addition to these reports, electronic data is submitted in the requested format. Higher level data packages may be requested at a future date by contacting the laboratory.

Unknown sample report

[Laboratory Name]			
Analyzed By:	[Signature 1]	**Reviewed By:**	[Signature 2]

Unknown Sample Report

Customer Request ID	:	[Analysis Request Name]	
Customer Sample ID	:	[Sample ID]	
Sample Type	:	[Sample Type]	
Sample Quantity	:	[Quantity as Analyzed]	[Quantity Unit]
Sample Date/Time	:	[Result Date]	
Analysis Method	:	[Analysis Methodology]	
Count Time	:	[Count Time]	Seconds

Analysis Results

Analyte	**Result**	**Uncertainty**	**{LC or MDA}**	**Lab Qualifier**
	[Result Unit]	**K=[coverage factor]**		
[Analyte]	[Result]	[Uncertainty]	[Lc] or [MDA]	[Lab Qualifier]
…	…	…	…	…

Lab control Sample Report

[Laboratory Name]			
Analyzed By:	[Signature 1]	**Reviewed By:**	[Signature 2]

Lab Control Sample Report

Customer Request ID	:	[Analysis Request Name]	
Customer Sample ID	:	LCS-[Analysis Request Name]	
Sample Type	:	Lab Control Sample	
Sample Quantity	:	1	ea.
Analysis Method	:	[Analysis Methodology]	
Count Time	:	[Count Time]	Seconds

Analysis Results

Analyte	**Bias**	**Pass/Fail**
	%	
[Analyte]	{LCS Bias}	
…	…	…

Method Blank Report

[Laboratory Name]			
Analyzed By:	[Signature 1]	**Reviewed By:**	[Signature 2]

Method Blank Sample Report

Customer Request ID	:	[Analysis Request Name]	
Customer Sample ID	:	MB-[Analysis Request Name]	
Sample Type	:	Method Blank	
Sample Quantity	:	1	ea.
Analysis Method	:	[Analysis Methodology]	
Count Time	:	[Count Time]	Seconds

Analysis Results

Analyte	**Result**	**Uncertainty**	**{LC or MDA}**	**Pass/Fail**
	[Result Unit]	**K=[coverage factor]**		
[Analyte]	=0.5*[Lc]*{20%fuzz} for pass =4*[Lc]* {20%fuzz} for fail	=0.5*[Lc]* {20%fuzz}	{Average of sample [Lc] or [MDA] reported for ARF}	{Pass} or {Fail}
…	…	…	…	…

Appendix IV: Rad Responder development needed to support full-integration/automation of the simulation process

To fully integrate the simulated data produced by this software, Rad Responder will need some development work done to minimize the data entry burden on the user. Listed below are some features that may be developed in the future to support the automation of sample result simulation.

- Develop an improved ARF import capability: inherit names and addresses from the event and laboratory; also, inherit the required critical level and unit from the linked mixture
- Develop a bulk import capability for In-Situ spectra measurements and their associated files
    - RadResponder currently allows for the bulk import of sample records and their metadata but does not include In-Situ measurements. A future import template that includes the metadata for an In-Situ spectra measurement would allow for the simulator user to easily import the injects into Rad Responder.
    - In addition to In-Situ spectra metadata, a bulk wise method for importing the spectra files that contain the unique identifier in the filename will be needed to expedite the data entry process.
- Develop ability to import hardcopy result files to created ARFs in bulk.
    - This simulator will develop EDD files containing simulated results for the ARFs and a .PDF of the hardcopy results. These EDD files can be imported in bulk but the individual files must be uploaded to each ARF individually. If there were a mechanism to bulk import the files and have them associate with the correct ARF, that would expedite the simulation process.
- Develop ability to schedule injects to upload during exercise play
    - To reduce the burden on the simulation cell, prestaged samples, ARFs, and results (along with their associated files) can be scheduled in an advanced importer script that would allow for an automated data transfer into the system on a set schedule defined by the exercise controllers. That would allow for simulation work to occur up front and during exercise play, injects would appear in the system in a realistic timeline. This would allow exercise players to see data stream in in near real-time adding a layer of realism that was not possible previously. With a tool like this, larger scale drills can be simulated with fewer players in the field helping responders get more familiar with realistically dense data sets.
- Full Sample, ARF, Result, file API available for future simulator development
    - A full API can be used by a future version of the simulator to make data connections more robust and seamless. This would of course, require development on both sides.

Appendix V: In-Situ Simulation in GADRAS

As an add-on to this simulator, a special batch processing add-in to GADRAS should be developed that will read in the export file from the Sample Control Module and batch-create the raw spectral files in GADRAS so that they may be imported into Rad Responder as if they were collected by field teams. The add-on to GADRAS will require the user to provide the following information:

1. Input file from the sample data simulator
2. Detector used for simulation – this will need to have been created in GADRAS
3. Model used for simulation – this will need to have been created in GADRAS
    a. In-Situ Disk or custom 1-D or 3-D model
4. Toggle gain adjustment bias (shift one way or the other for all) and fuzz (random about no shift)
5. Spectral file output type (.N42, .SPC, .PCF, etc.)
6. File drop location – file-folder where all spectral files will be saved

GADRAS would then run through each row of the input file, create a background spectrum based on the geocoordinates, then simulate the measurement given the count time, counting model, and source term. GADRAS would create a spectrum file, name it with the unique identifier in the file and save it to specified folder. The simulation user would need minimal training in GADRAS to perform this simulation for the most common In-Situ spectra generation. The user would then use the sample import template for Rad Responder entry and then import the files to Rad Responder to complete the simulation work.