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TECHNICAL SUPPORT DOCUMENT FOR

SECTION 194.34: USE OF CCDF FORMALISM IN THE WIPP PA: AN INTRODUCTION

U. S. ENVIRONMENTAL PROTECTION AGENCY
Office of Radiation and Indoor Air
Center for the Waste Isolation Pilot Plant
401 M. Street, S. W.
Washington, DC 20460

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1. INTRODUCTION

In 1979, Congress authorized construction of the Waste Isolation Pilot Plant (WIPP), a repository for the permanent disposal of the transuranic (TRU) wastes produced during the manufacture of nuclear weapons. (A TRU element is one with atomic number greater than 92, that of uranium.) By legal definition, TRU waste contains transuranic materials (in particular, certain isotopes of plutonium and of americium) and may contain non-TRU radionuclides mixed in, but does not include high-level waste or spent nuclear fuel. The WIPP consists of the surface projection of the repository proper and the "controlled area," as defined in the WIPP Land Withdrawal Act (LWA) of 1992. The disposal area is located 2,150 feet below the surface, with its waste disposal panels excavated from within a bed of halite (salt) nearly 2,000 feet thick. It is predicted that the halite will plastically deform over the course of several hundred years so as to encapsulate the waste permanently.

Before wastes can actually be placed in it, the Department of Energy (DOE) must demonstrate that the WIPP complies with the regulations at 40 CFR parts 191 and 194. These define upper bounds (expressed in terms of a nonstandard measure of radioactivity commonly called the *cumulative normalized release*) on the amounts of waste that might escape the repository and enter the *accessible environment*. The regulations also require that DOE carry out a comprehensive, quantitative analysis of the 10,000 year performance of the repository. The results of this Performance Assessment (PA) are presented in the form of *complementary cumulative distribution function* (CCDF) curves. The WIPP PA is a major component of the Compliance Certification Application (CCA) that DOE has submitted to EPA for approval (Docket A-93-02, II-G-1).

Aspects of the PA, and of the underlying modeling and other mathematical tools, are complex and technically demanding. Also, the most important ideas and information are not presented all together in one place, but rather appear in several chapters of the CCA, in a number of Appendices, and in supporting DOE documentation. It is to be expected that many readers of the CCA, and of EPA's review of the CCA, are not specialists in radioactive waste management, however, and also it could be difficult for someone not very familiar with the material to assemble quickly the relevant pieces that tell the story of the CCDF formalism. This document is intended to assist such people by providing an introductory overview of the generation and use of CCDF curves.

1.1. Cumulative Normalized Releases, Release Limits, and the Containment Requirements of *§191.13*

40 CFR part 191.13 presents specific design requirements, in the form of performance requirements, on the ability of the WIPP to contain TRU wastes: There must be "....reasonable expectation, based upon performance assessments, that the cumulative releases of radionuclides to the accessible environment for 10,000 years..... shall

(1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A); and

(2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A)."

The quantity calculated according to Table 1 (Appendix A), the primary measure of consequence, or seriousness, of a release resulting from an inadvertent human intrusion is the cumulative normalized release of radioactive waste that is estimated to occur over the 10,000 years following closure of the repository. "Cumulative normalized release," in turn, is defined in terms of three factors:

(1) the waste unit factor (number of units of TRU waste), which refers only to the total activity of the transuranic component of the waste in the WIPP;

(2) the release limit (per unit of TRU waste) for each of these TRU and non-TRU released nuclides; and

(3) a estimate (from mathematical modeling of the behavior of the WIPP over time) of the calculated activity of *every* radionuclide projected to be released or escaping from the repository for the scenario, both TRU and non-TRU;

One unit of TRU waste is defined in 40 CFR part 191 as that amount of radioactive waste that contains exactly one million curies of alpha-particle-emitting TRU radionuclides (with half-lives greater than 20 years) with a net TRU concentration of greater than 100 nCi/g — regardless of the amounts of other radionuclides present (*e.g.*, Sr-90, Ra-226, or Pu-241, which has a half-life of 14.4 years.)

Let C represent the total activity (in curies) of the TRU component of the waste in the repository at closure. (Prime contributors are Pu-238, Pu-239, Pu-240, Pu-241, and Am-241; Pu-241 does not add to C because its 14.4 year half-life is less than the 20 year cut-off for TRU waste). DOE calls the dimensionless entity $(C\ \text{Ci})/(10^6\ \text{Ci})$ the *number of units of TRU waste*, or the *waste unit factor* for WIPP. The calculation of C is discussed in **CARD 31 – Application of Release Limits**.

The *release limit* or, more precisely, the *release limit per unit of TRU waste*, for the j-th radionuclide, L_j, refers to the relevant normalizing factor (in curies per unit of TRU waste) listed in Table 1 of Appendix A., reproduced as Table 1 of **CARD 31 – Application of Release Limits**. For any TRU radionuclide, $L_j = 100$ Ci per unit of TRU waste, and it is at least that large for all other radionuclides, except for the isotopes of thorium.

40 CFR part 191 introduces an *adjusted* release limit for the j-th radionuclide, RL_j (in curies), defined as the product of the release limit for the j-th radionuclide and the number of units of TRU waste in the repository,

$$RL_j \ = \ L_j \times (\text{Ci} / 10^6\ \text{Ci}) \quad . \qquad (1)$$

RL_j, like L_j, is sometimes referred to as a release limit.

With an estimated repository TRU inventory of C Ci, and a 10,000 year scenario expected to cause the release if Q_j curies of the j-th radionuclide, the expression

$$nR_j = Q_j / RL_j = Q_j / (L_j \times C/10^6) \quad . \tag{2a}$$

is called the cumulative normalized release for the j-th radionuclide for the future under consideration, regardless of whether it is a TRU or a non-TRU radionuclide. Summing over all radionuclides released yields

$$nR = \sum_j nR_j \quad , \tag{2b}$$

the cumulative normalized release for the scenario under consideration. The cumulative normalized release is presented in equivalent form, in Eq. 1 of Chapter 1 of the CCA, as

$$nR = \sum_j (Q_j / L_j)(10^6/C). \tag{2c}$$

Note that if all the significant radionuclides have the same release limit, L, as may well be the case, this reduces to

$$nR = (10^6 / C\times L)(\sum_j Q_j) \quad . \tag{2d}$$

Cumulative normalized release is expressed in terms of a measure that DOE calls the *EPA unit*. The number of EPA units associated with the amount Q_j of the j-th radionuclide (in curies) is determined exactly the same way as is the cumulative normalized release itself— namely by computing $Q_j / (L_j \times C/10^6)$. EPA units are used to quantify not only the magnitude of a release of TRU waste, but also the amount of such waste in DOE's TRU inventory. Thus Q_j can represent the amount of the j-th radionuclide that either is projected to escape from the repository or that is being disposed of there.

The containment requirements of §191.13(a)(1) may now be expressed as

$$P[\, nR > 1 \,] < 0.1 \;, \tag{3a}$$

and

$$P[\, 10\times nR > 1 \,] < 0.001 \;, \tag{3b}$$

If it is likely for any future that $nR > 1$, or that $(Q_j / RL_j) > 1$ for a single radionuclide, then the containment requirement is automatically exceeded.

The cumulative normalized release finds its essential application in the calculation and display of CCDF curves for various release scenarios, and in the comparison of such curves with the applicable regulatory restrictions on permitted releases. Families of CCDF curves are shown and interpreted on a graph of cumulative probability *vs*. cumulative normalized release. The containment requirements are represented as an *exclusion region*[1] on the same graph. If the

[1] The regulations are formally defined in terms of two excluded horizontal *lines* that terminate on the left at

mean (average) CCDF curve does not enter the exclusion region, then the repository meets the requirements of 40 CFR part 191.13.

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the cited *points* in this space. In practice, however, because a CCDF curve is constructed to be single-valued and non-increasing, a curve consistent with Eqs. 3 cannot enter the exclusion region. (As will be seen below, however, it is statistically possible for a site to be in compliance even if a small number of CCDF curves do enter the exclusion region.)

2. THE ROLE OF CCDF CURVES IN THE WIPP PA

The basic objective of the WIPP PA process, and of the associated CCDF mathematical formalism, is to assess WIPP's ability to contain TRU waste. The PA involves estimating the amounts of TRU waste that might be released inadvertently from the repository to the accessible environment over 10,000 years under a wide variety of possible site conditions and human intrusion scenarios. The principal objective of the PA is to show that the sum total of all such releases over that time period complies with the containment requirements specified in 40 CFR part 191. The PA does this by:

(1) considering the universe of all possible physical events that conceivably might occur within the repository;

(2) restricting this to a much smaller set of plausible release scenarios;

(3) calculating the likelihood that any of these scenarios will occur, and the severity of any consequences; and

(4) displaying the results (for the restricted set of plausible scenarios) in the form of CCDF curves, as required by 40 CFR part 194.34.

A CCDF curve combines information on the *probabilities* of occurrence for a set of release or contamination scenarios with an appropriate measure of the magnitudes of their *consequences*. The CCDF can then be compared with the requirements of the applicable regulations, at 40 CFR parts 191.13(a) and 194.31, which are expressed in the same general form.

2.1 Realizations and Futures

To conduct the WIPP PA, DOE must create a large number of realistic, representative scenarios that describe what might happen at the WIPP over the next 10,000 years, for a broad set of possible *realizations* (modeled physical conditions within and near the repository). DOE must then demonstrate that it meets the containment requirements. To this end, DOE performed its studies and submitted its CCA to EPA in October of 1996 (A-93-02, II-G-1). EPA intends to publish its assessment of it (including the PA) as a proposed amendment to 40 CFR part 194.

The PA may be thought of as describing two large, somewhat independent blocks of phenomena. The first involves the interlinked, long-term natural physical processes ongoing within and near the repository following its closure. An example of these processes are the buildup of gas pressure caused by the degradation of metals or organic materials in brine over time. The second block deals with possible *futures*, or sequences of short-term human intrusion events, that are likely to take place over the next 10,000 years. Factors involved in defining a future include the time of drilling of a borehole, and the activities in the waste drums that it strikes. The two blocks come together when a series of intrusions occur for the repository when it is in a specific physical state that is evolving over time (CCA, Section 6.1.2). With a single realization, the information content for 10,000 futures are condensed into a single CCDF curve; and the principal result of the PA is three sets of 100 CCDF curves each, produced by 300 different randomly constructed realizations.

A future is an outline of a plausible, hypothetical chain of events that is highly likely to

involve drilling and/or mining intrusion(s) into the repository region, and to lead to the release of radioactive materials to the accessible environment. An endlessly diverse range of futures can arise, because these independent events can occur at different times and parts of the repository, under different conditions, and involving different types and activities of wastes. A future may thus involve several events, each of which may be characterized in terms of the *stochastic* parameters, numerical values for which are selected in the mathematical construction of the future. These seven variables are: (1) the time of intrusion; (2) which panel was hit; (3) the probability of striking waste material (as opposed to passing through a salt pillar); (4) the activities of the wastes; (5) the likelihood of subsequent penetration of a pocket of pressurized brine in the underlying Castile formation; (6) the type of borehole plugging used after the drilling; and (7) when (if at all) mining occurred nearby. (CCA, Section 6.4.12; Note that "location of each drilling intrusion" in the CCA actually refers to two parameters, determining the geographical location of the borehole and whether the borehole intersected an excavated panel) Thus by sampling random ly of values for the stochastic variables, DOE creates a universe of 10,000 futures for each realization.

2.2 Consequences of Events and Futures: Releases

The consequences of a future depend not only on the details of the sequence of intrusion events, but also on the physical conditions and processes within the repository over that time period. The physical characteristics of the repository at different times are determined by the conceptual/mathematical models and computer codes representing the various processes ongoing, in general, and by the particular, specific set of *subjective* parameters, which are also obtained through random sampling. — i.e., the realization. The subjective parameters describe and control the possible modes of flow of gas and brine throughout and near the repository, and the transport of radionuclides to the outside world, as modeled by the WIPP PA computer codes. It should be noted that the distinction between stochastic and subjective parameters is not conceptually rigid, but it is generally useful in carrying out computations. This is true also for the separation of FEPs into short-term intrusion events and processes that govern the behavior of the repository over thousands of years.

The PA process thus consists largely of determining the relevant futures for any realization, the probabilities of those futures, and their consequences. As such, the outcome of a PA may be expressed as a set of ordered triplets,

$$\{[S_i, pS_i, cS_i], \quad i = 1, 2, ..., nS\} , \tag{4}$$

where S_i refers to the i-th intrusion Scenario or future; pS_i is its probability of occurrence; cS_i is a suitable measure of the likely consequences; and nS is the number of futures under consideration (see Section 6.1.1 of the CCA, Eq. 1). The set of futures used in the PA are assumed to comprise a sufficiently "complete" set. For the CCA PA, this means that a representative set of futures are included, and arranged such that their probabilities sum to unity. The consequences of the futures are expressed quantitatively in terms of the cumulative normalized release (nR). This measure of the activity of radioactive waste released, modified according to the total amount of TRU radionuclides present in the repository at the time of WIPP closure in 2033 A.D., provides a gauge of the expected long-term hazards of the various released radionuclides. The regulation at 40 CFR part 194.34 may be viewed as stipulating that any release for which $nR < 1$ is acceptable, and the occasional release with $nR > 1$ may be, too;

but in the latter case, there must be a less than 0.001 probability of any release with nR > 10 occurring.

2.3 Generating a CCDF Curve -- A Simple Example

The WIPP PA process consists of determining the set of all possible, relevant futures and estimating the corresponding probabilities and consequences. By 40 CFR part 194.34(a), "The results of performance assessments shall be assembled into complementary, cumulative distribution functions (CCDFs) that represent the probability of exceeding various levels of cumulative normalized release caused by all significant processes and events." The CCA PA involves production of three hundred realizations (three *replicates* of one hundred realizations each), and of the associated 300 CCDF curves. The WIPP CCDF curve for any single realization involves the examination of 10,000 futures, each of which involves a number of intrusion events. For a given realization, the CCDF curve shows, for any and every particular value of cumulative normalized release, nR, the probability that a future created at random would lead to a release higher than that value of nR.

A simple example may be helpful here. A fair die has equal probability of showing any integer from 1 to 6 when it is thrown, as recorded in the probability graph ("histogram") of Fig. 1a . For a fair die, the probability of finding any particular one of the six first integers face-up is 1/6, as indicated on the vertical axis of the graph. This fact may be apparent from its cubic, sixfold symmetry, or it may be learned by throwing a die, say, 10,000 times. The area under the histogram curve is 1, since there is absolute certainty that *some* integer between 1 and 6 will occur; that is, there is a 1 in 6 chance that a "1" will come up, 1/6 chance for a "2", and so on up through the "6", so the probability of seeing a "1" or a "2" or a "3", "4", "5", or "6" is {1/6 + 1/6 + 1/6 + 1/6 + 1/6 + 1/6} = 1. The value of the CCDF ranges from 1 to 0 as the face value shown by the die steps from 1 to 6, where special provision is made for k = 0. That is, it steps down by 1/6, starting from 1 at the far left, for every increment in the face value shown by the die. Thus the CCDF is just a graph of the probability that the number displayed on the tossed die will be *greater than* that number, Fig. 1b. Thus, a CCDF curve provides exactly the same information content that a relative frequency histogram or a probability distribution function does, but it presents it in a different form. (The perhaps more familiar *cumulative distribution function* (*CDF*) is *exactly* the same as a CCDF, except that it climbs from a value of zero at the origin to unity, rather than falling from 1 to 0.)

Table 1.
CCDF for a Tossed Die.

k	P[k]	P[n > k]
(0)	0	1
1	1/6	5/6
2	1/6	4/6
3	1/6	3/6

k	P[k]	P[n > k]
4	1/6	2/6
5	1/6	1/6
6	1/6	0

DOE defines the CCDF curve for WIPP in terms of a simple equation (their Eq. 3 in Section 6.1.1 of the CCA), and it may be useful to illustrate its meaning by way of our simple example. For our purposes, DOE's expression may be viewed as being is equivalent to

$$CCDF(k) = P[n > k] = 1 - \sum_{n=1}^{k} P[n] \quad . \tag{5a}$$

This refers to a set of possible phenomena (throws of a die, events, futures, *etc.*) that are labeled with the index n, and n can assume the values 1, 2, ... up through k. The term P[n] refers to the probability that the n-th phenomenon occurs. For our die, P[n] would denote the probability of finding any one of the six first integers face-up, where n = 1,2, ...,6. That is, P[3] refers to the probability that a tossed fair die will display a "3". The Greek sigma with the "n=1" below and the "k" above is a simple mathematical prescription in standard scientific notation that says to sum a specific group of terms together: Replace the n with a 1, and write down the result, namely P[1]; then do the same for n=2, then for n=3, and so on until (and including) n reaches the value k; then, add up all the terms. In general, Eq. 5a would look like

$$CCDF(k) = P[n > k] = 1 - \sum_{n=1}^{k} P[n] = 1 - \{ P[1] + P[3] + ... + P[k] \} \tag{5b}$$

For the particular case of the CCDF for a fair die, we know that

$P[n] = 1/6$ for $n = 1, 2,.....6.$

and

$P[n] = 0$, all other n. ,

and that the largest meaningful value for k would be 6.

In Eqs. 5, the probability, P[n > k, where k = 0, 1, 2,....6], that the number coming up, n, will be *greater than* any particular value, k , defines the complementary cumulative distribution function, CCDF(k), for the die, shown in Table 1 and as the CCDF curve, Fig. 1b. It was obtained by working through Eq. 5b one value of k at a time. Consider:
The probability of throwing a 7, 8, *etc.*, which is to say a number greater than 6, is zero:

$P[n > 6] = 0.$

The probability of the tossed die displaying a six is 1/6 — but by the definition of CCDF, we are

to express this as $P[n > 5]$, so

$$P[n > 5] = P[6] = 1 - \{P[1] + P[2] + P[3] + P[4] + P[5]\} = 1/6 ,$$

Likewise, the probability of throwing greater than a four is

$$P[n > 4] = P[6] + P[5] = 1 - \{P[1] + P[2] + P[3] + P[4]\} = 2/6 ,$$

and

$$P[n > 3] = P[6] + P[5] + P[4] = 1 - \{P[1] + P[2] + P[3]\} = 3/6 ,$$

on down to

$$P[n > 0] = P[1] + P[2] + P[3] + P[4] + P[5] + P[6] = 1 - \{0\} = 1 ,$$

revealing that the probability of finding a number greater than zero is unity.[2]

To relate the CCDF for the die to that of a CCDF curve for the WIPP, think of the six different possible ways (*i.e.,* physical outcomes) of tossing the die as corresponding (loosely) to six different, one-event release futures over the 10,000 years following its closure. The number showing face-up on the die is analogous to the numerical value of the consequence of the future, *i.e.*, the amount of TRU waste released, expressed in terms of the cumulative normalized release, nR. Finally, the probability of a particular integer coming up on the die corresponds to the probability of occurrence of the particular WIPP future. After exploring all six possible outcomes, the single CCDF curve for the die recorded the probabilities (along the ordinate, or vertical axis) that a number coming up will be greater than each of the various integer consequence values lying along the abscissa. One simple way to do this is just to toss a die 10,000 times and track the results. Likewise, by incorporating information on 10,000 (rather than 6) different possible futures, a single CCDF curve reveals the probability that the cumulative normalized release for a ten thousand-year future will exceed any particular nR value.

For WIPP, a probability distribution function would indicate the relative number of physical scenarios, or futures, corresponding to any particular value of the cumulative normalized release. The associated function CCDF(nR) would show the relative number of physical scenarios with a cumulative normalized release *greater than* any particular value, such as nR, as suggested by Fig. 6-3 of the CCA, p. 6-25. Alternatively, the relevant computer code (CCDFGF) tracks the cumulative normalized releases for all 10,000 futures of a realization, and uses them as the raw material for constructing a CCDF curve: The value of CCDF(nR) is

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[2] Since *one* of the first six integers *must* come up, with 100% assurance,

$$\sum_{n=1}^{6} P[n] = \{P[1] + P[2] + P[3] + ... + P[6]\} = 1 .$$

calculated for any nR by counting the number of futures that result in cumulative normalized release greater than nR, then dividing the count by the total of 10,000 futures.

The CCDF formalism incorporates an automated system for computing the probabilities of occurrence and for modeling the consequences of millions of different sequences of possible intrusion events, with hundreds of possible sets of physical conditions within the repository — and then integrating and displaying this information in a relatively simple, physically meaningful form. While it is possible to compare the calculated value of the cumulative normalized release with the regulatory limiting values on it of nR = 1 or 10 future by future, a CCDF curve can display the results of this comparison for 10,000 futures at the same time. It allows, in particular, full consideration of very low-probability futures (down to a lower-bound probability cut-off, for WIPP, of 10^{-4}) for which the cumulative normalized releases may exceed 1, or even 10. Also, a statistically meaningful 'average' curve can be created out of a family of CCDF's, and it is to such a 'mean' curve that the tests of compliance apply. In this manner, the CCDF curves of the PA and the containment requirements of §194.34 can be expressed in essentially the same graphical format, and directly compared, Fig. 2.

For the very simple case of the fair die, there is only one possible CCDF curve, that shown in Fig. 1b. In the WIPP PA, by contrast, there were 300 CCDF curves, and any one of them could assume an infinite variety of shapes. A single WIPP CCDF curve shows, for a specific set of physical conditions in the repository (*i.e.*, for a specific realization), and for any given value of cumulative normalized release from it, nR′, the probability that the release for an arbitrary future or scenario will exceed that value — that is, CCDF(nR′) gives P [nR > nR′]. To obtain one such function or curve for WIPP, it is necessary to calculate for the realization, and for a

Table 2.

Conceptual Hierarchy of the Principal Components of the CCA PA

Term	Hierarchy of Components of the CCA PA
event	single intrusion (e.g., drilling of borehole) defined by a single set of values for the 7 *stochastic* variables, randomly sampled by CCDFGF with Monte Carlo program
future	sequence of intrusion events occurring over 10,000 years
realization	production of single CCDF curve, making use of the outputs of the WIPP PA codes.
replicate	100 realizations; 3 replicates in the CCA PA, 3 more in the PAVT

sufficiently large set (*i.e.*, 10,000) of appropriate futures, $\{S_i\}$, the set of probabilities of occurrence of the futures, {P}, and the set of associated cumulative normalized releases, $\{nR_i\}$. (Each future, in turn, may involve tens of intrusion events over 10,000 years.) The differences among CCDF curves reflect uncertainties in what is known about the physical conditions at the repository, and lack of knowledge of future intrusions; therefore the PA involves not only the consideration of 10,000 futures for each realization, but also 300 realizations. Three replicates of 100 realizations each were carried out by DOE, involving three

million futures and approximately one hundred million intrusion events, resulting in a grand total of 300 CCDF curves. Some of the terminology used in the PA is shown in Table 2.

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U.S. Department of Energy; Compliance Certification Application for the Waste Isolation Pilot Plant, Carlsbad, NM.; U.S. Department of Energy; Carlsbad Area Office; October, 1996. [Docket A-93-02, II-G-1]

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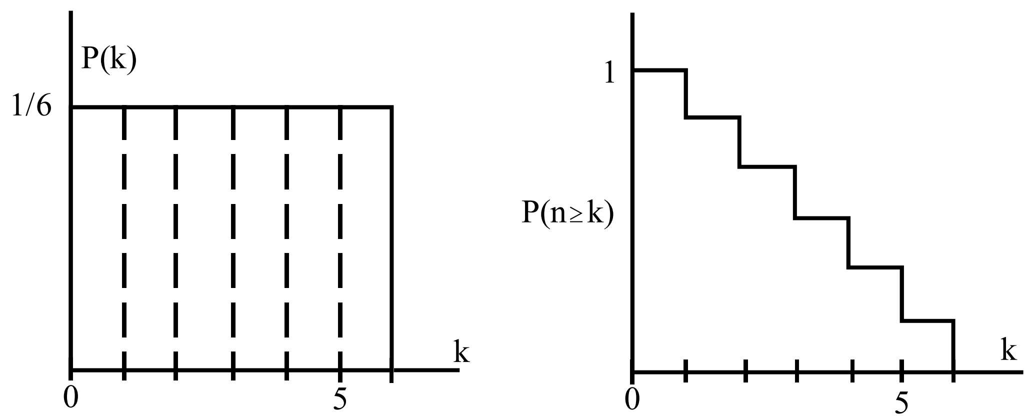
P(k)
1/6
k
0
5
1
P(n≥k)
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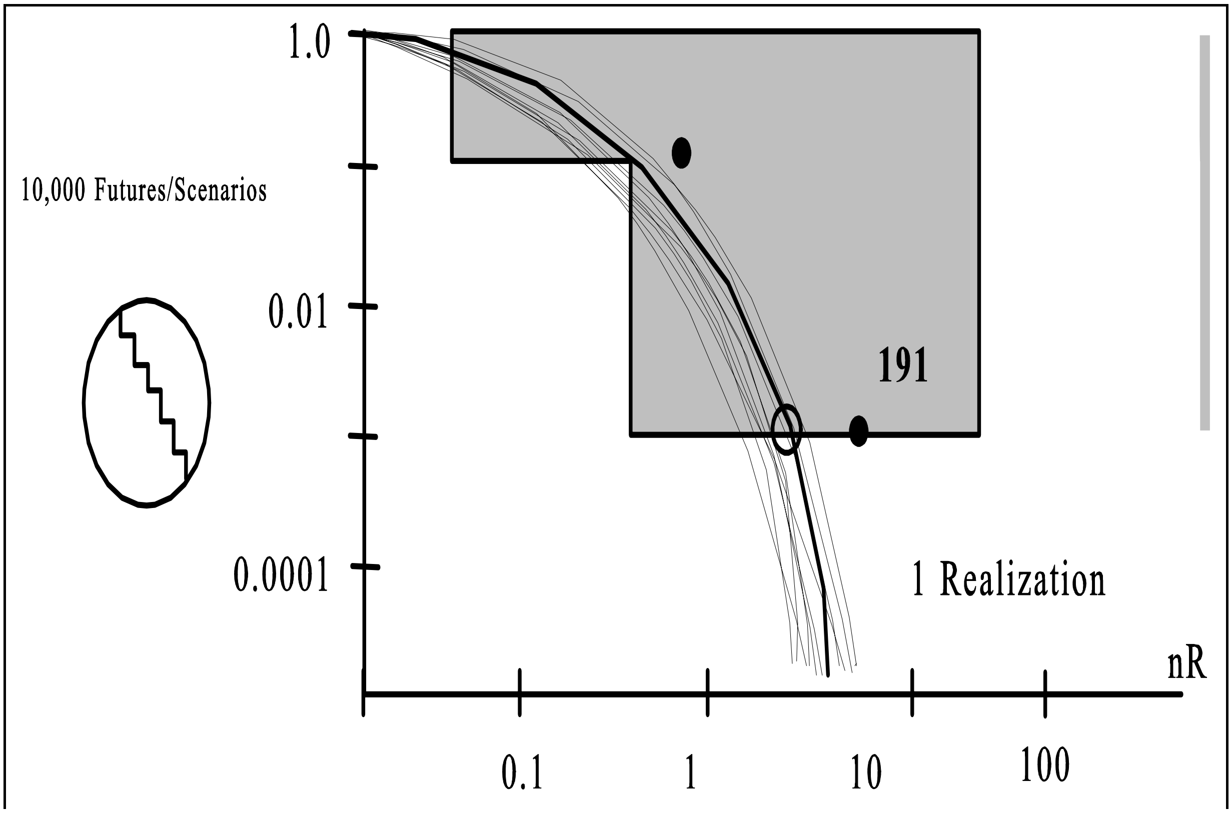

1.0
10,000 Futures/Scenarios
0.01
191
0.0001
1 Realization
nR
0.1
1
10
100