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Swedish Radiation Safety Authority

Research

Importance-Sampling Time-Domain Random Walk (ISTIDRAW) Version 1.0 User Guide

A Code for Radionuclide Transport in Pathway Networks

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Author: Stuart Stothoff, Osvaldo Pensado
Southwest Research Institute, San Antonio, Texas, United States

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SSM perspective

Background

To support regulatory review of post-closure safety assessments of geological disposal systems it is of importance to possess regulatory independent modelling capacity. Typically, SSM's independent modelling includes performing simple scoping calculations, utilizing the implementer's own models with other equation solvers, or defining alternative conceptual models.

In order to model radionuclide transport in safety assessments, the Swedish Nuclear Fuel & Waste Management Co. (SKB), has used time-domain particle tracking (TDRW) methods, algorithms that *e.g.* include the flexibility to account for variability and uncertainty in transport parameters. SSM has, to develop expertise in TDRW methods and to possess independent modelling tools in this respect, tasked Southwest Research Institute with developing a radionuclide transport model based on TDRW concepts in MATLAB®. The resulting code is titled ISTIDRAW (Importance Sampling Time Domain Random Walk). The following report includes a description of the model as well as a user guide for the developed computational tool.

Results

Southwest Research Institute has developed a code for radionuclide transport in pathway networks, Importance-Sampling Time-Domain Random Walk (ISTIDRAW) Version 1.0. The code offers an independent modelling tool for SSM to perform radionuclide transport analyses, to check radionuclide transport computations performed by SKB, to evaluate limitations and nonstated assumptions of numerical methods, to explore the importance of alternative release scenarios with *e.g.* different representations of variability and uncertainty, and develop an understanding of the strengths and limitations of TDRW methods.

Relevance

The outcome of the project rendered a computational exploratory tool that SSM can use for independent modelling in future reviews of safety assessments in *e.g.* license applications for geological disposal facilities for radioactive waste.

Need for further research

The set of algorithms derived in the present project to sample trajectories in channel networks will, within the framework of a recently initiated research project (SSM2020-2460), be developed in order to *e.g.* further simplify the radionuclide transport pathways. The sampling algorithms will be interfaced with channel networks developed by researchers at Uppsala University (SSM2019-1201), aiming to further assess the long-term implications of channel networks in safety assessments.

Project information

Contact persons SSM: Henrik Öberg and Maria Nordén
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This report concerns a study which has been conducted for the Swedish Radiation Safety Authority, SSM. The conclusions and viewpoints presented in the report are those of the author/authors and do not necessarily coincide with those of the SSM.

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1. Introduction

The Swedish Nuclear Fuel and Waste Management Company (SKB) implemented a time-domain particle tracking (TDRW) algorithm (i.e., an algorithm based on sampling of residence time for packets of mass) to compute radionuclide transport for performance assessments of geological disposal systems (e.g., SKB R-09-56; Painter and Mancillas, 2009). Stated advantages for TDRW algorithms include the flexibility to (1) account for variability and uncertainty in transport parameters, (2) account for downscale variability in flow paths, and (3) efficiently compute expected releases at a detection boundary without the need to resolve detailed radionuclide fluxes between individual streamline segments. It is possible for particles to move along fast pathways and reach the detection boundary sooner than would be predicted by computational methods considering average flow fields and transport properties (e.g., continuum porous medium pathways). In order to develop expertise in TDRW methods, the Swedish Radiation Safety Authority (SSM) commissioned the Center for Nuclear Waste Regulatory Analyses (CNWRA[®]) to develop a radionuclide transport model based on TDRW concepts in MATLAB[®], without relying on proprietary functions. The resulting code is titled ISTIDRAW (Importance Sampling Time Domain Random Walk). The goal of ISTIDRAW is to offer a tool for SSM to (1) perform radionuclide transport analyses; (2) verify radionuclide transport computations performed by licensees; (3) evaluate limitations and non-stated assumptions of numerical methods; (4) explore the importance of alternative release scenarios, possibly with different representations of variability and uncertainty; and (5) develop an understanding of the strengths and limitations of TDRW methods.

This report is a user guide for ISTIDRAW. Chapter 2 provides an overview of the basis of the time-domain random walk method, but original sources should be consulted for details. Chapter 2 also presents the basis of the importance sampling, which is intended as a strategy to resolve the leading edge of cumulative release and release rate curves with a relatively small number of realizations. Chapter 3 describes the Microsoft[®] Excel[®] input worksheets, providing inputs such as the source release rates, decay chains, and pathway network and radionuclide transport parameters. Chapter 4 describes how to execute the model. Example MATLAB m-files are provided with the ISTIDRAW distribution to (1) execute ISTIDRAW, (2) perform post-processing of particle arrivals into radionuclide release rates and cumulative radionuclide releases, and (3) extract a limited number of trajectories from channel network files describing TRUE-Block field tests computed by collaborators from Uppsala University. The list of references is presented in Chapter 5. The Appendix describes equations to compute radionuclide retention times in the matrix.

ISTIDRAW was developed as an exploratory code, outside a stringent quality assurance program. However, development included a level of basic control and testing. Radionuclide release rates were benchmarked against theoretical solutions, GoldSim[®], and TDRW Version 2.1 (a precursor to MARFA, sponsored by SKB). Radionuclide decay and ingrowth functions were tested against GoldSim. The matrix diffusion model was compared to TDRW Version 2.1 and GoldSim pipe elements. GoldSim pipe elements predict more matrix retention than TDRW Version 2.1. The ISTIDRAW matrix diffusion model produced nearly identical results to TDRW Version 2.1. The GoldSim pipe can be calibrated to TDRW Version 2.1 by decreasing the porewater matrix diffusion coefficient and increasing the fracture aperture, thus reducing the extent of matrix retention in the GoldSim pipe element. The reason for differences between GoldSim pipe elements and TDRW Version 2.1 should be further investigated. Again, ISTIDRAW produces consistent results with TDRW Version 2.1, which was a MARFA precursor.

ISTIDRAW was tested with MATLAB 2013, 2015, and 2018 in Microsoft Windows[®]. It does not require any special MATLAB toolbox. ISTIDRAW requires Microsoft Excel to provide inputs.

2. Model Description

ISTIDRAW implements algorithms to solve for radionuclide transport using TDRW concepts, following the description by Painter and Mancillas (2009) for the MARFA code. The model solves the advection-dispersion mass-balance equation along a one-dimensional (1D) flow path, accounting for diffusive exchange with stagnant water (matrix diffusion) perpendicular to the flow path. The boundary condition at the inlet of the path is a release rate,¹ in units of mass/time. The inlet release rate is the source term (e.g., radionuclide release from degraded waste containers). ISTIDRAW does not provide source term models; the source term must be independently computed with a model of the engineered barrier system and the near field of a waste disposal system. The initial condition for the transport path is zero mass in the path. The one-dimensional path may be an open fracture or a channel established between fracture planes.

ISTIDRAW considers radionuclide mass exchange between the fracture and the rock matrix. The mass exchange mechanism is diffusion perpendicular to the 1D direction of flow in the open fracture. The assumed geometry for the rock matrix is a planar slab. The planar slab can be semi-infinite with a zero concentration at infinity, or a finite slab with a zero flux at the far boundary. Equilibrium linear sorption (i.e., the K_d coefficient approach) can be considered in the rock matrix and in the fracture (for example, when the fracture contains a porous material).

One or more detection points are selected along a path, creating segments (the separation between detection points is referred to as the path “length”), and radionuclide fluxes or release rates are computed at the detection point(s). Complex paths can be considered, in the form of single streamlines, networks of streamlines, or network of channels in fracture planes. Streamlines and channels are comprised of one or more segments, with uniform transport properties in each segment.

The solution approach for the pathway networks concatenates radionuclide fluxes at the segment nodes.² In other words, the release rate computed at a segment terminus becomes the inlet release for the next segment downstream. Transport within each segment along the main fracture path is assumed to be described by a semi-infinite Green’s function, with a zero concentration at infinity. This solution approach is an approximation to the true solution, honouring continuity of radionuclide fluxes within segments and at nodes, but not enforcing continuity of radionuclide concentration at each node. The approximated releases are reasonable for systems with concentrations well below the solubility limit, which is true of most applications of interest. For applications of interest (waste disposal systems with far detection points), radionuclide fluxes at a point in a fracture are dominated by advection and only weakly depend on downstream conditions.

The ISTIDRAW solution algorithm is based on Green’s functions and convolutions. The solution for each segment is established given a Dirac delta in the release rate at the inlet (i.e., segment Green’s function), and the solution for the network of segments is computed by sequential convolution of segment solutions. Convolution integrations are efficiently computed using Monte Carlo sampling. Based on work by Painter and Mancillas (2009), the solution algorithm for transport of one species in a segment (path of uniform transport properties), is described as follows. The Green’s function for a species without decay is the flux at the segment outlet as a function of time in response to a Dirac delta flux at the inlet. The flux Green’s function (in units of mass/time) is interpreted as probability density function (PDF) of the residence times of particles in the segment. The cumulative output flux or cumulative release is interpreted as the cumulative density function (CDF) of the residence time of particles in the segment. The “particles” are not individual atoms but clusters or packets of mass.

Given a PDF or CDF for the source release time and each segment residence time, the arrival time for a given “particle” passing through a sequence of segments is the release time plus the sum of

¹ The release rate is a flux integrated over a cross section perpendicular to the average direction of motion.

² A *node* is a label assigned to a segment end. A simple segment is a path of uniform transport properties. A simple segment is bound by two *nodes*.

the individual segment residence times. The release time and the individual residence times are computed by sampling from the individual CDFs.

Sampling the segment residence time requires two steps to account for matrix diffusion. First, the travel time in the fracture is computed, τ , assuming no matrix diffusion and no retardation. Second, depending on τ , the retention time in the matrix, t_{ret} , is sampled from a pertinent CDF that is a function of τ . The segment residence time for the particle is $\tau + t_{ret}$. The solution approach is summarized as follows

1. Sample a random particle insertion time t_{in} from the normalized source $f_{in}(t_{in})$.
2. Sample the particle travel time in the fracture, τ , based on a 1D path with longitudinal dispersion and no-matrix diffusion.
3. Sample the retention time, t_{ret} , as a function of the travel time in the fracture, τ . Two retention models are included in ISTIDRAW: semi-infinite matrix diffusion and matrix diffusion in a finite-thickness slab. The retention function depends on τ , the fracture aperture, the matrix porewater diffusion coefficient, matrix porosity, matrix retardation coefficient, and matrix thickness. The sample scheme in ISTIDRAW employs quantiles that are precomputed from pertinent cumulative distributions and stored as lookup tables (see the Appendix). To sample from the retention time distribution, a random number uniformly distributed between 0 and 1 is selected and the corresponding quantile is then interpolated from the stored lookup table.
4. Calculate the particle residence time for the Segment 1 as

$$t_1 = \tau + t_{ret}$$

5. Repeat steps 3 to 4 to independently compute the particle residence times as it transfers through n independent segments: $t_1, t_2, t_3 \dots, t_n$
6. Calculate the particle arrival time or travel times as

$$t_{ar} = t_{in} + \sum_{i=1}^n t_i$$

This travel time t_{ar} represents one sample (one particle) from the arrival time distribution.

7. In the absence of importance sampling, each particle contributes an amount S_0/N_{part} to the cumulative mass discharge, where S_0 is the total moles released at the source.
8. Repeat from Step 1 to 6 for a total of N_{part} particles, and construct the empirical cumulative distribution of arrival times from the N_{part} arrival times.

In Step 2, the PDF and CDF for travel time in the fracture, τ , are given by the following functions (Painter and Mancillas, 2009; Painter et al., 2008):

$$PDF(\tau) = f_{\tau}(\tau) = \frac{1}{\tau} \frac{\sqrt{\eta}}{\sqrt{4\pi}} \tau^{-3/2} \exp\left[-\frac{\eta(1-\tau)^2}{4\tau}\right]$$

$$CDF(\tau) = F_{\tau}(\tau) = \frac{1}{2} \operatorname{erfc}\left(\frac{\sqrt{\eta}1-\tau}{2\sqrt{\tau}}\right) + \frac{1}{2} \exp(\eta) \operatorname{erfc}\left(\frac{\sqrt{\eta}1+\tau}{2\sqrt{\tau}}\right)$$

where η is the segment Peclet number [= flow velocity \times segment length / dispersion coefficient] and erfc is the complementary error function.

In Step 3, the retention time, t_{ret} , is sampled. Different functions are sampled, depending on the matrix retention model (unlimited or limited matrix diffusion). In the case of unlimited matrix diffusion, the cumulative distribution function of the retention time is (Painter and Mancillas, 2009; Painter et al., 2008; Cvetkovic et al., 1999)

$$G(t_{ret}) = \operatorname{erfc}\left(\sqrt{\frac{\tau_1}{4t_{ret}}}\right)$$

$$\tau_1 = \left(\frac{\tau \theta}{b}\right)^2 R_m D_m$$

where D_m is the porewater diffusion coefficient in the matrix, θ is the matrix porosity, R_m is the matrix retardation coefficient, and b is the fracture semi-aperture (aperture/2). For the case of limited matrix diffusion, the cumulative distribution function of the retention time is computed as the inverse Laplace transform of the function $F(s)$

$$F(s) = \frac{1}{s} \exp\{-(\tau_1 s)^{1/2} \tanh[(\tau_2 s)^{1/2}]\}$$

$$\tau_2 = \zeta^2 R_m / D_m$$

where s is the Laplace variable and ζ is the matrix thickness. See the Appendix for details.

ISTIDRAW can consider multiple trajectories (i.e., multiple sequences of segments with a common source node and outlet node). The total number of particles, N_{part} , is passed through each trajectory.

ISTIDRAW considers multiple sources with multiple nuclides at each source. For each source, ISTIDRAW systematically selects a trajectory associated with the source node location and uses the same trajectory until the particle reaches the trajectory terminus or final detection node.

ISTIDRAW considers sequential decay chains. Decay and the resulting transformation to the next species in the decay chain are simulated as random events that transform the particle entire molar mass to the offspring species at the time of the decay event. The decay time is sampled from an exponential distribution with the decay rate λ as the distribution parameter. If a decay event occurs in a segment, the total residence time of the offspring in the segment is calculated as a combination of sampled residence times for the parent and offspring species. The sampled residence time within a given segment must be perfectly correlated for all members of a decay chain (i.e., drawn from the same probability quantile) for the method to be correct. This perfect correlation is interpreted to mean that the particle stays on the same flow path as it decays. For example, if the decay time is t_d , measured from the time the particle enters the segment i , and t_i^p and t_i^c are the total segment residence times for the parent and child (including advection in the fracture and matrix diffusion, assuming corresponding transport parameters for the parent and child for the complete segment), sampled perfectly correlated,³ then the corrected child travel time, \bar{t}_i^c , is

$$\bar{t}_i^c = t_d + \left(1 - \frac{t_d}{t_i^p}\right) t_i^c$$

Since the decay event occurs in segment i , and the decay time is measured with respect to the time after the particle enters segment i , then necessarily $t_d \leq t_i^p$. A similar correction is applied for the next member of the decay chain, until the particle reaches the detection node of the trajectory. The decay times are sampled from the cumulative distribution function (or normalized cumulative decay function)

$$F(t) = 1 - \exp(-\lambda t)$$

where λ is radionuclide decay rate. At the detection node, both the particle travel time and the particle identity (i.e., member of the decay chain) are recorded.

³ To compute a particle travel time in a segment, two random numbers r are sampled ($0 < r < 1$). One random number is used to determine the fracture travel time, and the second random number for the matrix retention time. To attain *perfectly correlated sampling*, the same two random numbers are used for the parent and child.

2.1. Sampling Approach

ISTIDRAW permits importance sampling of any sampled parameter to improve the resolution of parameter tails that affect simulation results. Importance sampling can be applied to

- Release time from the source
- Travel time in the fracture
- Retention time in the matrix
- Decay time

In order to assure mass balance with the importance sampling, ISTIDRAW uses a nested strategy for sampling. The parameters affecting residence times are sampled in an “outer loop.” For each realization of the residence times, a complete set of particle release and decay realizations are created. This scheme is equivalent to a two-level event tree formulation. The cumulative mass release is calculated by

- Assigning a molar mass and probability weight to each particle
- Assigning a probability to each trajectory
- Assigning a probability to each decay chain
- Assigning conditional probabilities for the cumulative residence time to the nodes in each trajectory
- Assigning conditional probabilities for the cumulative decay time to arrive at the child products in each nuclide chain
- Comparing the cumulative residence times to the cumulative decay times to determine observed conditions for each particle (e.g., determining trajectory segments in which the decay events occur)
- Determining the molar mass and probability weight at the observation nodes for each particle

The probability-weighted molar mass for a particle arriving at an observation location is

$$m_{ar} = m_{rel}(w_{rel}P_{chain}w_{dec|chain})(P_{traj}w_{ret|traj})$$

m_{ar}	Probability-weighted molar mass for a particle arriving at an observation node
m_{rel}	Molar mass for a particle leaving the source
w_{rel}	Probability weight for the released particle
P_{chain}	Probability of the particle undergoing the nuclide decay chain
$w_{dec chain}$	Conditional cumulative probability of the particle arriving as the decay product in the chain
P_{traj}	Probability of the particle passing through the specific trajectory
$w_{ret traj}$	Conditional cumulative probability of the retention time in the trajectory

ISTIDRAW ensures that

$$\begin{aligned} \sum w_{ret|traj} &= 1 \\ \sum P_{traj} &= 1 \\ \sum w_{rel}w_{dec|chain} &= 1 \\ \sum P_{chain} &= 1 \end{aligned}$$

Because the calculations are performed in a nested manner, these restrictions ensure that the overall probability-weighted molar mass is consistent between the release and arrival.

2.2. Mass Release Sampling

ISTIDRAW requires as input the cumulative release versus time from the source for a set of radionuclides. Internally, ISTIDRAW creates a cumulative distribution function (CDF) for the mass release for each radionuclide. The realizations for the mass release of a radionuclide must obey

$$M_{tot} = \sum_{\text{all particles}} m_{rel} w_{rel}$$

Two mathematically equivalent options are provided. In one option, the CDF is used to partition M_{tot} into m_{rel} , with $w_{rel} = 1$ (the mass per particle is m_{rel} in this option). In the other, the CDF is used to calculate w_{rel} , with $m_{rel} = M_{tot}$ (the mass per particle is the product $M_{tot} w_{rel}$ in this option).

2.3. Importance Sampling

Each particle that passes through an observation point or detection node has (i) an arrival time, (ii) a molar mass, and (iii) a probability of arriving at that time. The probability of arrival is the product of probabilities from two categories: (i) probability of taking the particular trajectory from the source to the detection node and (ii) the probability of release and decay to the particular child-particle that is observed.

In the default MARFA approach to Monte Carlo sampling, each parameter that is sampled has a cumulative probability distribution. For each realization, a sample quantile F for the cumulative distribution is drawn from a 0-to-1 uniform distribution, and the parameter value corresponding to quantile F is calculated. Because all parameters are sampled using quantiles drawn from uniform distributions, the probability weight w for each particle arrival is the same, $w = 1/N_{part}$.

With importance sampling, the quantile value F can be selected using a non-uniform sampling strategy. This means that each sampled parameter (e.g., release time from the source, travel time in the fracture, retention time in the matrix, decay time) could have different probabilities of occurrence for different realizations. Importance sampling requires that two computational aspects be adjusted: (i) partitioning of the cumulative distribution range and (ii) assigning the probability weight to particles arriving at observation points, based on the partitioning.

Partitioning of the cumulative distribution range

ISTIDRAW draws values from a cumulative distribution using a binning approach. The binning approach subdivides the cumulative distribution range (from 0 to 1) into $N_{bin} + 1$ sequential values, creating N_{bin} bins. One value F_i is sampled for each of the probability bins, using either (i) a value drawn at random within the bin i range or (ii) the bin mid-point (i.e., no random sampling). The probability weight assigned to the F_i value is the difference in F over adjacent bins. This approach guarantees that every bin is sampled and that the sum of weights is 1. Importance sampling is useful for selectively sampling low-probability portions of a parameter (e.g., early decay times, early release times, short residence times) to enhance the resolution of the solution.

ISTIDRAW implements several allocation strategies for binning from two basic models, (i) arithmetic progression and (ii) geometric progression. In the arithmetic progression, the difference of width of two sequential or adjacent bins is a constant. In the geometric progression, the ratio of widths of two sequential bins is a constant. In practice, an allocation strategy based on the geometric progression is usually better for binning the tails of long-tailed distributions than a strategy based on the arithmetic progression.

In both progressions, a skewness parameter called f_{mid} is used to internally calculate the arithmetic progression factor or the geometric progression factor.

In the arithmetic progression, $0.25 < f_{mid} < 0.75$. The bin widths increase from $F = 0$ to $F = 1$ for $f_{mid} < 0.5$ (i.e., low values of the distribution are sampled more often when $f_{mid} < 0.5$), and increase from $F = 1$ to $F = 0$ for $f_{mid} > 0.5$ (i.e., high values of the distribution are sampled more often when $f_{mid} > 0.5$). All bin widths are the same for $f_{mid} = 0.5$, and skewing increases as f_{mid} is farther from 0.5.

The following formulas are used in the arithmetic progression. Consider adjacent bins that differ in width by $a+r$ (a is the first bin width) where r and a are computed as

$$r = \frac{4(1 - 2f_{mid})}{N^2}$$

$$a = \frac{1}{N} - \frac{r(N - 1)}{2}$$

With such definition for a , the sum of widths is 1:

$$1 = a + (a + r) + (a + 2r) + (a + 3r) + \dots + [a + (N - 1)r] = Na + \frac{(N - 1)N}{2}r$$

In the geometric progression, $0 < f_{mid} < 1$ with $f_{mid} \neq 0$. The bin widths increase from $F = 0$ to $F = 1$ for $f_{mid} < 0.5$ and increase from $F = 1$ to $F = 0$ for $f_{mid} > 0.5$ (i.e., low values of the distribution are sampled more often when $f_{mid} < 0.5$ and high values of the distribution are sampled more often when $f_{mid} > 0.5$). All bin widths are the same for $f_{mid} = 0.5$, and skewing increases as f_{mid} moves closer to 0 or to 1.

The following formulas are used in the geometric progression. N is the number of bins, the ratio of widths of adjacent bins is r , and a is the first bin width. The parameters r and a are computed as

$$r = \begin{cases} \left(\frac{1 - \sqrt{1 - 4f_{mid}(1 - f_{mid})}}{2f_{mid}} \right)^2 & \text{if } f_{mid} > 0.5 \\ \left(\frac{1 + \sqrt{1 - 4f_{mid}(1 - f_{mid})}}{2f_{mid}} \right)^2 & \text{if } f_{mid} \leq 0.5 \end{cases}$$

$$a = \frac{r - 1}{r^N - 1}$$

The sum of all bin widths is 1:

$$a + ra + r^2a + \dots + r^{N-1}a = a \frac{r^N - 1}{r - 1} = 1$$

The parameter f_{mid} can be any number between 0 and 1. To avoid numerical underflow in the geometric progression, in practice it is desirable to constrain $0.01 \leq f_{mid} \leq 0.99$.

ISTIDRAW includes the sampling methods specified in Table 1. Each sampling method is invoked by a keyword and a value of the bias parameter f_{mid} .

Table 1. Sampling models available in ISTIDRAW.

Method Key-word	Method for bin subsampling	Description
rand	N/A	Uniform random sampling
binunif	uniform	Bins of equal widths. For each bin, a value is uniformly randomly selected within the bin range. This method is equivalent to standard Latin Hypercube Sampling.
midunif	midpoint	Bins of equal widths. For each bin, a single value is selected as the bin mid-point.
binarith	uniform	Bins widths exhibit arithmetic progression. For each bin, a value is uniformly randomly selected within the bin range.
midarith	midpoint	Bins widths exhibit arithmetic progression. For each bin, a single value is selected as the bin mid-point.
bingeom	uniform	Bin widths exhibit geometric progression. For each bin, a value is uniformly randomly selected within the bin range.
midgeom	midpoint	Bin widths exhibit geometric progression. For each bin, a single value is selected as the bin mid-point.
binarith2s	uniform	Two-sided arithmetic progression symmetric around $F = 0.5$. For each bin, a value is uniformly randomly selected within the bin range. If $f_{mid} < 0.5$, low (close to 0) and high (close to 1) probability values are sampled more often. If $f_{mid} > 0.5$, values close to 0.5 are sampled more often than values close to 0 and 1.
midarith2s	midpoint	Two-sided arithmetic progression symmetric around $F = 0.5$. For each bin, a single value is selected as the bin mid-point. If $f_{mid} < 0.5$, low (close to 0) and high (close to 1) probability values are sampled more often. If $f_{mid} > 0.5$, values close to 0.5 are sampled more often than values close to 0 and 1.
bingeom2s	uniform	Two-sided geometric progression symmetric around $F = 0.5$. For each bin, a value is uniformly randomly selected within the bin range. If $f_{mid} < 0.5$, low (close to 0) and high (close to 1) probability values are sampled more often. If $f_{mid} > 0.5$, probability values close to 0.5 are sampled more often than values close to 0 and 1.
midgeom2s	midpoint	Two-sided geometric progression symmetric around $F = 0.5$. For each bin, a single value is selected as the bin mid-point. If $f_{mid} < 0.5$, low (close to 0) and high (close to 1) probability values are sampled more often. If $f_{mid} > 0.5$, values close to 0.5 are sampled more often than values close to 0 and 1.

Assigning the probability weight to particles arriving at detection nodes

ISTIDRAW allows arbitrary nodes in the fracture network to be observation locations or detection node. ISTIDRAW calculates the probability weight of particles arriving at an observation location using a renormalization of (i) the probability weights for the cumulative segment residence times upstream of the detection node, and (ii) the probability weights for particle release and cumulative decay times before arriving at the detection node.

Renormalization

Renormalization is required to properly assign cumulative weights over a series of segments. For example, consider a sequence of segments, each with N_{bin} sampled residence times t and associated weights w . For each segment, the weights assigned to the residence times must sum to one.

For each realization, the cumulative residence time after the second segment is the sum of residence times for the two segments ($t_{1+2} = t_1 + t_2$). A relative probability weight can be calculated by multiplying the weights for the two segments ($w_{1+2} = w_1 w_2$). The new weights w_{1+2} represent relative frequencies, but in general, relative weights will not sum to one over all realizations.

For example, assuming $w_1 = w_2 = 1/N_{bin}$ for all realizations, $w_{1+2} = (1/N_{bin})^2$, and the sum of all values for w_{1+2} is $1/N_{bin}$ instead of 1. Dividing the w_{1+2} value for each realization by the sum of weights ($1/N_{bin}$ in this example) renormalizes the weights to sum to 1.

The renormalization process is performed for

- The weights for residence times in each unique sequence of segments in each trajectory
- The weights for release and decay times in each unique decay chain for the released nuclides

Performing renormalization during execution requires that a set of realizations are created and stored for each probability bin. This pre-sampling is not necessary for standard Monte Carlo simulations (each particle has the same probability weight, $1/N_{part}$, allowing for sampling *on the fly*). The necessary memory storage can be reduced by using a smaller number of bins and replicating the bin sampling. For example, a simulation with 20,000 particles might generate 100 particles ($N_{bin} = 100$) per replicate, with 200 replicates. Each renormalization occurs 200 times, but is only performed on 100 realizations each time. This scheme results in each bin being sampled 200 times, and the probability of a particle calculated for each realization in a replicate must be divided by 200 (the number of replicates). In principle, it is possible to perform renormalization during post-processing. However, this would require accounting for the fate of every particle, including the particles decaying past the end of the decay chain before reaching detection nodes; thus, renormalizing as post-processing is not practical.

Branching segment networks

The input worksheet to ISTIDRAW defining the fracture network contains a list of transport segments, each segment with an upstream and downstream node. The worksheet also defines a number of transport parameters for each segment (e.g., porosity, retardation coefficients, Peclet number), and the input radionuclide release rate at the source node.

A sequence of segments connecting a source node to a terminal detection node is referred to as a *trajectory*. Each simulation considers a single source, which can be assigned to any node in the network. A network of segments is branching if multiple segments receive inputs from a single segment or if a single segment receives inputs from multiple segments.

ISTIDRAW has two options for defining trajectories in a network: (i) exhaustively creating all possible trajectories, and (ii) selecting a subset of the possible trajectories. Exhaustively creating all possible trajectories creates a prohibitively large number of combinations for complex systems.

When exhaustively creating all possible trajectories, ISTIDRAW analyses the network connectivity, creating all possible trajectories between the source node and each terminal output node. New trajectories are formed at each branch point, by replicating the upstream trajectory for each downstream segment. As a result, individual segments may belong in many possible trajectories. Segments that are not in any trajectory are ignored. The trajectories are assigned probabilities based on flow rates. To define trajectory probabilities, it is assumed that each downstream segment receives radionuclide outputs from the upstream segment proportional to its fraction of the total outflow. This fraction is used as the probability that a particle will enter the downstream segment. The overall probability of each trajectory is the product of the segment probabilities.

For more complicated networks, identifying all possible trajectories is not practical or even impossible. ISTIDRAW includes a post-processing MATLAB script to select a sample of the possible trajectories from the network. The user defines a target number of trajectories, and whether the trajectories should be unique or allow for repeats. The trajectory probabilities are renormalized based on the number of considered trajectories and relative flow rates. The MATLAB script generates a text file defining the finite number of trajectories, and including the relative probabilities. The input worksheet must declare the use of trajectories defined in an external text file as well as the

name of the text file. The text file defines the trajectories as a sequence of segments. Transport parameters for each segment are read from the original network, also provided in the input worksheet. An example to execute the MATLAB script is provided in this document, applied to the analysis of TRUE-Block scale field investigations at the Äspö Hard Rock Laboratory (SKB, 2003), in collaboration Uppsala University.

Branching decay chains

The input worksheet defining the radionuclides contains a list of radionuclides, half-lives, decay chains, and stoichiometric fractions of decay products. Certain radionuclides can have multiple decay products. Similarly as segment networks, decay chains may branch and join. ISTIDRAW handles the logic of decay networks in the same way as it handles fracture segment networks, creating multiple decay chains to represent all decay *trajectories* from parent to n-th child. Each decay trajectory is assigned a probability based on the stoichiometric fractions. If there is no branching, the decay trajectory probability is one.

3. Input Worksheets

Inputs to ISTIDRAW are defined using an Excel file organized in worksheets containing information on radionuclide decay chains and decay rates, pathway network, radionuclide transport parameters, source and detection nodes, and importance sampling strategies. Two files, `inputFile_examples.xlsx` and `InputFile_examplesNetwork.xlsx`, are provided with the ISTIDRAW distribution package, with examples.

The worksheets are described in the following sections. The distributed example input files include detailed comments describing the inputs.

3.1. Master Input Worksheet

The Master Worksheet is the main control for ISTIDRAW. It defines inputs such as auxiliary files, sampling strategies, sampling bias parameters, input worksheets with radionuclide information, pathway network information and radionuclide transport parameters, and output information. The Master Worksheet defines settings of individual simulations, with all settings for the simulation specified on a single column. The simulation columns start after the keyword *Table* (Column I in the next figure). Any entry in the simulation columns overrides default values on the column labelled with the *default* keyword. The radionuclide, pathway network, and source worksheets are read again at the start of each simulation, so that different inputs can be defined for different simulations.

	A	B	C	D	E	F	G	H	I	J
1	name	nuc	elem	node	seg	# desc	default		Table	
2	ysim					flag for running simulation	T		0	1
3	#					Label, suffix, for output result files				
4	# desc					description				
5	zoutDir					output directory name for simulation case	outputs			
6	zresfile					result file name	out.res			
7	ztravfile					travel time file name	out.trav			
8	zGsheet					worksheet with transport parameters and network definitions	oneSegment			
9	zNsheets					worksheet with radionuclide definitions	Radionuclides			
10	zpathfile					input trajectories				
11	ypathfile					T/F (=1/0) => use path file for trajectories	F			
12	ybrsplit					T/F (=1/0) => split particles at each chain branch vs. select 1 branch	F			
13	zpathSampMod					scheme for sampling path residence time (oneperseg/oneallseg)	oneperseg			
14	rngSeed					random number generator seed	1681538			
15						nuclide decay model (probrand/probinxxxx/probmidxxxx) Replace xxx with unif, arithm, or geom probinunif is equivalent to Latin Hypercube Sampling				
16	zdecaySampMod						probinunif			
17	zdecaySampMod	Ag108m					probinunif			
18	zdecaySampMod	C14					probrand			
19	zdecaySampMod	Cs135					probinunif			
20	zdecaySampMod	I129					probinunif			

The column with the keyword *default* (Column G in the previous figure) specifies default values for all settings. These defaults are overridden by values located after the column with the *Table* keyword (Column I) —the simulation columns. The simulation columns (from Column I and forward) are enabled by a value 1 or TRUE or T (for True) on Row 2. Each of the simulation columns defines a complete set of settings for one independent simulation. ISTIDRAW executes all of the simulations labelled with 1 (or T) on Row 2. To avoid overwriting output files by sequential runs, different names of the outputs files should be declared with different values for the variables `zresfile` and `ztravfile` (Rows 6 and 7 in the previous figure). If the values on Row 2 are 0 or FALSE or F (for False), the corresponding column simulations are not executed.

Column A defines variable names. The user must use the provided variable names in the examples. Column B is used to declare specific radionuclides. All variables include a default value to be

applied to all radionuclides (for variables that can be radionuclide specific). Entries in separate rows can overrule the default value for specified radionuclides. The following figure provides an example.

	A	B	C	D	E	F	G
1	name	nuc	elemnode	seg	#	desc	default
2	ysim					flag for running simulation	T
3	#					Label, suffix, for output result files	
4	# desc					description	
						nuclide decay model (probrand/probinxxxx/probmidxxxx) Replace xxx with unif, arith, or geom	
16	zdecaySampMod					probinunif is equivalent to Latin Hypercube Sampling	probinunif
17	zdecaySampMod	Ag108m					probbingeom
18	zdecaySampMod	C14					probrand
19	zdecaySampMod	Cs135					probbinarith

The variable zdecaySampMod (Column A) declares the sampling strategy for decay times. The default value on Row 16, Column G, probinunif, defines the default sampling strategy for all radionuclides. This default is overruled by radionuclide-specific values, when provided by the user. For example, on Row 18 the value probrand is applied to C-14, and on Row 19 probbinarith is applied to Cs-135.

The values probinunif, probbingeom, probrand, and probbinarith in the figure refer to methods described in Table 1. The “binunif,” “bingeom,” “rand,” and “binarith” suffixes to the prefix “prob” are method keywords listed on the first column in Table 1. These example keywords are abbreviations of uniform, geometric, random, and arithmetic, referring to uniform sampling, geometric progression, random sampling, and arithmetic progression. For example probbingeom for Ag-108m on Row 17 instructs ISTIDRAW to apply geometric progression binning, sampling values randomly within a bin to define decay times. The value probbinarith on Row 19 directs ISTIDRAW to apply arithmetic progression binning, sampling values randomly within a bin to define decay times for Cs-135. Another block in the Master Worksheet is used to declare the sampling bias parameters.

As described in Section 2.3.1, the arithmetic and geometric progression binning requires the definition of a bias sampling parameter, f_{mid} . If $f_{mid} > 0.5$, high values of the distribution are sampled more often. If $f_{mid} < 0.5$, low values of the distribution are sampled more often. If $f_{mid} = 0.5$, the frequency dictated by the distribution proper is implemented, without any bias.

The following figure continues the example for Ag-108m and Cs-135.

	A	B	C	D	E	F	G
1	name	nuc	elemnode	seg	#	desc	default
44							
45	decayFmid					weighting factor for decay sampling	0.5
46	decayFmid	Ag108m					0.1
47	decayFmid	C14					0.5
48	decayFmid	Cs135					0.75

The value of f_{mid} for Ag-108m is 0.1 (Row 46), instructing ISTIDRAW to sample short decay times more often. The value of f_{mid} for Cs-135 (Row 48) is 0.75, instructing ISTIDRAW to sample long decay times more often.

To declare sampling methods in the Master Worksheet in general, the two-block approach is consistently used. One block declares the sampling strategy via keywords in Table 1, first column,

added as suffixes to the prefix “prob.” In the cases of the travel time in the fracture and the matrix retention time, the “prob” suffix is not used. For example, the following words are used as values to declare sampling strategies for decay time and release times from the source:

- probrand
- probbinunif
- probbinarith
- probbingeom
- probbinarith2s
- probbingeom2s
- probmidunif
- probmidarith
- probmidgeom
- probmidarith2s
- probmidgeom2s

For fracture travel times (variable zFresSampMod) and matrix retention times (variable zMresSampMod), the same keywords in Table 1 are employed to invoke sampling strategies, without the “prob” suffix.

The top line of the block defining the sampling method defines the default strategy applied to all radionuclides. Following lines can be used to define optional radionuclide-specific sampling methods. Column B in the Master Worksheet is used to declare the radionuclide of interest.

A second block is used to input values of the bias parameter f_{mid} . The top line of the block defines the default value to apply to all radionuclides. Additional lines to the block are optional, and require specification of the radionuclide in Column B, as well as the value of f_{mid} . For arithmetic progression binning, $0.25 \leq f_{mid} \leq 0.75$, and the ISTIDRAW execution is interrupted if the user provides a value outside that range. For the arithmetic progression, $0 < f_{mid} < 1$.

The two-block strategy is applied to define sampled strategies for (i) radionuclide decay times, (ii) release times at the source, (iii) residence times in the fracture, and (iv) matrix retention times. The variable names used in Column A of the Master Worksheet, identifying the two blocks of inputs are summarized in Table 2.

Table 2. Times sampled in the ISTIDRAW algorithms

Time Parameter	Method Variable	Bias Variable, f_{mid}
Radionuclide decay times	zdecaySampMod	decayFmid
Release times at the source	zsrcRelSampMod	srcRelFmid
Residence time in the fracture	zFresSampMod	FresFmid
Retention time in the matrix	zMresSampMod	MresFmid

Besides the definition of sampling strategies, the Master Worksheet includes the following information

- Name of worksheet including radionuclide definitions (half-lives and decay chains)
- Node numbers to record incoming radionuclide transfer rates in units of mol/yr (variable ytraceNode)
- Number of repetitions or realizations (variable srcNReps)
- Number of sampled times at the source for each radionuclide (srcNRelT), or number of particles to represent the total mass released at the source
- Source node (srcNode)
- Worksheet with the source input radionuclide release rates (zSsheet)
- Identification of radionuclides to track in the run (ysrcNuc)
- Matrix retention model (zMresMod)

For the matrix retention model (zMrsMod), possible values of the variable are

- none: disables matrix diffusion (only transport through fractures)
- unlim: semi-infinite matrix diffusion
- lim0q: limited-thickness matrix diffusion (zero flux boundary condition at a depth inside the matrix)

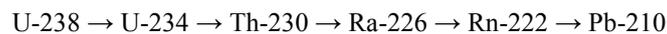
The files inputFile_examples.xlsx and InputFile_examplesNetwork.xlsx contain detailed comments to facilitate understanding of the inputs.

3.2. Radionuclides Worksheet

The Radionuclides Worksheet defines the decay chains and half-lives and the available set of radionuclides. The following figure presents an example of the worksheet structure.

	A	B	C	D	E	F	G	H	I
1	<i>Species ID</i>	<i>Isotope</i>	<i>Atomic Weight</i>	<i>Half-life</i>	<i>Radioactive</i>	<i>Daughter1</i>	<i>Stoichiometry1</i>	<i>Daughter2</i>	<i>Stoichiometry2</i>
2	Ag108m	N	108	438 yr	Y				
3	C14	N	14	5730 yr	Y				
4	Cs135	N	135	2.3e6 yr	Y				
5	I129	N	129	1.57e7 yr	Y				
6	Nb94	N	94	2.03E4 yr	Y				
7	Ni59	N	59	7.5E4 yr	Y				
8	Np237	N	237	2.14e6 yr	Y	U233	1		
9	Pb210	N	210	22.3 yr	Y				
10	Pu238	Y	238	87.7 yr	Y	U234	1		
11	Pu239	Y	239	24100 yr	Y	U235	1		
12	Pu240	Y	240	6560 yr	Y	U236	1		
13	Pu242	Y	242	3.73e5 yr	Y	U238	1		
14	Ra226	N	226	1.6E3 yr	Y	Rn222	1		
15	Rn222	N	222	0.010010475 yr	Y	Pb210	1		
16	Se79	N	79	3.77E5 yr	Y				
17	Tc99	N	99	2.11e5 yr	Y				
18	Th230	N	230	7.54E4 yr	Y	Ra226	1		
19	U232	Y	232	68.8 yr	Y				
20	U233	Y	233	159000 yr	Y				
21	U234	Y	234	246000 yr	Y	Th230	1		
22	U235	Y	235	7.04e8 yr	Y				
23	U236	Y	236	2.34e7 yr	Y				
24	U238	Y	238	4470000000 yr	Y	U234	1		

Decay products are declared along rows. For example, Row 8 defines the half-life of Np-237 and the reaction $\text{Np-237} \rightarrow \text{U-233}$. Information in other rows is used to specify decay chains such as



The row order in the Radionuclides Worksheet to specify decay chains is arbitrary. For decay chains with branching, all simultaneous children to a parent must be specified in the same row, as well as the corresponding molar stoichiometry. Information on the Column B (Isotope) and Column C (Atomic Weight) is not used in this version of ISTIDRAW.

Simulations are not required to use all of the radionuclides in the Radionuclides Worksheet. The Master Worksheet specifies which radionuclides are released from sources. A decay chain is internally constructed for each source radionuclide. A radionuclide is tracked during a simulation if it is part of any decay chain in the Radionuclide Worksheet (even if not declared by the user in the Master Worksheet). The tracked radionuclides can change from simulation to simulation.

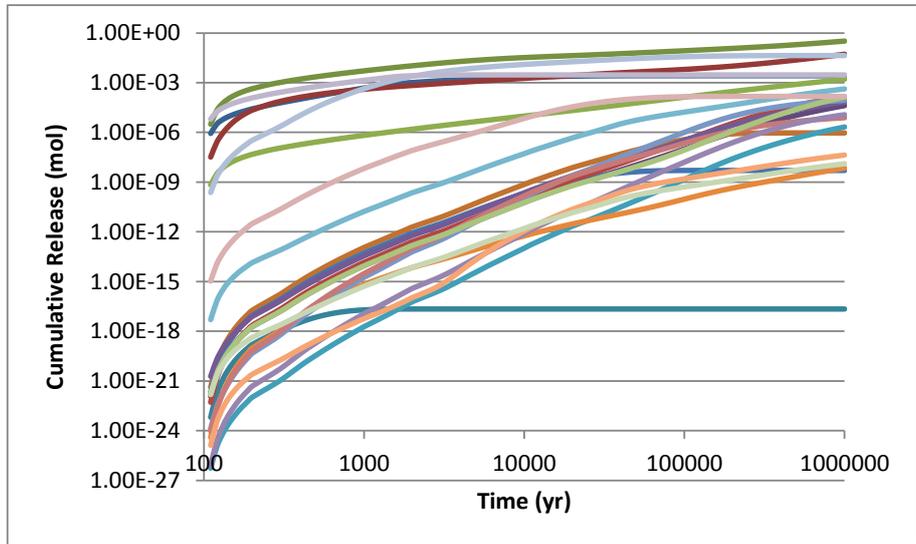
The name of the Radionuclides Worksheet can be any arbitrary name. The Master Worksheet must include the correct name of the Radionuclides Worksheet. The default worksheet name can be overridden in the simulation columns, allowing a different Radionuclides Worksheet to be used for each simulation.

3.3. Source Worksheet

The Source Worksheet specifies the cumulative radionuclide release rate input to the ISTIDRAW pathway network. The following figure is an example of the information in the Source Worksheet

	A	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Time	[1129]	[Np237]	[Pu238]	[Pu239]	[Pu240]	[Pu242]	[Se79]	[Tc99]	[U233]	[U234]	[U235]	[U236]	[U238]
2	yr	mol	mol	mol	mol	mol	mol	mol	mol	mol	mol	mol	mol	mol
21	80	0	0	0	0	0	0	0	0	0	0	0	0	0
22	90	0	0	0	0	0	0	0	0	0	0	0	0	0
23	100	0	0	0	0	0	0	0	0	0	0	0	0	0
24	110	0.000003134	1.17E-22	6.44E-24	4.18E-22	2.03E-22	5.20E-23	6.69E-10	1.88E-21	5.50E-27	3.87E-25	1.28E-24	9.58E-25	1.50E-22
25	120	0.00002062	2.42E-21	1.64E-22	1.12E-20	5.46E-21	1.40E-21	3.03E-09	1.90E-20	1.04E-25	1.74E-23	2.55E-23	2.17E-23	2.69E-21
26	130	0.0000534	1.36E-20	1.08E-21	7.90E-20	3.84E-20	9.83E-21	6.79E-09	8.14E-20	5.89E-25	1.68E-22	1.56E-22	1.51E-22	1.44E-20
27	140	0.00009656	4.54E-20	3.95E-21	3.10E-19	1.50E-19	3.85E-20	1.15E-08	2.36E-19	2.02E-24	8.32E-22	5.88E-22	6.35E-22	4.69E-20
28	150	0.0001463	1.14E-19	1.04E-20	8.68E-19	4.21E-19	1.08E-19	1.68E-08	5.45E-19	5.25E-24	2.79E-21	1.68E-21	1.96E-21	1.16E-19
29	160	0.0002002	2.43E-19	2.24E-20	2.00E-18	9.71E-19	2.49E-19	2.25E-08	1.09E-18	1.16E-23	7.45E-21	4.05E-21	5.06E-21	2.45E-19
30	170	0.0002568	4.55E-19	4.16E-20	3.98E-18	1.93E-18	4.95E-19	2.86E-08	1.97E-18	2.26E-23	1.66E-20	8.51E-21	1.12E-20	4.55E-19
31	180	0.000315	7.70E-19	6.93E-20	7.03E-18	3.40E-18	8.75E-19	3.48E-08	3.28E-18	3.96E-23	3.21E-20	1.59E-20	2.16E-20	7.67E-19
32	190	0.0003743	1.24E-18	1.08E-19	1.17E-17	5.67E-18	1.46E-18	4.12E-08	5.17E-18	6.60E-23	5.80E-20	2.82E-20	3.93E-20	1.23E-18
33	200	0.0004343	1.89E-18	1.60E-19	1.84E-17	8.89E-18	2.29E-18	4.77E-08	7.77E-18	1.04E-22	9.74E-20	4.70E-20	6.71E-20	1.87E-18
34	250	0.0007364	6.27E-18	4.86E-19	6.42E-17	3.10E-17	8.00E-18	8.06E-08	2.51E-17	3.73E-22	3.84E-19	1.85E-19	2.75E-19	6.17E-18
35	300	0.001041	1.63E-17	1.07E-18	1.75E-16	8.42E-17	2.18E-17	1.15E-07	6.81E-17	1.08E-21	1.18E-18	6.08E-19	9.40E-19	1.60E-17
36	350	0.001347	4.15E-17	2.09E-18	4.63E-16	2.23E-16	5.79E-17	1.50E-07	1.73E-16	3.18E-21	3.47E-18	2.03E-18	3.24E-18	4.05E-17
37	400	0.001651	9.37E-17	3.51E-18	1.07E-15	5.14E-16	1.34E-16	1.86E-07	3.79E-16	8.21E-21	8.49E-18	5.76E-18	9.99E-18	9.11E-17
38	450	0.001954	1.85E-16	5.19E-18	2.15E-15	1.03E-15	2.70E-16	2.22E-07	7.33E-16	1.81E-20	1.73E-17	1.36E-17	2.24E-17	1.79E-16
39	500	0.002256	3.24E-16	7.02E-18	3.83E-15	1.82E-15	4.81E-16	2.60E-07	1.29E-15	3.50E-20	3.09E-17	2.74E-17	4.56E-17	3.15E-16
40	550	0.002556	5.37E-16	8.89E-18	6.41E-15	3.04E-15	8.05E-16	2.98E-07	2.12E-15	6.35E-20	5.10E-17	5.16E-17	8.62E-17	5.21E-16
41	600	0.002854	8.39E-16	1.07E-17	1.01E-14	4.76E-15	1.27E-15	3.36E-07	3.28E-15	1.07E-19	7.85E-17	9.01E-17	1.51E-16	8.12E-16
42	650	0.003151	1.25E-15	1.24E-17	1.51E-14	7.11E-15	1.90E-15	3.76E-07	4.86E-15	1.72E-19	1.15E-16	1.48E-16	2.49E-16	1.21E-15
43	700	0.003447	1.79E-15	1.39E-17	2.17E-14	1.02E-14	2.74E-15	4.15E-07	6.94E-15	2.65E-19	1.60E-16	2.32E-16	3.91E-16	1.73E-15
44	750	0.003741	2.49E-15	1.53E-17	3.03E-14	1.42E-14	3.82E-15	4.55E-07	9.62E-15	3.92E-19	2.17E-16	3.50E-16	5.90E-16	2.41E-15
45	800	0.004033	3.37E-15	1.64E-17	4.12E-14	1.92E-14	5.20E-15	4.96E-07	1.30E-14	5.62E-19	2.85E-16	5.11E-16	8.62E-16	3.25E-15
46	850	0.004323	4.45E-15	1.74E-17	5.46E-14	2.54E-14	6.90E-15	5.37E-07	1.71E-14	7.86E-19	3.65E-16	7.24E-16	1.22E-15	4.30E-15
47	900	0.004612	5.78E-15	1.82E-17	7.10E-14	3.29E-14	8.98E-15	5.79E-07	2.22E-14	1.08E-18	4.59E-16	1.00E-15	1.69E-15	5.88E-15

The first column specifies time instants, and the other columns specify the cumulative radionuclide release, in mole units, at the specified time instants for individual radionuclides. The following plot is an example of the information in the Source Worksheet.



Each curve corresponds to a specific radionuclide. Cumulative releases must be increasing functions of time [i.e., if $time_2 > time_1$, then $release(time_2) \geq release(time_1)$], otherwise, ISTIDRAW may produce errors.

ISTIDRAW does not include a source term model. Source term releases must be computed with external models of the near field. Source term models can include roundup errors that could cause cumulative releases to be non-increasing functions of time. The user should check that cumulative releases properly increase with time. The time instants must increase monotonically, but intervals

between time instants are arbitrary. ISTIDRAW linearly interpolates between time instants to define the insertion times of particles and the molar mass carried by each particle.

The name of the Source Worksheet is arbitrary. However, the Master Worksheet must correctly identify the Source Worksheet by the assigned name. The Master Worksheet specifies how radionuclide sources are assigned to the network nodes. The default worksheet name can be overridden in the simulation columns, allowing a different Source Worksheet to be used for each simulation.

3.4. Pathway Network Worksheet

The Pathway Network Worksheet is used to specify (i) transport properties of segments, and (ii) the network connectivity. Several examples are provided in this section. The following figure presents an example of a transport pathway of a single segment.

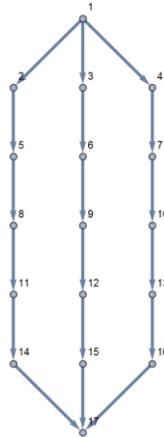
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1						[m ³ /yr/m]			[m ² /yr]	[m]	[m]			Rf	Rf	Rf	Rf	Rf	Rf
2	segment	n1	n2	Q	V/L/D	V/L	w	porM	DcoefM	aperF	thkM	Rf	Rm	C	Cs	I	Nb	Ni	Np
3	1	1	2	1	10	0.01	1	0.1	0.001	0.000667	0.05995	1	1		100				
4																			
5																			

Column A is a numeric label for the segment. Columns B and C are node numbers. In this example, Segment 1 is enclosed by Nodes 1 and 2. Node 1 is the pathway inlet (source node), and Node 2 is the pathway outlet. The first three columns are used to define the network connectivity. The columns after Column C are used to define the transport parameters. The transport parameters are explained in Table 3. Note that ISTIDRAW does not perform unit conversions. Units must be consistent, including the unit of time considered in the Source Worksheet. In the units in Table 3, it is assumed that units of time steps in the Source Worksheet are years.

Table 3. Description transport parameters defined in the Network Worksheet. The units in the description assume that time steps in the Source Worksheet are specified in years.

Parameter	Description
Q	Flow rate through the segment (m ³ /yr)
V L/D	Peclet number, equal to velocity (m/yr) × segment length (m) / dispersion (m ² /yr). If the Peclet number is large, the dispersion in the segment is negligible. If the Peclet number is small, the dispersion is significant.
V/L	Flow velocity (m/yr) / segment length (m) = inverse of travel time
w	Segment width (m), perpendicular to the flow direction and pathway aperture
porM	Matrix porosity (dimensionless)
DcoefM	Porewater diffusion coefficient (m ² /yr) in the matrix. This coefficient should not be confused with the effective matrix diffusion coefficient, which is equal to the porewater diffusion coefficient times the matrix porosity.
aperF	Pathway aperture or fracture aperture (m).
thkM	Thickness of matrix diffusion zone (m). This parameter is used only if zMresMod = lim0q in the master worksheet (i.e., limited matrix diffusion is enabled)
Rf	Default retardation coefficient for transport in the fracture (dimensionless). This retardation is used to consider the presence of porous infill inside the fracture. For most applications of interest Rf=1. The default value is used for all radionuclides without specified values.
Rm	Default retardation coefficient for transport in the matrix (dimensionless). This default value is used for all radionuclides without specified values.
Rf, Rm	The Worksheet allows specifying radionuclide specific values for Rf and Rm. In the example in the previous figure, Column O defines a value of Rf equal to 100 for Cs. A similar approach is used to define radionuclide specific values of Rm

Additional examples are provided to present the structure of simple networks. Consider the following network



The numbers in the graph are the nodes. This network is specified as follows

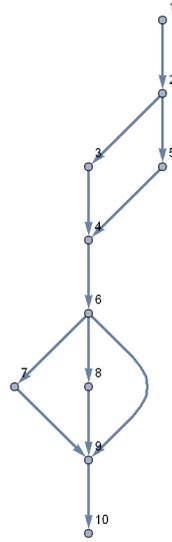
	A	B	C	D	E	F	G	H	I	J	K	L	M	
1						[m/yr/m]				[m ² /yr]	[m]	[m]		
2	segment	n1	n2	Q	VL/D	V/L	w	porM	DcoefM	aperF	thkM	Rf	Rm	
3	1	1	4	1	1.666667	0.06	1		0.1	0.001	0.000667	0.05995	1	1
4	2	4	7	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
5	3	7	10	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
6	4	10	13	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
7	5	13	16	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
8	6	16	17	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
9	7	1	2	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
10	8	2	5	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
11	9	5	8	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
12	10	8	11	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
13	11	11	14	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
14	12	14	17	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
15	13	1	3	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
16	14	3	6	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
17	15	6	9	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
18	16	9	12	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
19	17	12	15	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	
20	18	15	17	1	1.666667	0.06	1	0.1	0.001	0.000667	0.05995	1	1	

The node sequence in columns B and C (1 to 4, 4 to 7, 7 to 3, and etcetera) represents the three trajectories in the network. The three outflows from Node 1 are identical, and therefore the three possible trajectories are equally likely. For this network, ISTIDRAW identifies the three possible trajectories, and in each different trajectory all source particles are inserted for each decay chain (decay chains are split into multiple decay chains in case of branching).

ISTIDRAW does not compute a water balance. Information on the flow column is only used to define branching probabilities and trajectory weights, by computing the relative flow at branching points (Node 1 in the previous example). ISTIDRAW does not check for recirculation. In case of inconsistent flow directions resulting in flow returns to the same node, erroneous results will be produced.

The source node must be explicitly identified in the Master Worksheet, using the variable srcNode. In the previous example, if Node 1 is defined as the source node, then ISTIDRAW will identify three possible trajectories for the radionuclides. If any other node is identified as the source, ISTIDRAW will ignore the two trajectories not participating in radionuclide transport.

The detection node must also be identified in the Master Worksheet (variable ytraceNode). Multiple detection nodes can be specified, in case there is interest in analysing intermediate transfers. ISTIDRAW only tracks trajectories including the source node and the detection nodes. The following simple network includes six different trajectories.



This network may be defined as

	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2	segment	n1	n2	Q	VL/D	V/L	w	porM	DcoefM	aperF	thkM	Rf	Rm
3	1	1	2	1	0.1	100	1	0.01	0.06	0.001	0.1	1	1
4	2	2	3	1	0.1	1	1	0.01	0.06	0.001	0.1	1	1
5	3	3	4	1	0.1	10	1	0.01	0.06	0.001	0.1	1	1
6	4	2	5	1	0.1	2	1	0.01	0.06	0.001	0.1	1	1
7	5	5	4	1	0.1	0.1	1	0.01	0.06	0.001	0.1	1	1
8	6	4	6	1	0.1	1.00E-04	1	0.01	0.06	0.001	0.1	1	1
9	7	6	7	1	0.1	1	1	0.01	0.06	0.001	0.1	1	1
10	8	6	8	1	0.1	8	1	0.01	0.06	0.001	0.1	1	1
11	9	7	9	1	0.1	9	1	0.01	0.06	0.001	0.1	1	1
12	10	8	9	1	0.1	1.00E-04	1	0.01	0.06	0.001	0.1	1	1
13	11	9	10	1	0.1	11	1	0.01	0.06	0.001	0.1	1	1
14	12	6	9	1	0.1	12	1	0.01	0.06	0.001	0.1	1	1

ISTIDRAW counts all possible trajectories, unless instructed not to do so in the Master Worksheet. For networks of a given level of complexity, it can become impractical or even impossible to enumerate all trajectories. For those cases, the variable `yfilepath` can be assigned a value T (=True) in the Master Worksheet, to instruct ISTIDRAW to rely on an external file explicitly defining a finite number of trajectories. The file name is set by the value of the variable `zfilepath` in the Master Worksheet. ISTIDRAW relies on the Network Worksheet for the specification of transport parameters; thus, the Network Worksheet is always required as input.

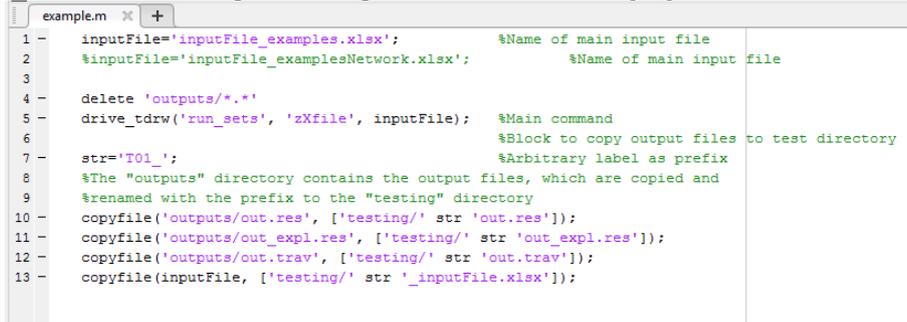
The code execution section includes an example to generate external trajectory files.

4. Code Execution

Examples are presented in this section to run the code and generate graphic displays. A level of familiarity with MATLAB is assumed in the following sections.

4.1. Executing ISTIDRAW

An example m-file is provided in the distribution of ISTIDRAW, main directory, named example.m. The contents of example.m are reproduced in the following figure.



```
1 - inputFile='inputFile_examples.xlsx';           %Name of main input file
2 - %inputFile='inputFile_examplesNetwork.xlsx';   %Name of main input file
3
4 - delete 'outputs/*.*'
5 - drive_tdrw('run_sets', 'zXfile', inputFile); %Main command
6 - %Block to copy output files to test directory
7 - str='T01_';                                     %Arbitrary label as prefix
8 - %The "outputs" directory contains the output files, which are copied and
9 - %renamed with the prefix to the "testing" directory
10 - copyfile('outputs/out.res', ['testing/' str 'out.res']);
11 - copyfile('outputs/out_expl.res', ['testing/' str 'out_expl.res']);
12 - copyfile('outputs/out.trav', ['testing/' str 'out.trav']);
13 - copyfile(inputFile, ['testing/' str '_inputFile.xlsx']);
```

Line 1 defines the name of the input Excel file (inputFile_examples.xlsx). Lines starting with % are comment lines, ignored by MATLAB. The command

```
delete 'outputs/*.*'
```

erases any files located at the default directory for outputs (directory name specified by the variable zoutDir in the Master Worksheet). The command

```
drive_tdrw('run_sets', 'zXfile', inputFile)
```

is the main driver of the ISTIDRAW code. The string 'run_sets' specifies the execution of all simulations in the Master Worksheet, without generating lookup tables for distributions.

The commands after Line 6 are simply to move input and output files to a different location (*testing* folder), renamed by adding a prefix (string 'T01_' defined on Line 7). It is assumed that only one simulation was executed, and that the default output files are named out.res, out_expl.res, and out.trav. If more than one simulation is executed in the Master Worksheet, the user must specify different names for the output files, to avoid losing information by file rewrites. The template in the m-file example.m can be followed to move and rename additional output files to the *testing* directory.

To execute the code, point MATLAB to the main directory of ISTIDRAW, open the file example.m, and click on the run icon.

The prefix string 'T01_' is intended as a label to identify different runs, their input and outputs. The prefix string is used by graphic post-processing routines accompanying ISTIDRAW. The user must change the value of the prefix string to identify and track different runs.

4.2. Output Files

The file named by default out_expl.res is a dictionary file, explaining the content of the of the main output file out.res. An example of the dictionary file is presented in the following figure

Column 1: source node
 Column 2: tracking node
 Column 3: path ID
 Column 4: nuclide ID of parent at source node
 Column 5: nuclide ID of child at tracking node
 Column 6: release time
 Column 7: travel time
 Column 8: particle mass
 Column 9: particle unnormalized probability weight
 Column 10: probability-weighted particle mass

ID	Nuclide	Element
9	Pb210	Pb
14	Ra226	Ra
18	Th230	Th
21	U234	U
24	U238	U

The column numbers refer to column in the main output file out.res. The column explanations remain constant in all simulations. The only difference from simulation to simulation are the radionuclides tracked and the numeric label assigned to each radionuclide. The column explanations are further expanded in Table 4.

Table 4. Explanation of information by columns in the main output file

Column	Explanation
1	Source node number. The source must be inserted at a single node.
2	Tracking node. The Master Worksheet can specify multiple tracking nodes, to identify mass transfers at key nodes of the pathway network.
3	Path ID is a numeric label assigned to the different trajectories
4	Numeric label to identify the radionuclide identity of the particle at the source. As the particle moves along a trajectory, the radionuclide identity changes because of decay. The correspondence of numeric labels to radionuclides is listed at the end of the dictionary file out_expl.res.
5	Numeric label to identify the radionuclide identity of the particle at the intermediate or final tracking node. The correspondence of numeric labels to radionuclides is listed at the end of the dictionary file out_expl.res.
6	Release time of the particle at the source.
7	Travel time of the particle measured from the time of insertion to the time of detection at the tracking node. In other words, the travel time does not include the release time in Column 6.
8	Particle molar mass
9	Probability weight of the particle. Several factors participate in probability weights including bias sampling of travel time and matrix residence times, decay times, trajectory probability, and decay chain probability in case of decay chains with branching
10	Product of molar masses on Column 8 and probability weights on Column 9

The following figure is an example of information contained in the main output file out.res

```

1 2 1 14 14 597904 11691.1 0.0004199 2e-05 8.398e-09
1 2 1 14 14 734022 11691.1 0.0004199 2e-05 8.398e-09
1 2 1 14 14 973346 11691.1 0.0004199 2e-05 8.398e-09
1 2 1 18 18 83175 170208 1.167e-05 1.6285e-06 1.90046e-11
1 2 1 18 18 99749 170208 1.167e-05 2.14683e-06 2.50535e-11
1 2 1 18 18 128104 170208 1.167e-05 3.16772e-06 3.69673e-11
1 2 1 18 18 129214 170208 1.167e-05 3.41884e-06 3.98978e-11
1 2 1 18 18 158076 170208 1.167e-05 5.75754e-06 6.71905e-11
1 2 1 18 18 160239 170208 1.167e-05 5.57628e-06 6.50752e-11
1 2 1 18 18 185015 170208 1.167e-05 9.16893e-06 1.07001e-10
1 2 1 18 18 190097 170208 1.167e-05 9.61294e-06 1.12183e-10
1 2 1 18 18 193075 170208 1.167e-05 9.64342e-06 1.12539e-10
1 2 1 18 18 200994 170208 1.167e-05 1.16739e-05 1.36234e-10
1 2 1 18 18 208435 170208 1.167e-05 1.47227e-05 1.71813e-10
1 2 1 18 18 209616 170208 1.167e-05 1.52951e-05 1.78494e-10
1 2 1 18 18 219361 170208 1.167e-05 1.68596e-05 1.96752e-10
1 2 1 18 14 231177 170208 1.167e-05 1.6677e-05 1.94621e-10
1 2 1 18 18 236097 170208 1.167e-05 2.19078e-05 2.55664e-10
1 2 1 18 18 240757 170208 1.167e-05 1.98366e-05 2.31494e-10
1 2 1 18 18 245807 170208 1.167e-05 2.36571e-05 2.76079e-10
1 2 1 18 18 299730 170208 1.167e-05 4.12803e-05 4.81741e-10
1 2 1 18 18 411275 170208 1.167e-05 0.000101607 1.18576e-09
1 2 1 18 18 420392 170208 1.167e-05 0.000104966 1.22496e-09
1 2 1 18 18 434208 170208 1.167e-05 0.000125557 1.46525e-09
1 2 1 18 9 444384 170208 1.167e-05 0.000103811 1.21147e-09
1 2 1 18 18 482993 170208 1.167e-05 0.000129823 1.51503e-09
1 2 1 18 18 515466 170208 1.167e-05 0.000160903 1.87774e-09
1 2 1 18 18 670300 170208 1.167e-05 0.000294102 3.43217e-09
1 2 1 18 18 721598 170208 1.167e-05 0.000328949 3.83884e-09
1 2 1 18 18 775167 170208 1.167e-05 0.000315917 3.68676e-09
1 2 1 18 18 857859 170208 1.167e-05 0.00045067 5.25932e-09
1 2 1 18 14 124053 221707 1.167e-05 3.02246e-06 3.52722e-11
1 2 1 18 14 133037 221707 1.167e-05 3.59574e-06 4.19623e-11
1 2 1 18 18 162115 221707 1.167e-05 6.57352e-06 7.67129e-11
1 2 1 18 18 173913 221707 1.167e-05 8.34294e-06 9.73621e-11
1 2 1 18 18 189972 221707 1.167e-05 1.04684e-05 1.22166e-10
1 2 1 18 18 190995 221707 1.167e-05 1.1364e-05 1.32618e-10
1 2 1 18 18 201623 221707 1.167e-05 1.27508e-05 1.48802e-10

```

Each row carries information on a single particle. The data in each column is explained in Table 4. The total time is computed by adding Columns 6 and 7 (release time and travel time). The raw output data must be post-processed to generate graphic displays.

The file out.trav is a diagnostic file containing travel times. Information in this file was used only for testing during development of ISTIDRAW. Users may delete the file out.trav.

4.3. Data Post-Processing

In the description that follows, it is assumed that output files are located in the folder named *testing*, with different prefix labels assigned to individual runs. The folder testing includes an m-file, example_plot.m, with an example of plot commands. MATLAB must point to this directory as the main execution directory, in order for output files to be properly generated and placed.

The following figure reproduces the content of the file example_plot.m.

```

1 %Additional controls and flags are available in smoothDriver.m
2
3 - outputFile='T01_out'; %Output file name without res extension
4 - GEVDflag=true; %Use generalized extreme value distribution for tails?
5 - createExcelFlag=true; %Create excel file with release rates and cumulative releases?
6 - %maxTime=1E-10; %Max time for graphic display and Excel file.
7 %Select a very small time for automatic detection
8 %of maximum
9 -
10 - maxTime=1E7;
11 - plotUnit='mol'; %'Bq' or 'mol'. For any other string, the output defaults to mol.
12 - scaleY=1E8; %Orders of magnitude to include in plots
13 -
14 - if GEVDflag
15 - suffix='_GEVD'; %suffix label for png files
16 - else
17 - suffix='_norm';
18 - end
19 -
20 - smoothDriver(outputFile, GEVDflag, createExcelFlag, maxTime, plotUnit, suffix, scaleY);
21 %Additional controls and flags are available in smoothDriver.m

```

As previously stated, text after the symbol % is comment text, ignored by MATLAB. Table 5 defines the variables the used is expected to modify in the file `example_plot.m`.

Table 5. User-defined variables to be modified in `example_plot.m`

Variable	Description
<code>outputFile</code>	Prefix label identifying the output files. In the example, <p style="text-align: center;"><code>outputFile='T01_out'</code></p> indicates that the output files generated previously by ISTIDRAW are named <code>T01_out.res</code> and <code>T01_out_expl.red</code> . This prefix label is also used to name graphic files and an Excel file.
<code>GEVDflag</code>	Logical variable that can take values <i>true</i> or <i>false</i> . <p>If <i>false</i>, a kernel density estimator (KDE) algorithm is employed to compute derivatives of cumulative releases relying exclusively on Gaussian functions.</p> <p>If <i>true</i>, the Gaussian KDE algorithm is complemented with the use of the generalized extreme value distribution (GEVD) to fit the extremes (left and right) of the cumulative release functions.</p>
<code>createExcelFlag</code>	Logical variable that can take values <i>true</i> or <i>false</i> . <p>If <i>true</i>, then an Excel file is created containing the cumulative releases versus time and release rates versus time, using regular time steps.</p> <p>If <i>false</i>, the Excel file is not created.</p>
<code>maxTime</code>	Maximum time to include in the plots and in the Excel output file. The same time units as the Source Worksheet must be used. <p>To allow the MATLAB script to automatically select the maximum time, the value of this variable can be set to an arbitrarily small value.</p>
<code>plotUnit</code>	String variable that can take the values <code>'mol'</code> or <code>'Bq'</code> . <p>If <code>'mol'</code> then cumulative releases are output in units of mol, and instant release rates in units of mol/year (assuming the unit of time in the Source Worksheet is years), in both the graphic displays and the generated Excel file.</p> <p>If <code>'Bq'</code> then cumulative releases are output in units of Bq, and instant release rates in units of Bq/yr.</p>
<code>scaleY</code>	Range to display in the plots. This variable does not affect the output Excel file.

The command

```
smoothDriver(outputFile, GEVDflag, createExcelFlag, maxTime, plotUnit,
suffix, scaleY)
```

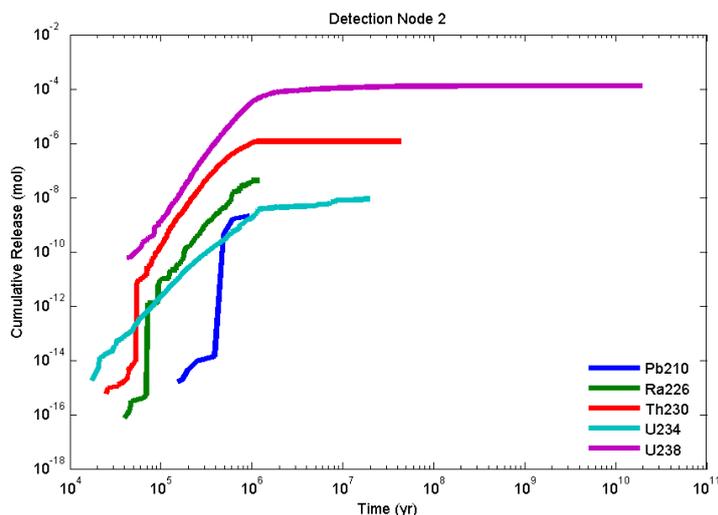
is the main instruction driving the smooth kernel density estimator, the graphic displays, and the generation of the Excel file with cumulative releases and release rates. The m-file containing the function `smoothDriver` must be consulted for additional fine controls, simulation settings, and KDE algorithms.

Unit conversions controlled by the variable `plotUnit` require an additional auxiliary file. This file is named `RadionuclideHalfLives.xlsx`, and must be located in the `testing` directory. The content of this auxiliary file is self-explanatory and is reproduced in the following figure.

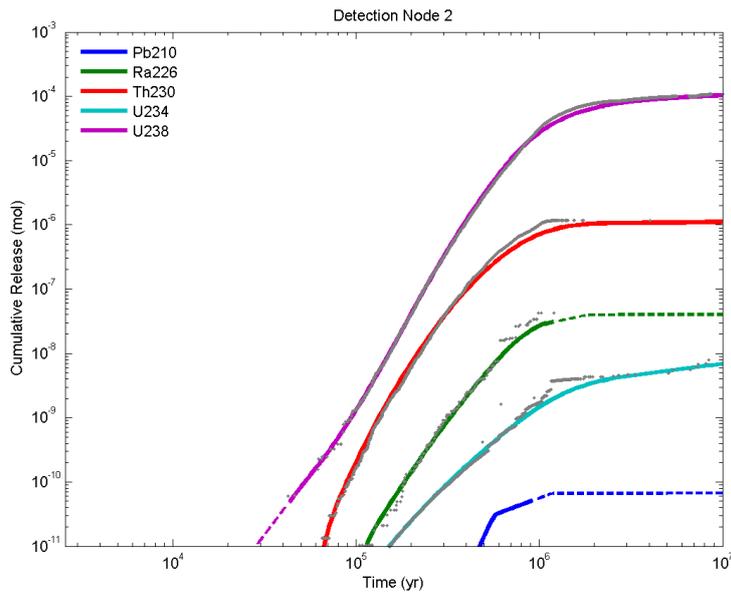
	A	B	C	D	E	F
1	Species ID	Atomic Weight (g/mol)	Half-life (yr)	Decay Rate (1/s)	Activity (Bq/mol)	Specific Activity (Bq/g)
2	Ag108m	108	438	5.01816E-11	3.0220E+13	2.7982E+11
3	Cl14	14	5730	3.83587E-12	2.3100E+12	1.6500E+11
4	Cs135	135	2.30E+06	9.55633E-15	5.7550E+09	4.2629E+07
5	I129	129	1.57E+07	1.39997E-15	8.4308E+08	6.5355E+06
6	Nb94	94	2.03E+04	1.08274E-12	6.5204E+11	6.9366E+09
7	Ni59	59	7.50E+04	2.93061E-13	1.7649E+11	2.9913E+09
8	Np237	237	2.14E+06	1.02708E-14	6.1852E+09	2.6098E+07
9	Pb210	210	22.3	9.8563E-10	5.9356E+14	2.8265E+12
10	Pu238	238	87.7	2.50622E-10	1.5093E+14	6.3415E+11
11	Pu239	239	24100	9.12015E-13	5.4923E+11	2.2980E+09
12	Pu240	240	6560	3.35054E-12	2.0177E+12	8.4073E+09
13	Pu242	242	3.73E+05	5.89264E-14	3.5486E+10	1.4664E+08
14	Ra226	226	1.60E+03	1.37372E-11	8.2727E+12	3.6605E+10
15	Rn222	222	0.010010475	2.19566E-06	1.3223E+18	5.9561E+15
16	Se79	79	3.77E+05	5.83012E-14	3.5110E+10	4.4443E+08
17	Tc99	99	2.11E+05	1.04168E-13	6.2732E+10	6.3365E+08
18	Th230	230	7.54E+04	2.91506E-13	1.7555E+11	7.6326E+08
19	U232	232	68.8	3.1947E-10	1.9239E+14	8.2927E+11
20	U233	233	159000	1.38236E-13	8.3248E+10	3.5729E+08
21	U234	234	246000	8.93478E-14	5.3806E+10	2.2994E+08
22	U235	235	7.04E+08	3.1221E-17	1.8802E+07	8.0007E+04
23	U236	236	2.34E+07	9.39297E-16	5.6566E+08	2.3969E+06
24	U238	238	447000000	4.91713E-18	2.9612E+06	1.2442E+04

If more or different radionuclides are considered, the corresponding information for the additional radionuclides must be incorporated in the file RadionuclideHalfLives.xlsx to ensure appropriate unit conversions from mole to Bq.

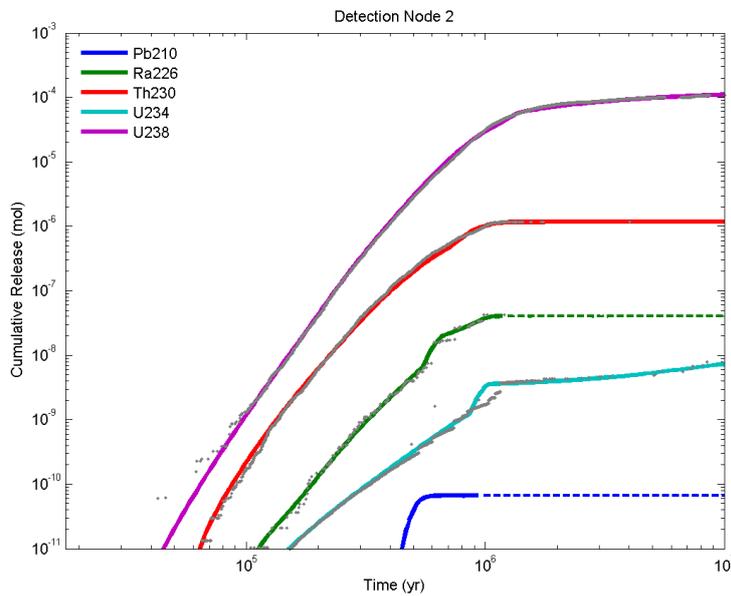
The next plots were generated by executing example_plot.m. The following plot is the raw data in the file T01_out.res. To prepare such plot, the arrival times at Node 2 are identified and classified by radionuclide. For each radionuclide, the total arrival times (source injection time plus travel time) are sorted in increasing order, and the cumulative probability-weighted mass for each arrival time is computed. The cumulative releases are defined as the cumulative probability-weighted mass versus the sorted particle arrival times.



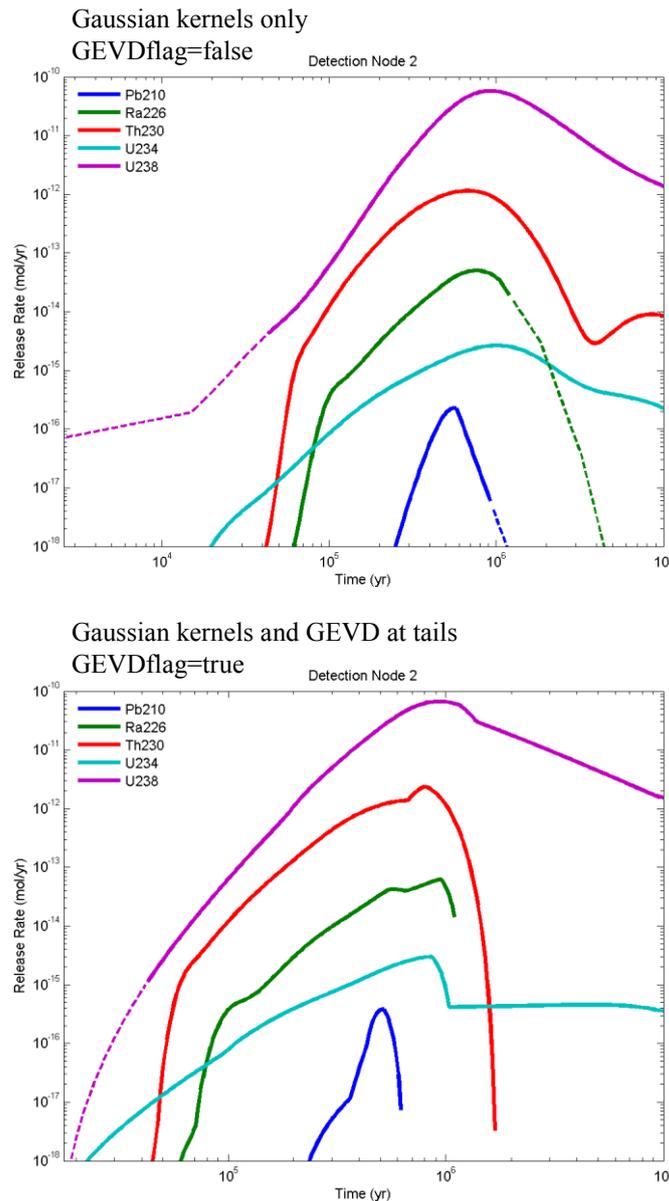
The following plot was produced with the logical variable GEVDflag=false (only Gaussian kernels used). The objective of the smoothing algorithm is producing smooth approximations to the cumulative releases, to facilitate the computation of instant release rates as time derivatives.



The plot includes the original raw data to facilitate the analyst deciding whether the smooth fit is adequate. The dashed lines indicate extrapolations beyond the raw data. Note that the right tails of the functions differ from the raw data. The following example employed `GEVDflag=true` (Gaussian kernels used in the central points and GEVD used in the left and right tails), which improved fits to the right tails.



Different radionuclide release rates are computed depending on the smoothing algorithm. The next two figures compare radionuclide releases computed with the setting `GEVDflag=false` and `GEVDflag=true`.



The analyst must decide which smoothing algorithm fits best the data. Additional simulation controls are available in the m-files `makeSmooth.m` and `makeSmoothGEVD.m`, available in the folder *testing/private*. Using GEVD is recommended when cumulative releases attain a full sigmoidal shape (i.e., cumulative release attain a full plateau at the right tail). Fitting to tails becomes poor when cumulative releases are still increasing at the detection node.

There is a level of uncertainty in the release rate computation introduced by the need to use smoothing algorithms. The uncertainty is reduced by using more particles, but it can never be completely eliminated. This is a fundamental limitation of time-domain particle tracking methods.

The following figure is fragment of information contained in an example output Excel file. The information is self-explanatory. At the end of the file, radionuclide release rates are reported, identified by the label "Rate."

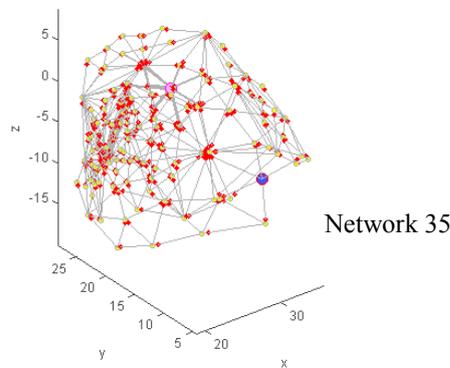
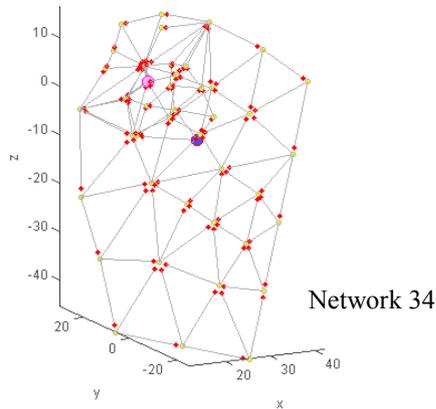
	A	B	C	D	E	F	G
1	Node Number	2					
2	Release Type	Time	Pb210	Ra226	Th230	U234	U238
3	Cumulative	17508.61	0	7.6E-135	1.5E-17	8.66E-16	2.51E-16
4	Cumulative	17960.69	0	1.6E-131	1.54E-17	9.67E-16	3.96E-16
5	Cumulative	18424.44	0	3.4E-128	1.58E-17	1.08E-15	6.1E-16
6	Cumulative	18900.16	0	7.3E-125	1.63E-17	1.2E-15	9.17E-16
7	Cumulative	19388.17	0	1.6E-121	1.71E-17	1.43E-15	1.51E-15
8	Cumulative	19888.78	0	3.3E-118	1.81E-17	1.71E-15	2.44E-15
9	Cumulative	20402.31	0	7E-115	1.92E-17	2.03E-15	3.81E-15
10	Cumulative	20929.1	0	1.5E-111	2.03E-17	2.41E-15	5.81E-15
11	Cumulative	21469.5	0	3.2E-108	2.17E-17	2.83E-15	8.62E-15
12	Cumulative	22023.85	0	6.7E-105	2.31E-17	3.32E-15	1.25E-14
13	Cumulative	22592.51	0	1.4E-101	2.47E-17	3.88E-15	1.79E-14
14	Cumulative	23175.85	0	3.03E-98	2.65E-17	4.51E-15	2.51E-14
15	Cumulative	23774.26	0	6.44E-95	2.86E-17	5.23E-15	3.47E-14
16	Cumulative	24388.12	0	1.37E-91	3.09E-17	6.05E-15	4.73E-14
17	Cumulative	25017.83	0	2.91E-88	3.34E-17	6.97E-15	6.38E-14
18	Cumulative	25663.79	0	6.17E-85	3.64E-17	8.02E-15	8.5E-14
19	Cumulative	26326.44	0	1.31E-81	3.98E-17	9.19E-15	1.12E-13
20	Cumulative	27006.2	0	2.79E-78	4.36E-17	1.05E-14	1.47E-13
21	Cumulative	27703.5	0	5.92E-75	4.81E-17	1.2E-14	1.9E-13
22	Cumulative	28418.81	0	1.26E-71	5.33E-17	1.37E-14	2.45E-13
23	Cumulative	29152.6	0	2.67E-68	5.94E-17	1.55E-14	3.13E-13
24	Cumulative	29905.32	0	5.68E-65	6.66E-17	1.76E-14	3.97E-13
25	Cumulative	30677.49	0	1.21E-61	7.52E-17	1.99E-14	5.01E-13
26	Cumulative	31469.59	0	2.56E-58	8.55E-17	2.25E-14	6.29E-13
27	Cumulative	32282.14	0	5.44E-55	9.79E-17	2.54E-14	7.85E-13

All of the input files, graphic output files, and Excel file include the same prefix label (T01_ in the example in Table 5 and the figure preceding Table 5).

4.4. TRUE-Block Network Example

Benoit Dessirier, Chin-Fu Tsang, Bruno Figueiredo, Jonas Pedersen, and Auli Niemi of Uppsala University examined the TRUE-Block Scale field experiment at Äspö (SKB, 2003). They proposed the formation of flow channels within a fracture network, as alternative explanation of pressure tests, dilution tests, and tracer tests of the TRUE-Block Scale field experiment. They constructed a pathway network made of flow channels embedded in a fracture network. The channel network can be input to ISTIDRAW for the analysis of tracer tests.

To collaborate in the development of ISTIDRAW, Uppsala University provided two sets of channel networks, referred to as Network 34 and Network 35. Network 34 is a backbone channel network embedded in 10 fracture planes. Network 35 is a denser network built by considering smaller fractures in addition to the 10 main fracture planes. Networks 34 and 35 are depicted in the following figures. The injection node is represented by the blue dot and the extraction node by the pink node. The downstream end of each segment is indicated by a red dot. Most of the network is excluded from the figures; only the nodes and channels that belong in trajectories connecting the injection node to the extraction node are depicted. The length units in the axes are meters.



The number of trajectories connecting the injection and extraction nodes is approximately calculated by raising the average number of outflow segments per node to a power equal to the average number of segments in a trajectory. Even the relatively simple Network 34 produces tens of thousands of possible trajectories connecting the injection and extraction nodes, and it is not computationally feasible to identify all possible trajectories for Network 35. However, for radionuclide transport computations, the most likely trajectories (trajectories with high flows along all segments) capture the majority of the release. Less likely trajectories (longer trajectories with a number of segments of low flow) are associated with delayed particle arrival times at the extraction node.

The most likely trajectories can be identified by following particles randomly moving from the injection to the extraction node. The most likely trajectories tend to have higher flows across all segments (the probability for a particle to transfer into a segment at branching nodes is assumed proportional to the segment flow) and fewer segments. It is more practical to compute radionuclide transport considering only a subset of the trajectories. Radionuclide releases computed on the basis of a subset skewed to the most likely trajectories will yield shorter arrival times at the extraction node, which is adequate (conservative) for performance assessments.

The ISTIDRAW distribution includes scripts to extract a limited number of trajectories from Network 34 and Network 35. The base channel network was computed by collaborators from Uppsala University, with corresponding electronic files archived inside the folder called *TRUEBlock*, and subfolders named *sample_34_v2* and *sample_35*. The MATLAB script, located in the *TRUEBlock* folder is named *example_network.m*. Contents of the m-file are reproduced in the following screen capture.

```

example_network.m x +
1 %First parameter: 's34' or 's35' for 10 fracture planes of 200 fracture planes
2 %Reads inputs from existing directories sample_34_v2 or sample_35
3 %No other input file is needed
4
5 %'zsamp': 'monte' or 'unique' // Monte Carlo (random) or unique (different) trajectories
6 %'nsamp': number of trajectories
7 %'zwght': 'renorm' or 'monte' // renormalize by flow (preferred) or use Monte Carlo frequency
8 %'zpfle': 'fileName.dat' // file name with trajectories definition for ISTIDRAW input
9 %'zxls': 'fileName.xlsx' // file name with network nodes, input to ISTIDRAW
10 %'zsht': 'sheetName' // Sheet name of 'fileName.xlsx'
11
12 % Additional options such as diffusion coefficient, matrix porosity,
13 % retardation coefficients are controlled in extract_sample. Providing
14 % corresponding inputs/options in drive_extract overrules default inputs
15
16 drive_extract('s35', ...
17     'zsamp', 'unique', ...
18     'nsamp', 200, ...
19     'zwght', 'renorm', ...
20     'zpfle', 's35_200unique.dat', ...
21     'zxls', 'inputFile.xlsx', ...
22     'zsht', '200u')
23

```

To execute the m-file, the MATLAB main directory must point to the *TRUEBlock* folder. The parameters of the function `drive_extract` are explained in Table 6.

Table 6. Inputs to the `drive_extract` MATLAB function to post-process channel network information of the TRUE-Block field test

Variable name	Value
First entry	's34' : process channel network based on 10 fracture planes 's35' : process channel network based on 10 fracture planes and secondary fractures
'zsamp'	'monte' : find random trajectories allowing for repeats 'unique' : find unique (different) trajectories
'nsamp'	Number of trajectories
'zwght'	'monte' : assign weight to trajectories based on the frequency they are identified 'renorm' : assign weight to trajectories based on the relative flows (preferred method)
'zpfle'	'trajectories.dat' : name of trajectory file. The arbitrary file name is declared in the Master Worksheet via the variable <code>zpathfile</code> , and the variable <code>ypathfile</code> set to <code>T (=true)</code> or <code>1</code> . In the example in the previous figure the trajectory file is named <code>'s35_200unique.dat'</code> .
'zxls'	'transportParameters.xlsx' : name of the Excel file to contain information on transport parameters. In the example in the previous figure, the Excel file is named <code>'inputFile.xlsx'</code> .
'zsht'	'worksheet' : name of the worksheet, within the Excel file 'transportParameters.xlsx' to contain network information related to transport parameters. This worksheet must be copied to the Master Worksheet. The name of the transport parameter worksheet, in the Master Worksheet, must be identified by the variable <code>zGsheet</code> . In the example in the previous figure, the worksheet is named <code>'200u'</code> within the file <code>'input-File.xlsx'</code> .

The m-file `extract_sample.m` includes additional flags and default values of transport parameters such as porosity, dispersion coefficient, matrix diffusion coefficient, matrix thickness, and matrix retardation coefficient.

After executing `example_network.m`, the script outputs the following information in the MATLAB command screen:

```

Command Window
New to MATLAB? See resources for Getting Started.

>> example_network
inj = 4731 (4.1667e-07)
pmp = 4733 (-3.25e-05)
extracted minj = 6
extracted mpmp = 115
extracted nnode = 147
extracted nchan = 403
.....*.....*
fx >>

```

The integer after the string ‘minj’ is the injection node (6 in the example), and the integer after the string ‘mpmp’ is the extraction node (115 in the example). **The injection node must be declared in the Master Worksheet as the source node, via the variable srcNode.** The extraction node must be identified in the Master Worksheet as a recording node, via the variable ytraceNode.

The structure of the trajectory file is explained with an example with 10 trajectories, as follows

```

10 %Number of trajectories
138 %Number of nodes
66 %Number of segments
9 %Maximum number of segments for a trajectory
9 6 5 7 9 6 6 6 6 6 % Number of number of segments for each trajectory
6 5 10 26 55 94 118 131 104 115 %Node sequence for trajectory 1
6 16 40 96 138 134 115 0 0 0 %Node sequence for trajectory 2
6 19 51 107 136 115 0 0 0 0 %Node sequence for trajectory 3
6 16 19 40 96 138 120 115 0 0 %Node sequence for trajectory 4
6 19 26 51 89 130 132 131 104 115 %Node sequence for trajectory 5
6 16 19 62 107 136 115 0 0 0 %Node sequence for trajectory 6
6 19 51 107 136 125 115 0 0 0 %Node sequence for trajectory 7
6 16 40 62 107 136 115 0 0 0 %Node sequence for trajectory 8
6 19 40 96 138 120 115 0 0 0 %Node sequence for trajectory 9
6 5 19 62 107 136 115 0 0 0 %Node sequence for trajectory 10
1 11 21 31 41 51 60 63 65 %Segment sequence for trajectory 1
2 12 22 32 42 52 0 0 0 %Segment sequence for trajectory 2
3 13 23 33 43 0 0 0 0 %Segment sequence for trajectory 3
4 14 24 34 44 53 61 0 0 %Segment sequence for trajectory 4
5 15 25 35 45 54 62 64 66 %Segment sequence for trajectory 5
6 16 26 36 46 55 0 0 0 %Segment sequence for trajectory 6
7 17 27 37 47 56 0 0 0 %Segment sequence for trajectory 7
8 18 28 38 48 57 0 0 0 %Segment sequence for trajectory 8
9 19 29 39 49 58 0 0 0 %Segment sequence for trajectory 9
10 20 30 40 50 59 0 0 0 %Segment sequence for trajectory 10
0.0707116 %Weight or probability of trajectory 1
0.113976 %Weight or probability of trajectory 2
0.16771 %Weight or probability of trajectory 3
0.0426361 %Weight or probability of trajectory 4
0.0960976 %Weight or probability of trajectory 5
0.105344 %Weight or probability of trajectory 6
0.0830558 %Weight or probability of trajectory 7
0.120691 %Weight or probability of trajectory 8
0.0674522 %Weight or probability of trajectory 9
0.132326 %Weight or probability of trajectory 10

```

The top lines in the trajectory file (blue font), tells ISTIDRAW the structure of the file. The second block (green font) is the list of 10 trajectories. Note that all trajectories start at 6 (injection node) and end at 115 (detection node). The third block (red font) is the sequence of segment numbers, for each of the 10 trajectories. For each segment, the transport properties for each radionuclide are defined in the output Excel file. (As stated in Table 6, Information in the Excel file must be copied to the Master Worksheet to input the transport parameters to ISTIDRAW.) The fourth block (grey font) is the probability of each trajectory. This probability is applied as a weight factor to each particle tracked in the radionuclide transport model. Each trajectory is independently simulated in ISTIDRAW; each trajectory includes the same number of particles.

The distributed files with ISTIDRAW contains an example Master Worksheet, InputFile_examplesNetwork.xlsx, including examples of pathway networks prepared using Network 35. Several trajectory files are included s35_05unique.dat, s35_10unique.dat, s35_100unique.dat, s35_1000unique.dat, where the numbers 5, 10, 100, and 1000 represent the number of different trajectories in each trajectory file. Each trajectory file must be properly paired with a Pathway Network Worksheet. The input file InputFile_examplesNetwork.xlsx provides several examples to probably establish the pairing. The input file in the worksheet Source_s34 is a simple pulse input, as a first approximation to simulate injection-extraction tests of conservative tracers in the TRUE-Block field experiments.

In the *testing* folder, examples with the prefixes “N01” and “N01” provide examples of cumulative releases and instant release rates for conservative tracers, considering Network 35.

5. References

Painter, S., V. Cvetkovic, J.W. Mancillas, and O. Pensado. "Time Domain Particle Tracking Methods for Simulating Transport with Retention and First-Order Transformation." *Water Resources Research*. Vol. 44. p. 1,406. 2008.

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SKB. "Äspö Hard Rock Laboratory, Äspö Task Force on modelling of groundwater flow and transport of solutes. Task 6c: A semi-synthetic model of block scale conductive structures at the Äspö HRL." International Progress Report IPR-03-13. Svensk Kärnbränslehantering AB: Stockholm, Sweden. 2003.

Appendix

The ISTIDRAW mathematical model for retention time in a matrix is based on the Cvetkovic et al. (1999) analytical model, which considered particle transport in a fracture and surrounding matrix. The model considers diffusion in the matrix, advection in the fracture, and reversible sorption within the matrix and on the fracture walls. Cvetkovic et al. (1999) solved the model in Laplace space, which must be inverted to the time domain. An inverse Laplace transform can be analytically derived for the case of a semi-infinite matrix domain, but not for more complex conditions with a finite domain.

Neglecting particle decay and assuming uniform fracture aperture, the general form of the Cvetkovic et al. (1999) model for normalized return flux with a no-flow boundary at full matrix depth can be expressed in Laplace space as

$$f(s) = \frac{\hat{q}}{\Delta M} = \exp[-\tau G_f(s)] \exp\left[-\frac{\tau\theta}{b} (D_m G_m(s))^{1/2} A(s)\right] \quad (\text{A-1})$$

$$G_i(s) = s \left(1 + \frac{K_d^i \alpha_i}{s + \alpha_i}\right) \approx s R_i \text{ for equilibrium sorption } (\alpha_i \rightarrow \infty) \quad (\text{A-2})$$

$$A(s) = \tanh \left[\zeta \left(\frac{G_m(s)}{D_m} \right)^{1/2} \right] \quad (\text{A-3})$$

where

s	Laplace variable [1/T]
\hat{q}	Mass returning from the matrix to the fracture [M]
ΔM	Mass instantaneously transferred from the fracture to matrix [M]
τ	Residence time for a nonsorbing tracer in the fracture system [T]
θ	Matrix porosity
D_m	Porewater diffusivity in the matrix [L ² /T]. (Note that the effective diffusivity is θD .)
b	Fracture aperture [L]
ζ	Thickness of matrix domain [L]
K_d^m	Dimensionless sorption coefficient in the matrix ($K_d^m = \rho_b K_d / \theta$, where ρ_b is the bulk density and K_d is the partition coefficient)
K_d^f	Dimensionless sorption coefficient on the fracture wall ($K_d^f = K_a b_a / b$, where K_a is a dimensionless sorption coefficient at a reference aperture b_a)
α_m	Rate coefficient for reversible sorption in the rock matrix [1/L]
α_f	Rate coefficient for reversible sorption on the fracture wall [1/L]
R_m	Retardation factor in the matrix ($1 + K_d^m$)
R_f	Retardation factor due to surface adsorption on the fracture wall ($1 + K_d^f$)

Cvetkovic et al. (1999) assert that the same expression holds for the case of zero concentration at full matrix depth, except that $A(s)$ is replaced with $1/A(s)$.

When equilibrium fracture-wall and matrix sorption is considered, Eq. (A-1) simplifies to

$$f(s) = \frac{\hat{q}}{\Delta M} = \exp[-\tau R_f s] \exp[-(\tau_1 s)^{1/2} \tanh[(\tau_2 s)^{1/2}]] \quad (\text{A-4})$$

$$\tau_1 = \left(\frac{\tau\theta}{b}\right)^2 R_m D_m \quad (\text{A-5})$$

$$\tau_2 = \zeta^2 \frac{R_m}{D} \quad (\text{A-6})$$

The matrix and fracture components of the Cvetkovic et al. (1999) model can be separated using the time-shifting property of Laplace transforms, where $\mathcal{L}^{-1}[e^{-as}F(s)] = F(t - a)u(t - a)$. In this expression, $\mathcal{L}^{-1}[\cdot]$ indicates the inverse Laplace transform and $u(t)$ is the Heaviside step function.

The cumulative distribution function for particle return time after an instantaneous pulse transferred to the matrix is

$$F(t) = \mathcal{L}^{-1}[F(s)] = \mathcal{L}^{-1}[f(s)/s] \quad (\text{A-7})$$

The general solution to Eq. (A-4) is therefore

$$F(s) = \frac{1}{s} \exp[-(\tau_1 s)^{1/2} \tanh[(\tau_2 s)^{1/2}]] \quad (\text{A-8})$$

In the limit as $x \rightarrow \infty$, $\tanh[x] = 1$, and $\tanh[x] = x$ in the limit as $x \rightarrow 0$. ISTIDRAW uses the analytical solution for the case of infinite matrix depth ($\zeta \rightarrow \infty$, thus $\tau_2 \rightarrow \infty$). For this case, regardless of the matrix boundary condition Eq. (A-8) reduces to

$$F(s) = \frac{\exp[-(\tau_1 s)^{1/2}]}{s} \quad (\text{A-9})$$

$$F(t) = \text{erfc}\left[\left(\frac{\tau_1}{4t}\right)^{1/2}\right] \quad (\text{A-10})$$

For the case where the matrix depth is small ($\zeta \rightarrow 0$, thus $\tau_2 \rightarrow 0$), Eq. (A-8) reduces to

$$F(s) = \frac{\exp[-(\tau_1 \tau_2)^{1/2} s]}{s} \quad (\text{A-11})$$

$$F(t) = u[t - (\tau_1 \tau_2)^{1/2}] \quad (\text{A-12})$$

If the far-field matrix boundary condition is zero concentration, instead of no flow, the corresponding matrix equation for a small matrix depth is

$$F(s) = \frac{\exp[-(\tau_1 s)^{1/2} \coth[(\tau_2 s)^{1/2}]]}{s} = \frac{\exp[-(\tau_1/\tau_2)^{1/2}]}{s} \quad (\text{A-13})$$

$$F(t) = \exp[-(\tau_1/\tau_2)^{1/2}] \quad (\text{A-14})$$

Valsa and Brančik (1998) developed an approach to numerical Laplace transform inversion based on high-pass filters, rather than most common approached relying on approximation polynomials. Valsa uploaded a MATLAB routine exemplifying the solution approach to the MathWorks® file exchange in 2011 (<https://www.mathworks.com/matlabcentral/fileexchange/32824-numerical-inversion-of-laplace-transforms-in-matlab>). Confirmatory testing of the model against several analytical solutions suggests that solutions can be obtained that are accurate to at least nine decimal places with suitable selection of coefficients. However, the approach does exhibit aliasing effects when the solution in time has nearly discontinuous derivatives (e.g., a Dirac delta function or a Heaviside function). The uploaded example version of the MATLAB numerical inversion routine internally generated output times and accepted a character string defining the function to be inverted. The routine was revised to improve generality and robustness.

The Laplace transforms has the following time-scaling property

$$\mathcal{L}[f(at)] = \frac{1}{a} f_{\mathcal{L}}\left(\frac{s}{a}\right) \quad (\text{A-15})$$

where $\mathcal{L}[f(t)] = f_{\mathcal{L}}(s)$. Equation (A-8) has two time constants (τ_1 and τ_2). The inverse Laplace solver by Valsa and Brančik was applied to Eq. (A-8) over a wide range of τ_1 and τ_2 to generate a lookup table for $F(t_s)$, where $t_s = t/(\tau_1\tau_2)^{1/2}$. The table employed a combined parameter $T = (\tau_2/\tau_1)^{1/2}$, and tabulates $\log[F(t_s)]$, $\log[T]$, and $\log[t_s]$ for selected values of $F(t_s)$. The tabulation process assumes τ_1 is 1. To calculate $F(t)$, the interpolated t_s values based on τ_1 and τ_2 are multiplied by τ_1 .

$$t_s = \frac{t}{(\tau_1\tau_2)^{1/2}} = \frac{t}{R_m} \left(\frac{b}{\tau \theta \zeta} \right) \quad (\text{A-16})$$

$$T = \left(\frac{\tau_2}{\tau_1} \right)^{1/2} = \frac{\zeta b}{\tau \theta D_m} \quad (\text{A-17})$$

The created table employed 76 values for T and 603 values for $F(t_s)$ to assure accuracy. The table spans the range that can be accurately calculated with the inverse Laplace transform solver.

Figure A-1 shows selected values of the interpolation table, increasing a by an order of magnitude for each successive curve from blue to yellow. Figures A-2 and A-3 compare the interpolated and directly calculated responses for a case with a matrix thickness of 0.01 (Figure A-2) and 10 (Figure A-3).

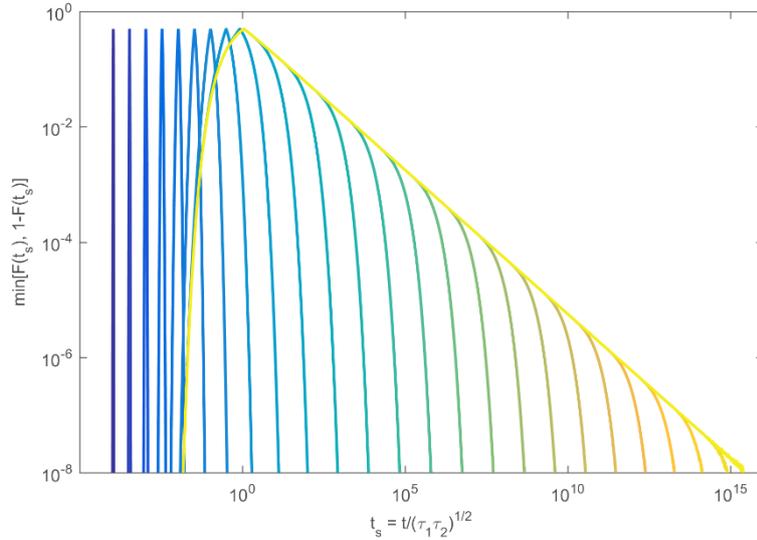


Figure A-1. Tabulated CDF for particle retention time in the matrix. The CDF is plotted as $\min(F, 1-F)$ to facilitate logarithmic scaling. Curves use scaled time for selected values of $a = \tau_2/\tau_1$ ranging from 10^{-8} to 10^{17} . Each curve increases by one order of magnitude moving from blue to yellow.

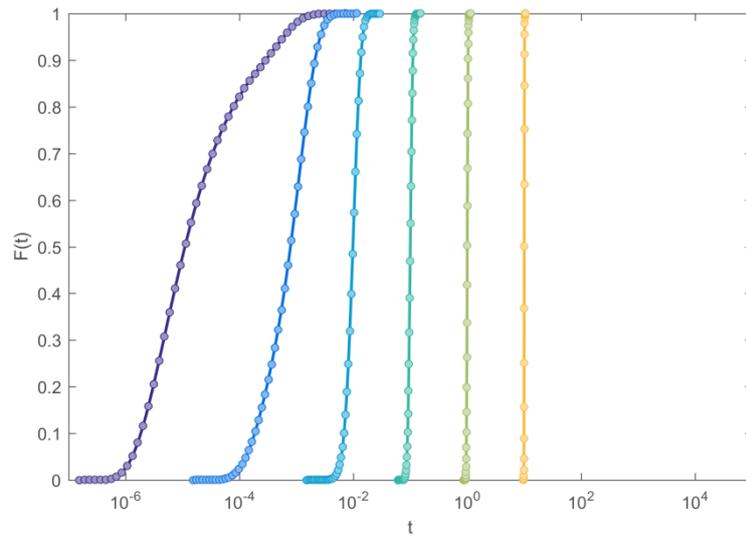


Figure A-2. Interpolated and directly calculated matrix retention time CDF with matrix thickness of 0.01. Each curve represents a different τ (fracture travel time), increasing from 10^{-3} to 10^2 by a factor of 10 from blue to yellow.

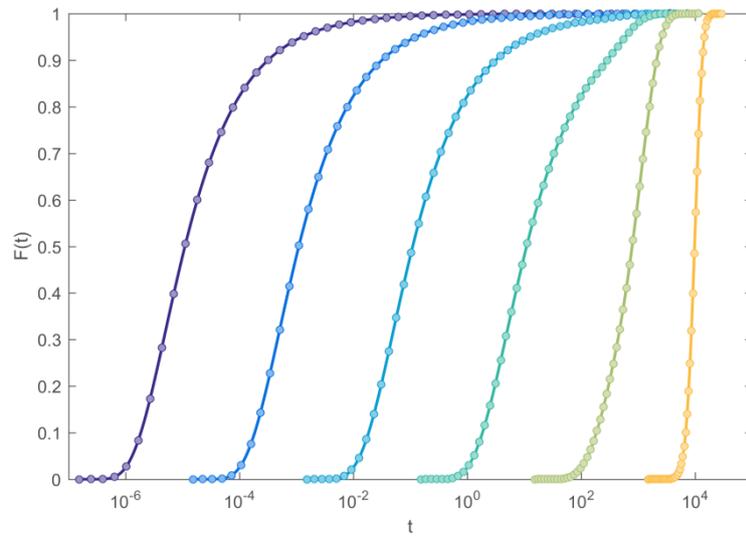


Figure A-3. Interpolated and directly calculated matrix retention time CDF with matrix thickness of 10. Each curve represents a different τ (travel time in the fracture), increasing from 10^{-3} to 10^2 by a factor of 10 from blue to yellow.

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