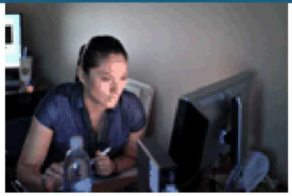
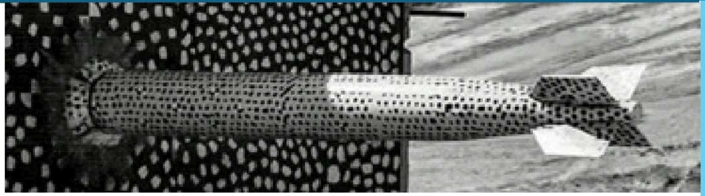
SAND2020-0797PE

CCDFGF - Overview





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PRECCDFGF

PRECCDFGF

- Collates the output from other WIPP PA codes into a single release table (RELTAB) file

Key Capabilities:

- Read multiple input file formats
- Retrieve information from the WIPP PA Parameter Database (PAPDB)

Key Inputs:

- Release Data
  - Direct brine release tables from BRAGFLO_DBR
  - Direct solids release table from CUTTINGS_S
  - Salado transport release tables from NUTS and PANEL
  - Culebra transport release tables from SECOTP2D
- Inventory Data
  - CH and RH waste stream data from EPAUNI
  - Mobilized radionuclide files from PANEL
  - Colloidal mobilization fractions from PANEL
- Parameter Data
  - Sampled parameter values from LHS
  - Constant parameter values from the PA Parameter Database (PAPDB)

Key Outputs:

- One RELTAB file for each replicate (e.g. ccgf_CRA19_reltab_r1.dat)

Downstream Use of Output:

- CCDFGF input files

CCDFGF

CCDFGF – CCDF Generating Function

- Assembles results to produce complementary cumulative distribution functions (CCDFs)

Key Capabilities:

- Uses a Monte Carlo procedure to evaluate stochastic uncertainty about future states of the repository

Key Inputs:

- One RELTAB file for each replicate, created by PRECCDFGF
  - e.g. ccgf_CRA19_reltab_r1.dat
- One control file for each replicate, user-defined
  - e.g. ccgf_CRA19_control_r1.inp

Key Outputs:

- One output file for each replicate
  - e.g. ccgf_CRA19_r1.out
- Outputs written to the database PA_Results
- Final CCDFGF curves

Downstream Use of Output:

- Post-processing, regulatory evaluation

CCDFGF – Code Overview

Assembles results from other WIPP PA codes

- BRAGFLO_DBR, PANEL, NUTS, SECOTP2D, CUTTINGS_S, EPAUNI

Simulates drilling of boreholes at the surface of the repository

- Drilling location, depth (whether the brine pocket is penetrated), plugging pattern vary

Produces one complementary cumulative distribution function (CCDF) for each set of sampled values

A CCDF defines the probability that cumulative normalized releases will exceed a given level

An individual CCDF represents 10,000 randomly chosen futures for each vector

- 10,000 points per CCDF
- Each future is equally probable
- 100 vectors per replicate, 3 replicates

WIPP compliance is based on the mean CCDF over 3 replicates

- An individual CCDF is NOT relevant for compliance

CCDFGF – Stochastic Elements

Stochastic Uncertainty – Uncertainty related to predicting future events

- Drilling and mining are the only disruptive events that are both sufficiently likely and consequential
- Assumes drilling intrusions and mining within the LWB occur randomly in space and time

Stochastic Elements:

- Time (yr)
- Location
- Activity level (Ci/m^2)
- Diameter (m)
- Brine pocket intrusion
- Plugging pattern of each intrusion
- Time that mining occurs

CCDFGF – Epistemic Uncertainty

Epistemic Uncertainty – Uncertainty related to values of parameters

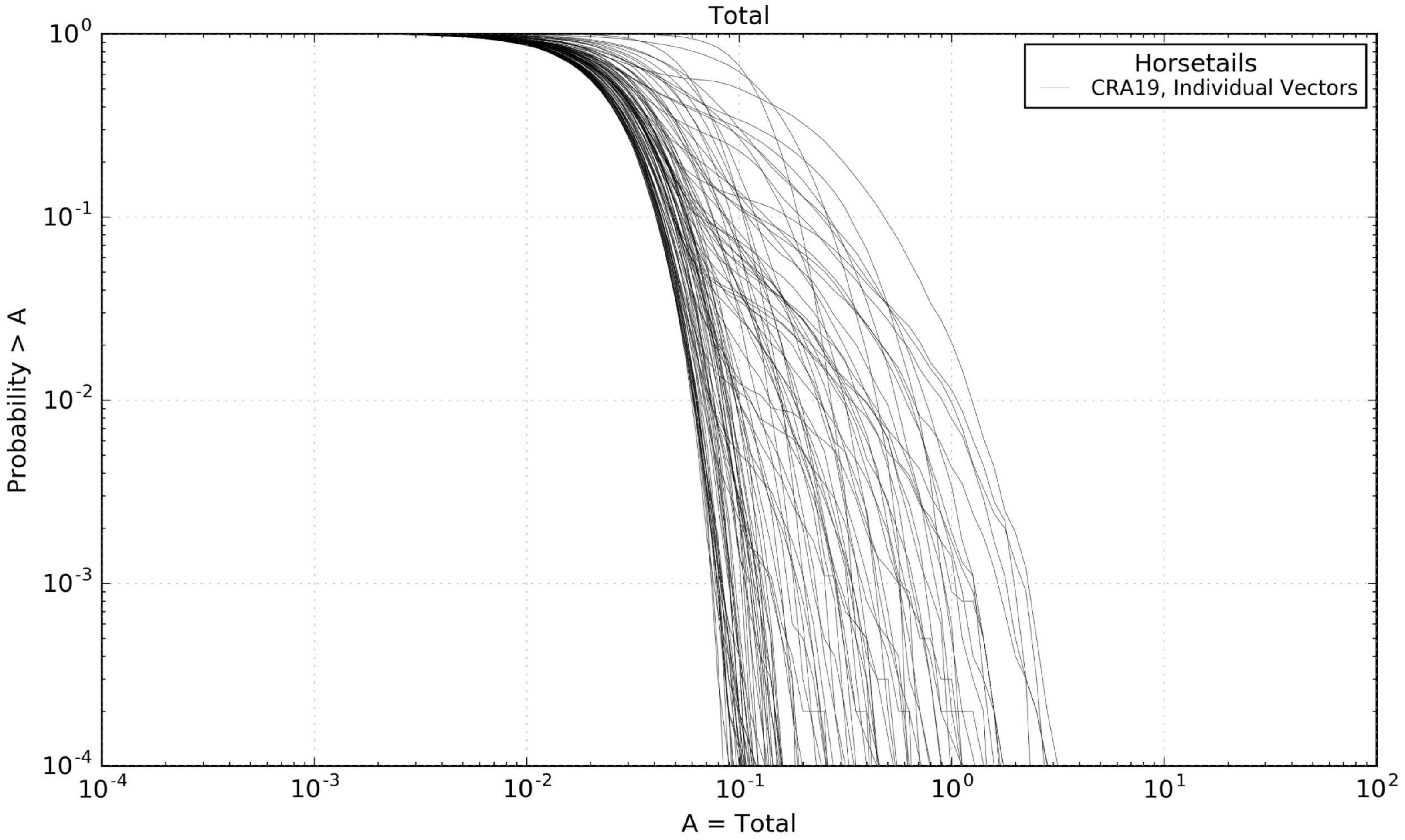
Sampled parameters (64 in CRA19)

Assigned a distribution that characterizes the uncertainty in that variable

One CCDF curve represents:

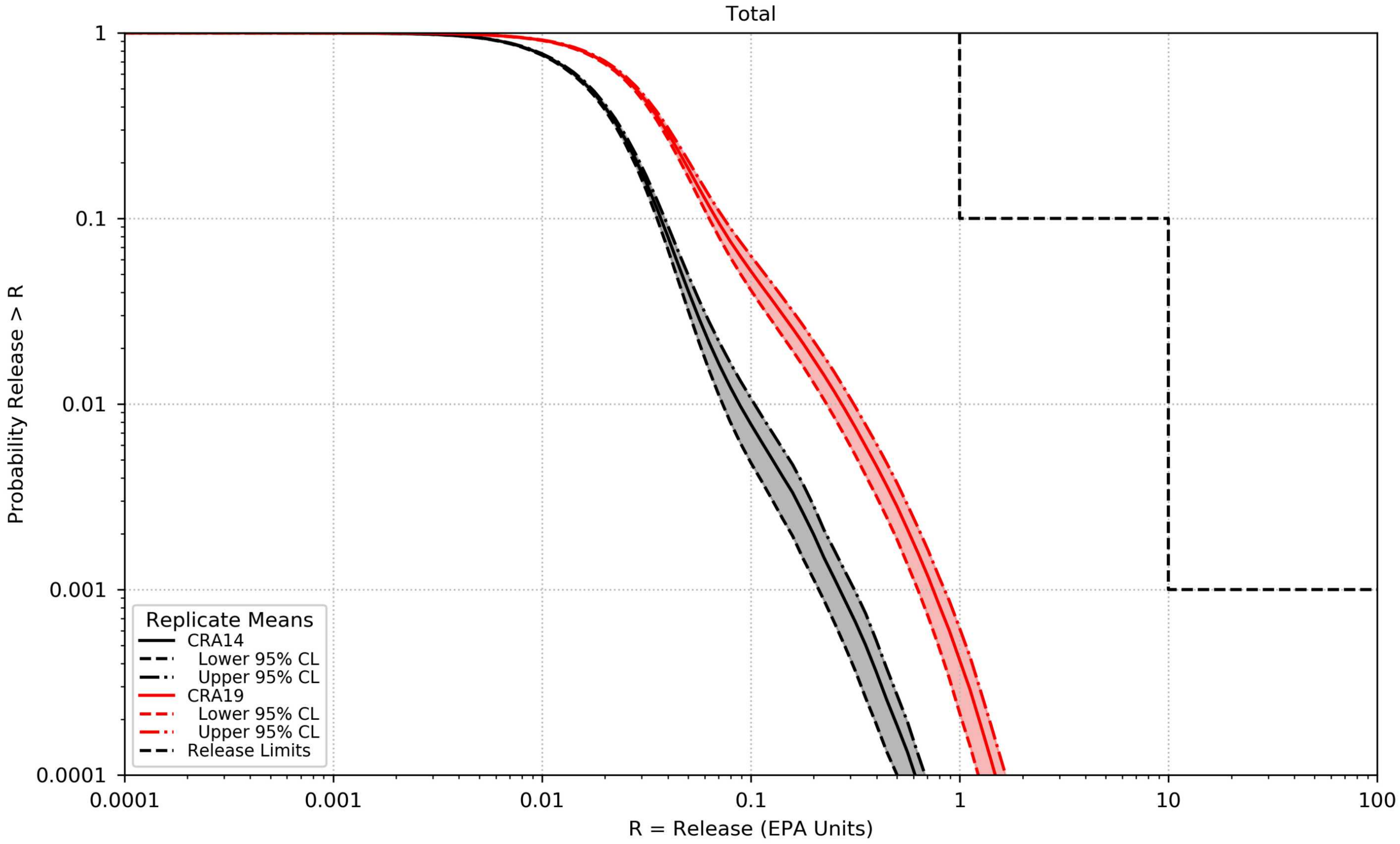
- One set of values for each vector
- 10,000 possible futures for that set of values

CRA-2019, Replicate 1



100 CCDFs, each constructed from 10,000 data points (futures)

CRA-2014 vs. CRA-2019, Mean CCDFs



CCDFGF – Sampling of Futures

Sample the uncertainty of events occurring over 10,000 years

Make the following assumptions:

- Drilling intrusions occur randomly in time and space
- Different plugging patterns are used for different drilling intrusions
  - Full, two, three plug configurations possible
- Varying waste activity levels distributed within the repository
  - Different waste streams
  - RH vs. CH waste
- There is a distribution of drill bit diameters in use
- Selection of which waste panel is intruded is random
- An intrusion may or may not penetrate pressurized brine in the Castile Formation
- Potash mining occurs randomly in space and time

CCDFGF – Creating a Specific Future

Four processes control the generation of individual futures

- Drilling and mining intrusions
- Penetration of CH or RH waste
- Plugging of boreholes
- Penetration of the brine pocket

CCDFGF – Drilling and Mining Intrusions

100 years of administrative control assumed

Drilling and mining rates used to generate times for intrusions

- Rates are PAPDB parameters

Mining intrusions determine which Culebra release scenarios are selected

Location of drilling intrusions

- Randomly selected at execution time
- Based on panel probabilities defined in the control file

Borehole diameter

- Varies for each intrusion
- Output from CUTTINGS_S for each intrusion
- Used by CUTTINGS_S to calculate the volume of cuttings and cavings

CCDFGF – Penetration of Waste

Three stochastic processes involved:

- Is an excavated area penetrated?
  - Probability = (CH waste area + RH waste area)/Total area
    - All parameters are from PAPDB
- Is CH or RH waste penetrated?
  - CH Probability = CH waste area/(CH waste area + RH waste area)
  - RH Probability = RH waste area/(CH waste area + RH waste area)
    - All parameters are from PAPDB
- Which waste stream is encountered?
  - Each stream assigned a probability of being encountered
    - Calculated by PRECCDFGF from output produced by EPAUNI
  - Number of streams to be averaged
    - Specified in control file
    - 3 CH waste streams may be penetrated in one intrusion
    - Waste stream data output from EPAUNI

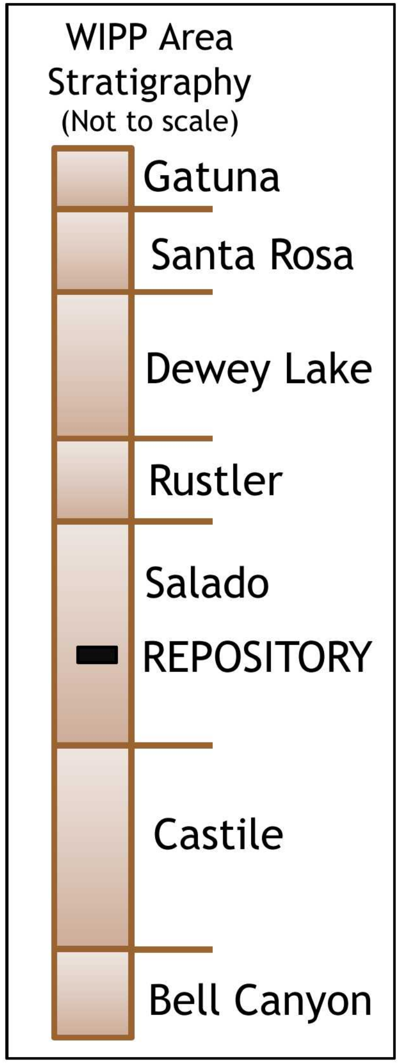
CCDFGF – Plugging Pattern

3 potential borehole plugging patterns
- Full concrete plug
  - Through Salado formation to Bell Canyon formation
- Two-plug configuration
  - Rustler/Salado Interface
  - Castile/Bell Canyon Interface
- Three-plug configuration
  - Rustler/Salado interface
  - Salado/Castile interface
  - Castile/Bell Canyon interface

Randomly selected based on probabilities

Probabilities defined in PAPDB

Used to set type of intrusion scenario



CCDFGF – Penetration of Brine

Probability of penetrating a brine pocket is a sampled parameter from PAPDB

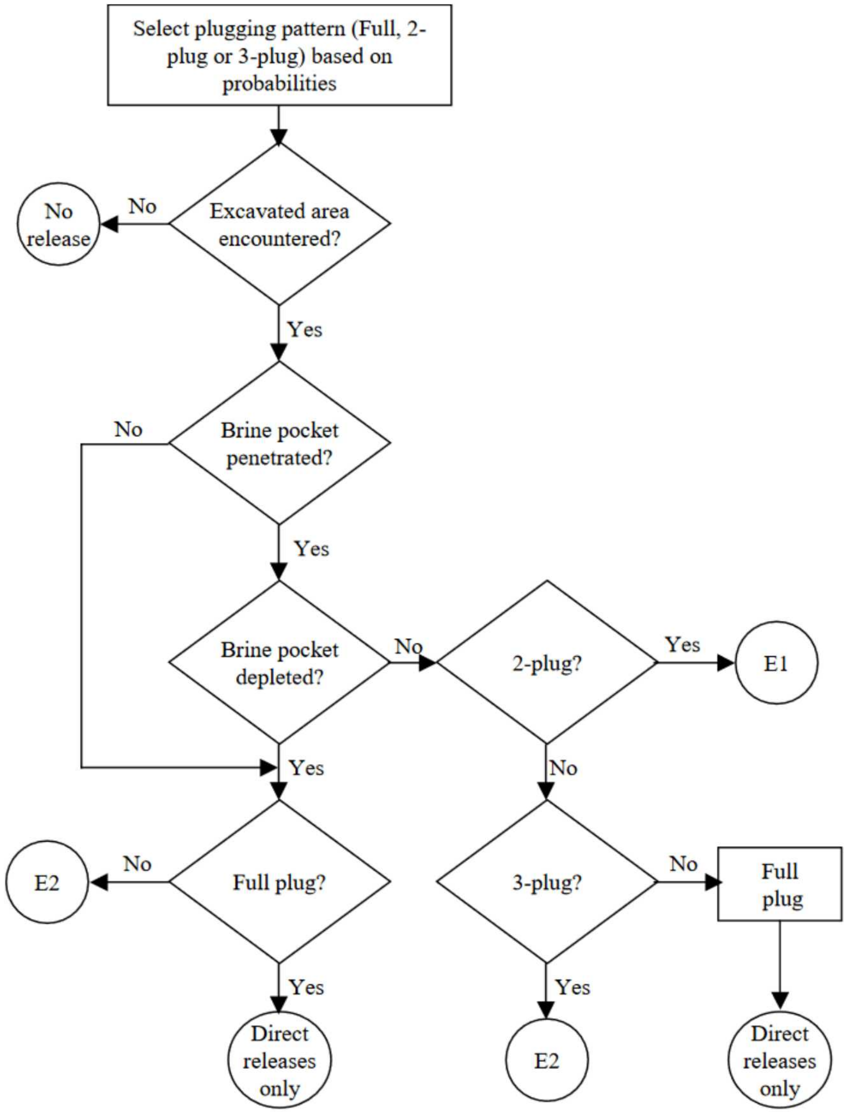
If an intrusion penetrates brine pocket:

- Check to see if excavated area is penetrated
- Check to see if brine pocket depleted
- Check plugging pattern:
  - Full plug –> E0 Scenario (Direct Releases Only)
  - Two plug –> E1 Scenario
  - Three plug, given no previous E1 intrusions –> E2 Scenario

If an intrusion does not penetrate brine

- Check to see if excavated area is penetrated
- Check plugging pattern:
  - Full plug –> E0 Scenario
  - Two or Three plug –> E2 Scenario

CCDFGF – Scenario Selection



Results for Specific Futures

Each sampled future requires the determination of a normalized release to the accessible environment

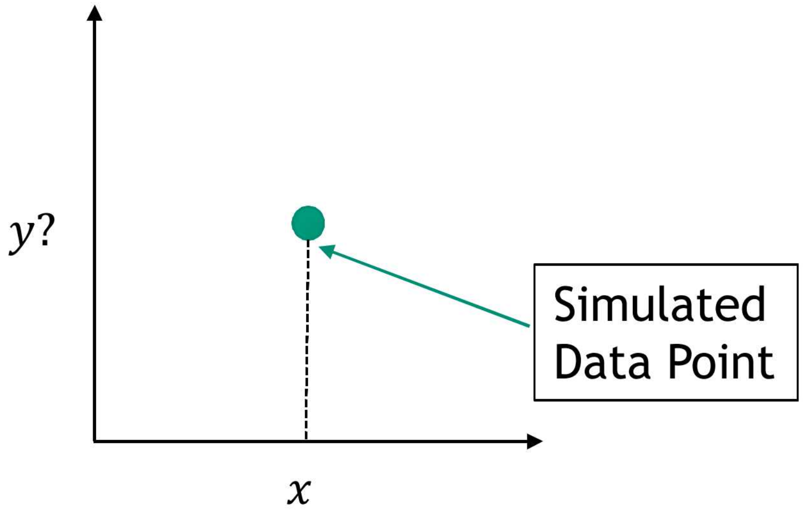
Each replicate represents a full PA

Computing these results requires the use of interpolation.

CCDFGF – Linear Interpolation

Computationally too intensive to model each possible scenario explicitly

Model representative points, interpolate when needed to determine the simulated values.



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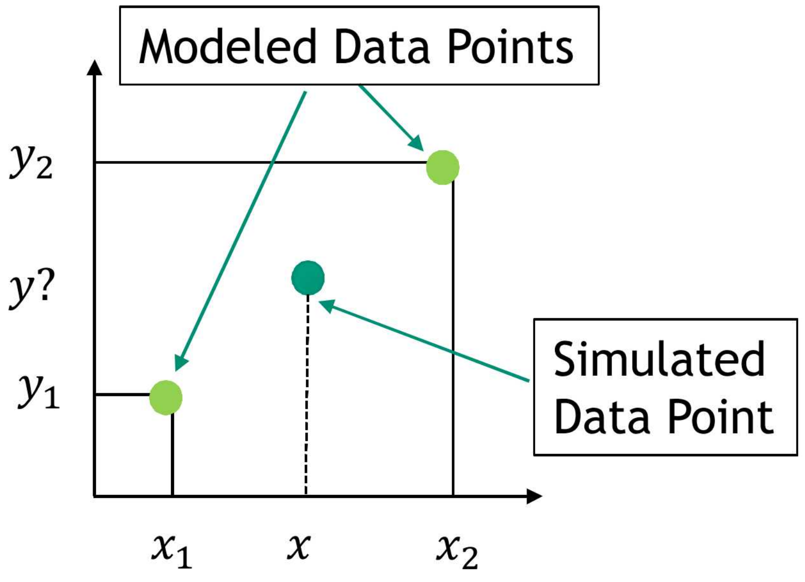

1. Find two modeled data points that bracket the simulated data point.

CCDFGF – Linear Interpolation

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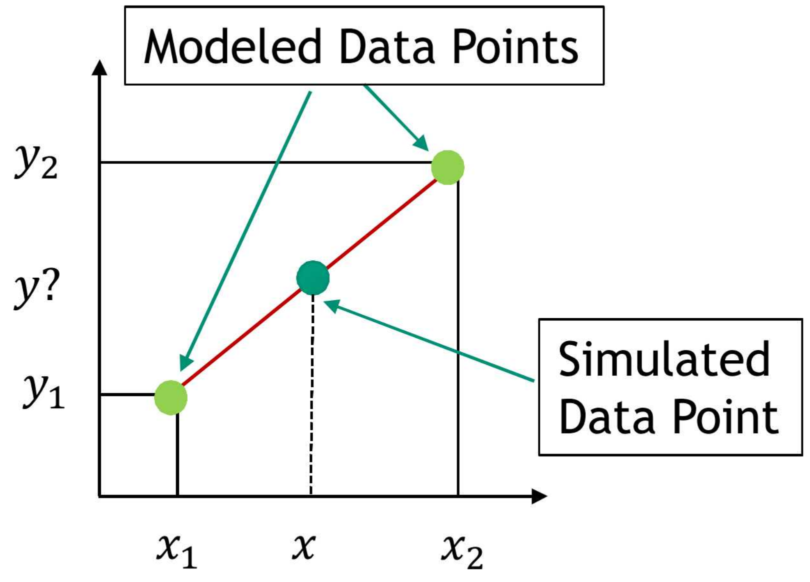

1. Find two modeled data points that bracket the simulated data point.
2. Draw a straight line between those two points.

CCDFGF – Linear Interpolation

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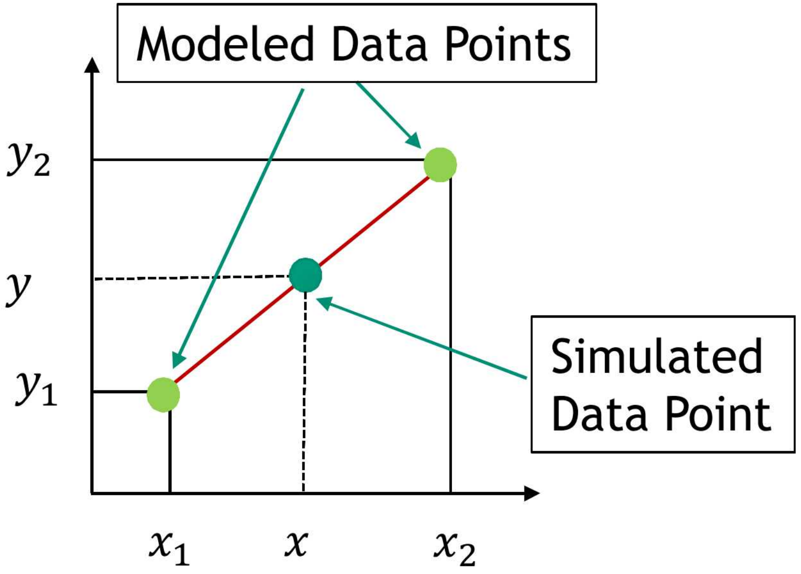


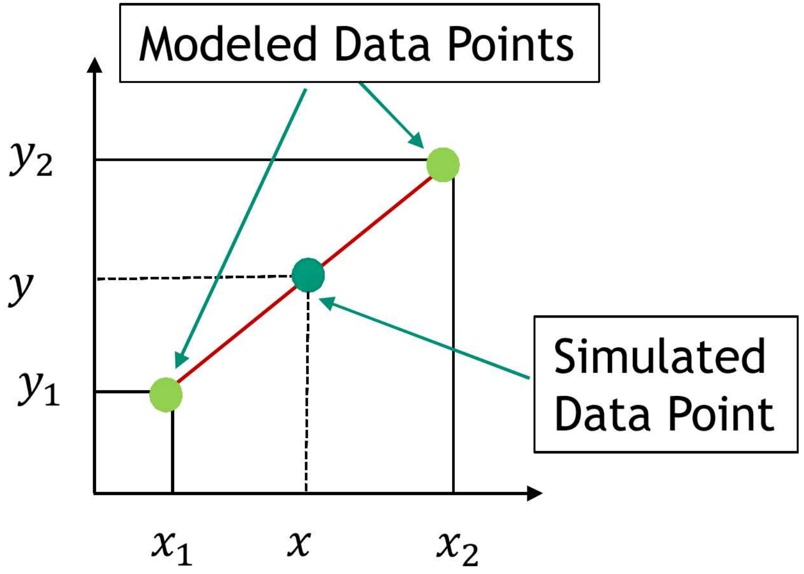
1. Find two modeled data points that bracket the simulated data point.
2. Draw a straight line between those two points.
3. Determine the ***y***-value at that point for our simulated ***x***-value.

$$y = y_1 + (x - x_1)\left(\frac{y_2 - y_1}{x_2 - x_1}\right)$$

CCDFGF – Linear Interpolation

Computationally too intensive to model each possible scenario explicitly

Model representative points, interpolate when needed to determine the simulated values.



1. Find two modeled data points that bracket the simulated data point.
2. Draw a straight line between those two points.
3. Determine the *y*-value at that point for our simulated *x*-value.
4. Repeat if needed to obtain additional reference points.

$$y = y_1 + (x - x_1)\left(\frac{y_2 - y_1}{x_2 - x_1}\right)$$

CCDFGF – Linear Interpolation

Example - Interpolation for direct brine, cuttings, and spallings volumes

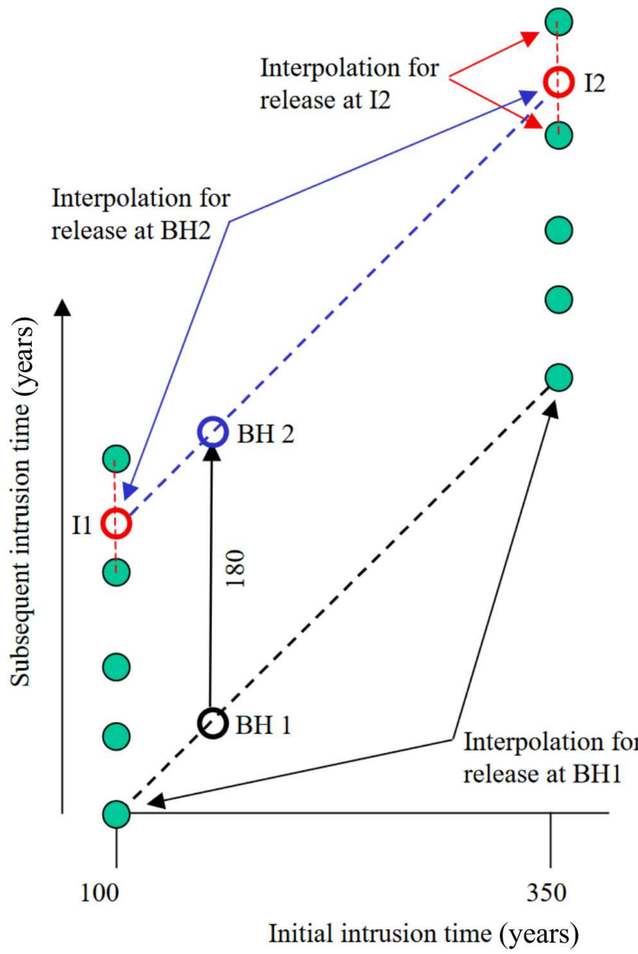
Based on time of the original intrusion and time to the subsequent intrusion

Data tables consist of release volumes and panel volumes at a series of intrusion times

Initial release volume and initial panel volume at any arbitrary time are computed by linear interpolation

Release and panel volumes are interpolated from corresponding release volumes for the appropriate panel location

CCDFGF – Linear Interpolation

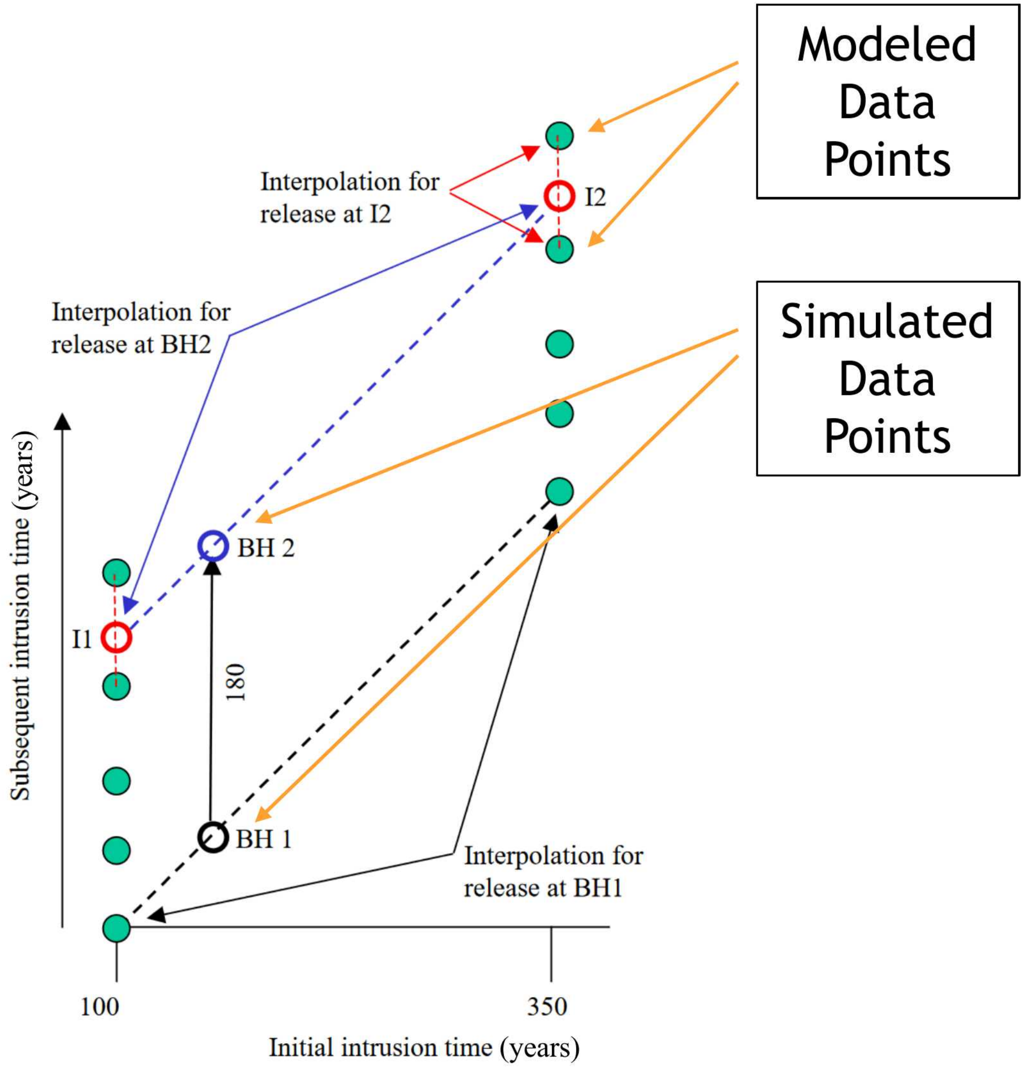


Initial intrusion located at BH1 at time 160.

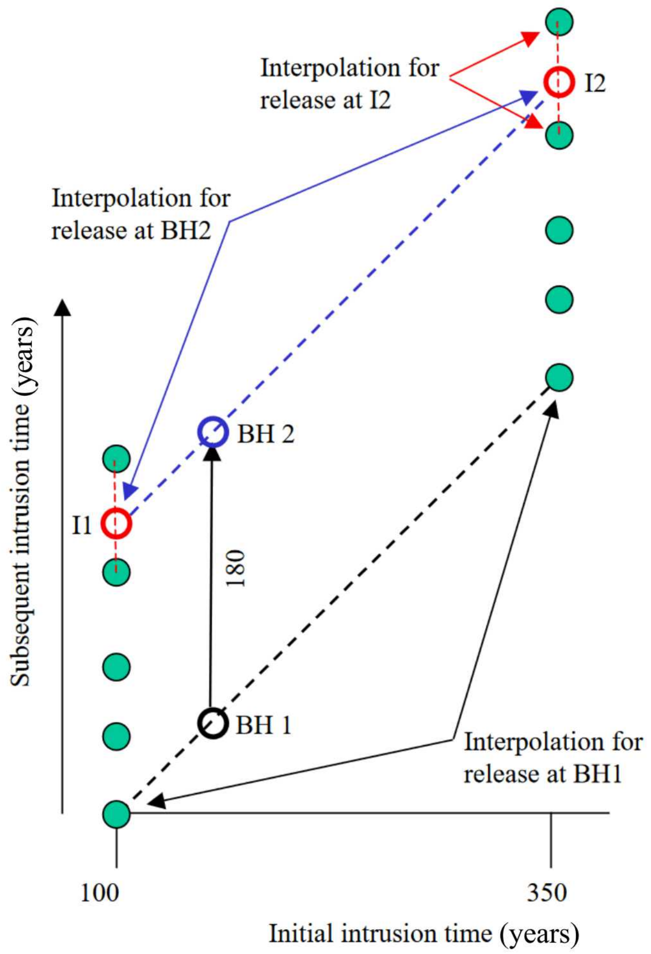
Subsequent intrusion at BH2 at time 340 years (180 years after the initial intrusion).

Need to use linear interpolation to find the (x,y) values at those two points to calculate release volumes.

CCDFGF – Linear Interpolation

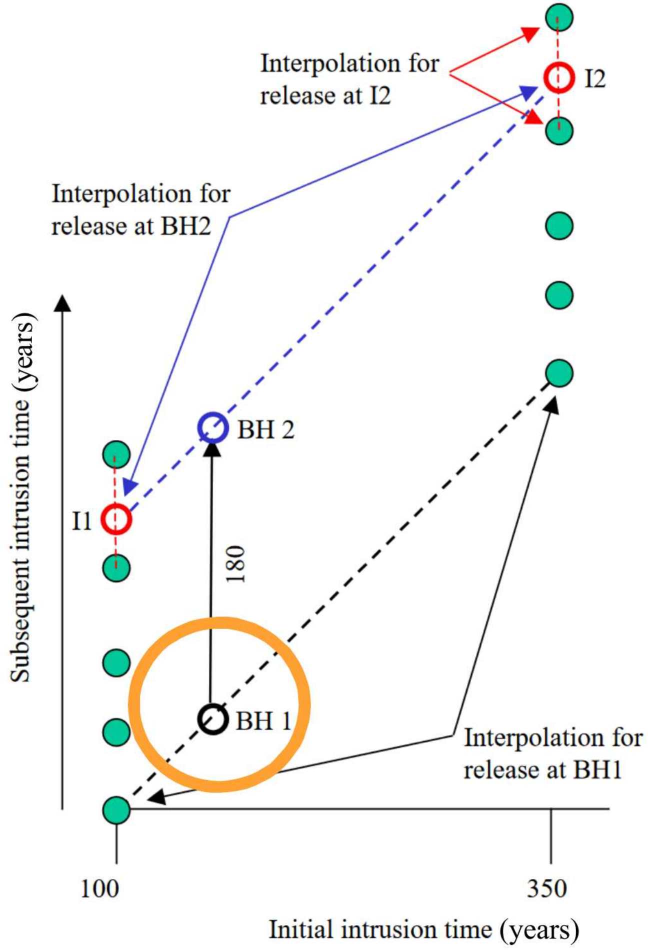


CCDFGF – Linear Interpolation



This represents 4 steps:

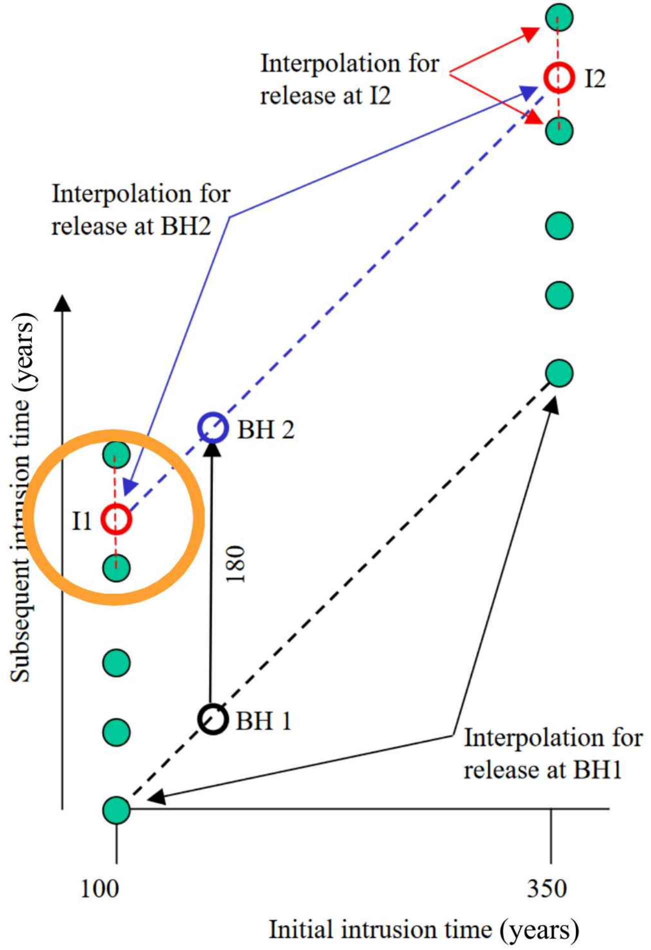
CCDFGF – Linear Interpolation



This represents 4 steps:

1. BH1

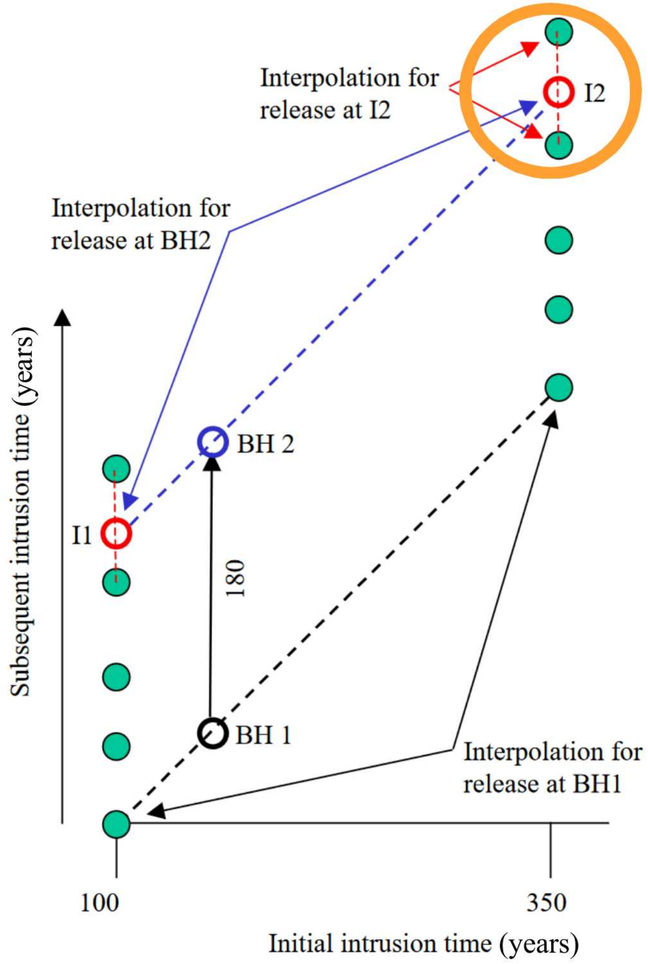
CCDFGF – Linear Interpolation



This represents 4 steps:

1. BH1
2. I1

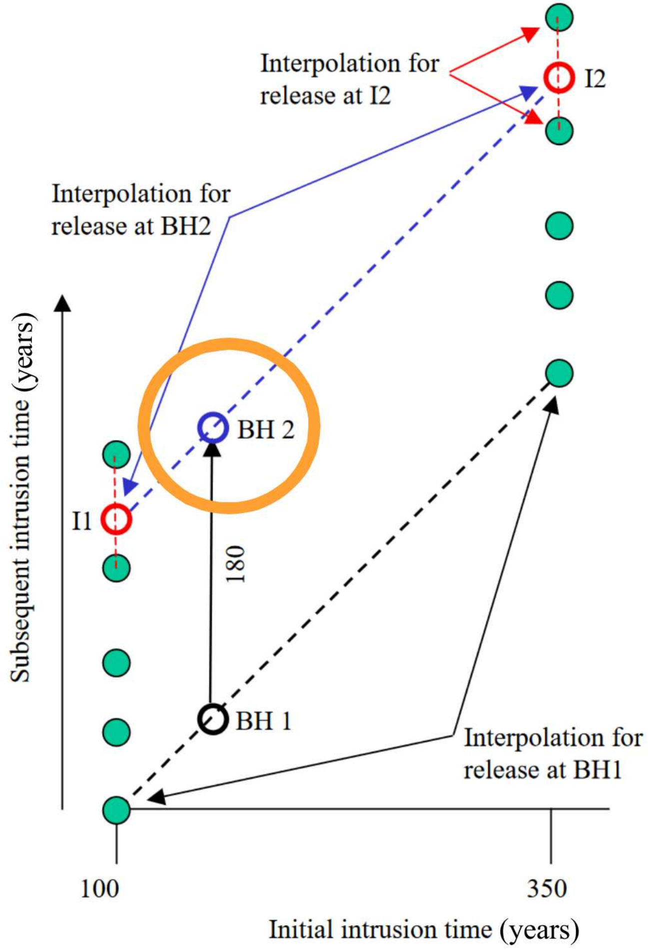
CCDFGF – Linear Interpolation



This represents 4 steps:

1. BH1
2. I1
3. I2

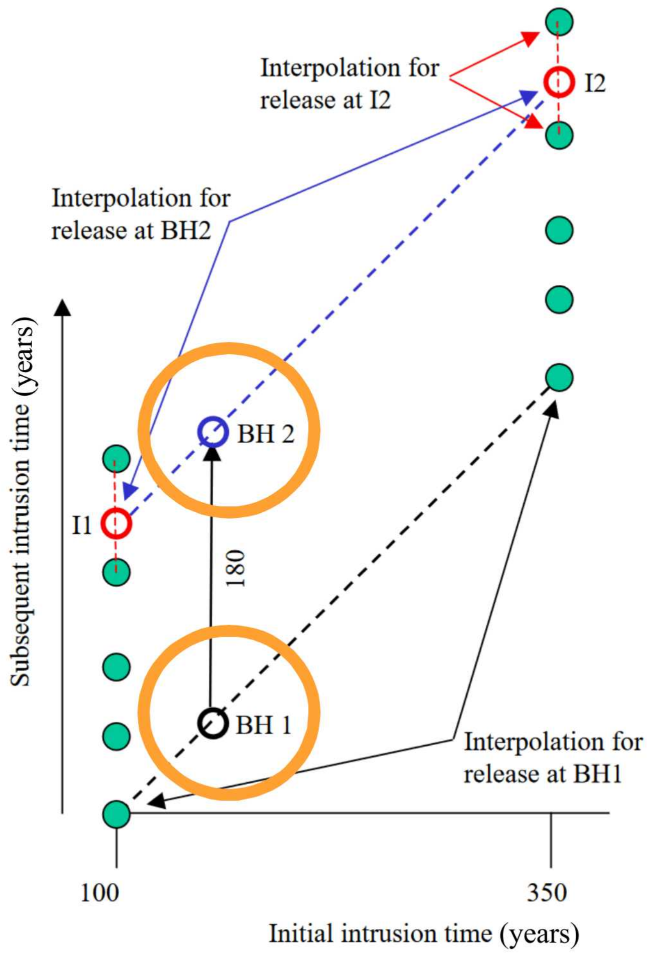
CCDFGF – Linear Interpolation



This represents 4 steps:

1. BH1
2. I1
3. I2
4. BH2

CCDFGF – Linear Interpolation



This represents 4 steps:

1. BH1
2. I1
3. I2
4. BH2

Releases are then computed based on these final interpolated values

CCDFGF – Cuttings Releases

Obtain waste type (CH or RH) based on PAPDB probabilities

Loop across number of waste streams to be averaged

Final releases computed as the volume of waste scaled by a weighting factor

3 table files, 1 per replicate

CCDFGF – Direct Releases and Transport

Direct (DBR and spallings) releases depend on conditions at the time of intrusion:

- Location of previous intrusions
- Conditions in the intruded panel
- Repository condition

Other WIPP PA models calculate releases for initial intrusion and for the second intrusion

CCDFGF calculates releases from the subsequent intrusions from the data for releases for the second intrusion

Repository and panel conditions are updated for each intrusion

CCDFGF – Direct Releases and Transport

CCDFGF assigns the following conditions:

Panel Condition – Determines releases through the Culebra

- E0 – Panel not intruded by drilling
- E1 – Panel has at least one previous E1 intrusion
  - At least one intersects brine
- E2 – Panel has at least one previous E2 intrusion
  - None intersect brine
- E1E2 – At least two previous intrusions, at least one E1 intrusion

Repository Condition – Determines DBR and Spallings releases

- E0 – Repository is undisturbed by drilling
- E1 – Repository has at least one E1 intrusion
- E2 – Repository has at least one E2 intrusion, no E1 intrusions

CCDFGF – Direct Releases and Transport

Direct releases also depend on the distance between current intrusion and previous intrusions

Use BRAGFLO_DBR release tables for these three cases:

- Same panel
  - Represents an intrusion into a previously intruded panel
- Adjacent panel
  - Represents an intrusion into an undisturbed panel adjacent to a previously intruded panel
- Non-adjacent panel
  - Represents an intrusion into an undisturbed panel not adjacent to a previously intruded panel

Panel adjacency is determined by the number of panel closures

CCDFGF – DBR Releases

Calculated for all intrusions that encounter CH waste

Constructed from:

- Brine releases to the surface from BRAGFLO_DBR
- Radionuclide concentrations in brine from PANEL

Volume of brine in the panel and volume of brine released depend on time of initial intrusion

234 DBR table files:

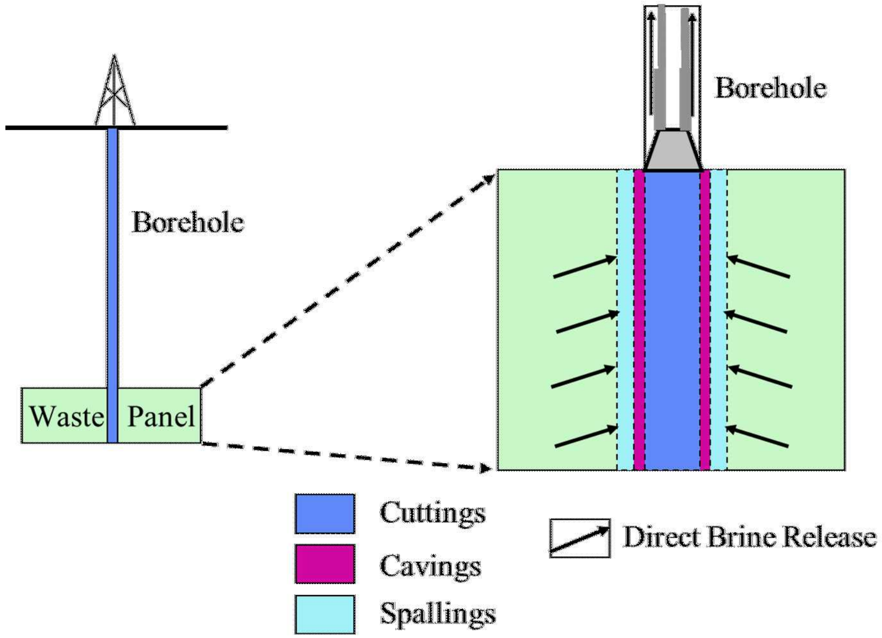
- 78 per replicate for 3 replicates
- Scenario, time, panel group (L,M,U)

CCDFGF – Spallings Releases

Calculated for all intrusions that encounter CH waste

Constructed from

- Volumes of solids released to the surface from CUTTINGS_S
- Radionuclide concentrations calculated from EPAUNI output by PRECCDFGF



CCDFGF – Radionuclide Transport

Similar to cuttings and DBR releases

Assumes primary paths for radionuclide transport are:

- Through boreholes to the Culebra (NUTS and PANEL)
- Through Culebra to LWB (SECOTP2D)

Releases are cumulative across:

- Each radionuclide species
- Each point in time
- All release pathways

CCDFGF – Releases to the Culebra

Constructs series of values for cumulative activity releases to the Culebra

Activity release data depends on:

- Panel condition (E0, E1, or E1E2)
- Radionuclide species
- Time for start of the release

Cumulative activity releases are summed from:

- Time of the intrusion until the next E1 or E1E2 intrusion into the same panel OR
- Until the end of the regulatory period

Accumulates a total release to the Culebra for each time interval and each radionuclide

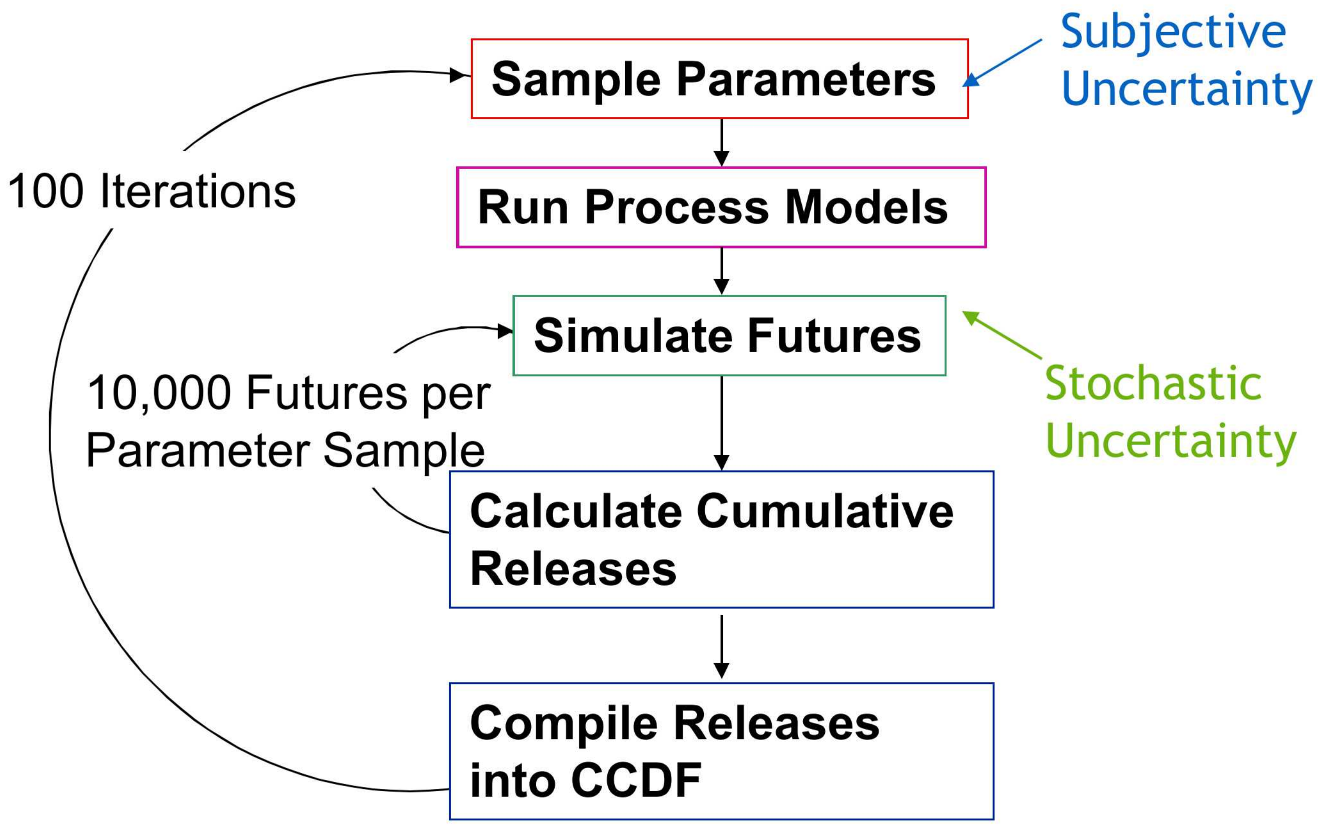
CCDFGF – Releases From the Culebra

Transport through the Culebra is calculated for each radionuclide

Releases through the LWB are based on the fraction of the mass of the radionuclide that reaches the LWB

These mass fractions are calculated by SECOTP2D

CCDFGF – Constructing CCDFs



CCDFGF – Results

Writes data to the PA_Results database

- Table CCDF_Data – Binned raw results

CCDFVECTORSTATS

- Reads results from CCDF_Data
- Calculates statistics
  - Mean, median, 10th and 90th percentiles*, standard deviation, and standard error
- Writes results to the database PA_Results
  - Vector statistics are written to the table StatsAcrossVectors
  - Replicate statistics are written to the table StatsAcrossReplicates

*Percentiles based on order statistics