Factors Affecting Risk Predictions: Proposed Rule and Other Risk Metrics

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Abstract – *Risk predictions must meet regulatory requirements for the type of contamination at a site and are typically made based upon one or more performance metrics (e.g., peak-of-the-mean, mean-of-the-peaks, and cumulative release). A performance metric for a repository containing high-level radioactive waste at Yucca Mountain, Nevada, was proposed by the U.S. Environmental Protection Agency (EPA) in 40 CFR Part 197 [1] and the implementation of that proposed rule presented by the U.S. Nuclear Regulatory Commission (NRC) in 10 CFR Part 63 [2]. The proposed rule requires that compliance in the first 10,000 years be determined using the arithmetic mean of the dose estimates (i.e., peak-of-the-mean performance metric); while after 10,000 years, compliance is determined using the peak of the median of the dose estimates. The risk predicted by each performance metric may be affected differently by uncertainties and model biases. In a risk analysis, it is common to identify parameters that have the greatest impact on the performance measure (i.e., are the most sensitive) and devote resources to decrease their uncertainty. However, there are instances when decreasing the uncertainty can yield a higher estimate of risk, depending on the metric. These instances are counter-intuitive and result in unexpected outcomes that are known as "risk dilution." Previous analyses investigated the stability and accuracy of the peak-of-the-mean, mean-of-the-peaks, and cumulative release performance metrics in relation to the nominal risk at a range of uncertainties and model biases [3,4]. Stability of the risk metric relates to its behavior over a range of factors such as uncertainty, bias, and containment time. Accuracy of the risk metric is its ability to predict the nominal risk. These analyses concluded that the peak-of-the-mean metric provides the least stable and least accurate risk predictions, whereas the cumulative release metric is the most stable and the most accurate. The peak-of-the-mean metric also exhibits risk dilution (i.e., a decrease in the predicted risk with increased uncertainty). Additionally, these results illustrated how risk predictions made using what may be considered "conservative" assumptions can be moved in a direction that may or may not be expected or intended. This paper assesses the stability and accuracy of risk predictions determined using the proposed risk metric which is based on a peak of a quantile (i.e., the peak of the median dose estimates). These risk predictions are compared with results from the previous analyses which evaluated the peak-of-the-mean, mean-of-the-peaks, and cumulative release risk metrics. The differences between the behavior of the risk metrics at varying levels of model bias and uncertainty illustrate the impacts of a particular risk metric on evaluating performance of the disposal system. These results suggest how risk predictions for a metric are related to the actual or true risk from the site.*

I. INTRODUCTION

In this paper, we consider the case where risk assessments are performed by predicting a contaminant release, dose, or concentration in the environment as a function of time (a realization) and where uncertainty is assessed by running multiple realizations using different model input parameter values. The questions to be ascertained are: How should the results from multiple realizations released to the environment over time be simplified or summarized (averaged, summed, etc) to allow comparison with a regulatory dose, concentration, or release standard (the metric)? Given our current method of generating multiple realizations do some metrics provide more accurate and stable predictions of the actual risk? How does the accuracy and precision of the different risk metrics depend upon the amount of uncertainty in the models and/or the degree of bias in parameter selection? How is risk prediction changed by the longevity of the contaminants of concern?

The risk predicted by each performance metric may be affected differently by uncertainties and model biases. Previous analyses investigated the stability and accuracy of the peak-of-the-mean, mean-of-the-peaks, and cumulative release performance metrics in relation to the nominal risk at a range of uncertainties and model biases [3,4]. Stability of the risk metric relates to its behavior over a range of factors such as uncertainty, bias, and containment time. Accuracy of the risk metric is its ability to predict the nominal risk. These analyses concluded that the peak-of-the-mean metric provides the least stable and least accurate risk predictions, whereas the cumulative release metric is the most stable and the most accurate. The peak-of-the-mean metric also exhibits risk dilution (i.e., a decrease in the predicted risk with increased uncertainty). Additionally, these results illustrated how risk predictions made using what may be considered "conservative" assumptions can sometimes lead to an under prediction of risk.

With the exception of these analyses, there has not been a general quantitative analysis of risk predictions and factors that impact those risk predictions reported in the literature. Codell et al. [5] present a discussion of the sensitivity of risk predictions for the peak-of-the-mean metric. A number of studies discuss the importance of separating uncertainty and variability. These studies also offer examples of approaches to separate uncertainty and variability [6-11].

II. PERFORMANCE METRICS

Performance metrics from multiple realizations chosen for investigation in this work are cumulative release, the peak-of-the-mean, the mean-of-the-peaks and the peak of the 50th and 95th quantiles. The first three of these metrics are common and a performance measure based on a quantile has been proposed [1]. In this work, the peak-of-the-mean, the mean-of-the-peaks, and peak of quantile metrics are determined using release rates. However, these metrics could also be considered as measures of the dose rate since release rates can be converted to dose rates using a multiplicative factor that takes the ultimate use of the contaminated water into account (i.e., a dose model). Therefore, the results presented in this work for the performance metrics, which are determined from release rates, can be interpreted as risks.

An important consideration when evaluating risk metrics is that, in the presence of uncertainty, all of the metrics considered herein are nonphysical – none of them are predicted by the models to literally occur. When uncertainty is present, each realization is a prediction of one path which may occur in the future. When one travels to the grocery store to purchase a loaf of bread one may take many alternative paths from the door of one's house to the shelf holding the bread and then back – but if one only takes one trip to the store, only one of those possible paths is actually taken. An a priori probabilistic prediction of the trip might consider different exact pathways in each realization (e.g., had to change lanes around a stalled car), but the average of those possible pathways cannot physically occur in one individual trip. Likewise, a waste disposal site in actuality will have only one future path, we simply do not know exactly what that path will be.

II.A. Cumulative Release Metric

The cumulative release metric is determined by integrating the release from each realization over the time period of interest. This metric was applied to the licensing of the Waste Isolation Pilot Plant [12] and is most useful for calculating risk to populations over the compliance period, such as 10 CFR 60.

II.B. Mean-of-the-Peaks Metric

The mean-of-the-peaks is calculated by averaging the peak concentration from all Monte Carlo realizations. This metric is useful for regulations written in terms of the risk to any individual exposed to releases from the disposal system, regardless of the time at which the individual is exposed. This metric averages the peak doses, even though those peak doses may be widely spaced over time.

II.C. Peak-of-the-Mean Metric

The peak-of-the-mean is determined by calculating the mean concentration at each time step from all realizations and then selecting the peak of that calculated mean concentration over all time steps.

II.D. Peak of Quantile Metric

A quantile metric is assessed in this paper for the 50th and 95th quantile of concentration. At each time from all realizations, the 50th and 95th quantile is determined by finding the peak for the quantile over the entire simulation time. The 50th quantile (median) is selected because it is proposed as a performance measure at times greater than 10,000 years [1]. The 95th quantile is selected because it provides a perspective on the relationship between the proposed quantile (i.e., median) and the other performance measures for the cumulative release, mean-of-the-peaks, and peak-of-the-mean.

III. MODELING APPROACH

In order to facilitate the multiple probabilistic computer runs required in the analysis, a simplified conceptualization of a disposal system is employed that uses near-field containment, delayed release, and far-field transport factors. A FORTRAN computer program was developed and tested to simulate this conceptual model using Monte Carlo sampling of probability distributions for all model input parameters. The near-field factors are the time of container failure and the first-order release rate constant. Far-field transport factors are the groundwater travel time and retardation coefficient. These four factors are general and, because the factors are modeled stochastically, may be considered "lumped" parameters whose probability distributions encompass detailed processes. The simplicity of the model allows a clear demonstration of the behavior of risk predictions for the metrics without confounding effects from a more complicated model.

Risks at the receptor are calculated using a first-order release rate model. The released material is then transported to the exposed individual assuming plug flow, a retardation factor, steady flow, and a first-order reaction that could represent hydrolysis, biodegradation, or radioactive decay.

The general equation used to compute the risk at the receptor, $R(t)_{receptor}$, accounts for the near-field factors (k and t_{fail}) and transport factors (t_{gwtt} and r_d):

$$R(t)_{receptor} = 0 \quad for \quad t < t_{fail} + t_{gwtt} r_d \qquad (1)$$

$$R(t)_{receptor} = k\, e^{-k\left[t - \left(t_{fail} + t_{gwtt} r_d\right)\right]} e^{-\lambda t} \quad for\ t \geq t_{fail} + t_{gwtt} r_d \qquad (2)$$

where,

t	=	time [T]
k	=	release rate constant [1/T]
λ	=	decay constant (= $\ln(2)/t_{1/2}$) [1/T]
$t_{1/2}$	=	half-life [T]
t_{fail}	=	time of container failure [T]
t_{gwtt}	=	groundwater travel time [T]
r_d	=	retardation factor [ ]

The governing equation is confusing in the sense that we are comparing dose or health effect risk which is assumed to be proportional to concentration. Since all results are normalized relative to the nominal concentration, the relative concentration and thus dose is proportional to relative release. The release rate constant, container failure time, groundwater travel time, and retardation factor are sampled stochastically and used in Equations 1 and 2 to calculate $R(t)_{receptor}$. The means and the associated variances of these four parameters and model variables are assigned values in units based on a containment time. The containment time is defined as the sum of the mean time required for a container to fail and the mean time for the release to arrive at the receptor using the mean values for each parameter. The variables and parameters in Equations 1 and 2 are defined with respect to the nominal containment time [T] to make them non-dimensional. This approach allows the results to be interpreted in the useful context of the protection afforded by natural barriers and engineered barriers of the system.

The computer code automatically calculates the effect of contaminat lifetime by considering three ratios of contaminant half-life to the nominal containment time of the disposal system. The values are chosen as 0.1, 0.5, and 2.5 of the containment time. The half-life of 0.1 represents a “well contained” contaminant, because basically all of the contaminant decays or biodegrades (i.e., 10 half-lives) prior to being released into the environment. The contaminant with a half-life of 2.5 is classified as “poorly contained”, because there is little decay or biodegradation prior to being released into the environment.

Values of the four near-field and transport factors are also non-dimensionalized with respect to the containment time. Both near-field and transport factors are assumed to contribute equally and each delays the release by one-half of the containment time. Therefore, the mean container failure time is set at one-half of the containment time, while the mean groundwater travel time is specified as 0.05 of the containment time with a mean retardation factor of 10. Consequently, using mean values, the transport factors account for one-half of the containment time, since the transport travel time is the product of the groundwater travel time and the retardation factor.

Similarly, the mean value for the release rate constant is set at a value that results in 50% release at 0.25 of the containment time for a conservative (i.e., nondecaying) contaminant. This mean value of the release rate constant yields 75% and 94% releases at 0.50 and 1.0 of the containment time, respectively.

III.A. Nominal Case

For the simplified model presented in this paper, the nominal case is deterministic based on the mean values of the model parameters. The nominal case represents the “true” performance of the disposal system against which all results are compared and normalized. The disposal system could be modeled differently by representing multiple sources of release, multiple failure times, or multiple flow paths for transport. However, for simplicity and clarity the current model includes neither spatial nor temporal variability. Future work will consider both uncertainty and variability.

III.B. Bias and Uncertainty

The analyses account for model bias and uncertainty. The bias is specified with a factor that is multiplied by the mean value of the parameter. A factor that increases the container failure time, groundwater travel time, or retardation or that decreases the release rate constant is classified as a “nonconservative” bias, whereas a “conservative” bias is a factor that decreases the container failure time, groundwater travel time, or retardation factor and increases the release rate. Uncertainty is a lack of complete information for a parameter and is modeled as an increase in the variance. As more information becomes available (e.g., experiments are conducted), the uncertainty decreases and the variance of the parameter would also decrease. The “uncertainty” in a parameter is modified using a factor that is multiplied by its variance. A factor of zero corresponds to zero uncertainty.

All values calculated for a risk metric are normalized with respect to a nominal case. The nominal case is deterministic based on the mean values of the model parameters and represents the “true” performance of the disposal system.

III.C. Parameters Distributions

In this analysis, it is assumed that the nominal means of the parameters are known and a reference value for the variance is set to allow the variance (uncertainty) to be scaled in the calculations. Lognormal distributions are typical distributions for environmental data [13] and are utilized in risk assessments. Therefore, lognormal distributions are used in the Monte Carlo sampling conducted in this analysis. Table 1 provides the nominal mean and reference variances.

Uncertainty is modeled using a multiplicative factor that is applied to the reference variance; however, increasing the variance also increases the mean of the distribution. To ensure that when uncertainty (i.e., variance) increases, the arithmetic mean remains the same, the mean of the lognormal distribution is adjusted according to Bowen and Bennett [14].

For the distributions in Table 1, variances are assigned to ensure that, at three standard deviations less than the mean, the minimum bias together with the maximum uncertainty cases yield physically-feasible values (e.g., the retardation factor is not less than 1.0).

The distributions provided in Table 1 are input values for Equations 1 and 2. Monte Carlo simulations with 4,000 realizations were conducted and yield release rates at times from 0 to the maximum simulation time at time steps equal to 0.002 of the containment time. Convergence testing of this Monte Carlo analysis determined that 4,000 realizations was a reasonable number for convergence of these Monte Carlo results.

TABLE 1. Sampled parameter means and variances as a fraction of the compliance time, T.

Sampled Parameter	Distribution Type	Mean	Standard Deviation
Release rate constant [1/T]	lognormal	2.75	0.12
Container failure time [T]	lognormal	0.5	0.022
Groundwater travel time [T]	lognormal	0.05	0.0022
Retardation factor [ ]	lognormal	10.0	0.33

The maximum simulation time was 10 times the longest half-life (i.e., 25 times the nominal containment time). The nominal containment time was comprised of equal contributions from nominal values for the container failure time and the contaminant transport time. The contaminant transport time is the product of the groundwater transport time and the contaminant retardation factor.

Factors representing "bias" are multiplied by the means in Table 1. The 10 bias factors are 2.50, 2.03, 1.66, 1.35, 1.10, 0.90, 0.74, 0.60, 0.49, and 0.40. Similarly, factors representing "uncertainty" are multiplied by the variances (i.e., the square of the standard deviations in Table 1). The 11 uncertainty factors are 1.00, 2.09, 4.37, 9.15, 19.13, 40.00, 83.66, 174.97, 365.91, 765.25, and 1600.00.

Simulation output includes values from 110 sets of 4,000 realizations for each of the three performance metrics. These values are calculated over the simulation time and represent all possible combinations of the 10 biases and the 11 uncertainties. Additionally, the logarithm (base 10) of the ratio of the performance metric with respect to its nominal value is calculated over the simulation time. The nominal value represents reality and is defined as having no bias and zero uncertainty. Thus, a value of 1.0 is interpreted as a one order-of-magnitude overestimation of the nominal risk. Similarly, a value of -3.0 is interpreted as a three order-of-magnitude underestimation of the nominal or true risk.

IV. RESULTS

Simulation output is plotted and contoured in figures presented in this section with each colored square in the figure resulting from 110 simulations each having 4,000 realizations. To facilitate the explanation and interpretation of these figures, the following example is presented.

IV.A. Example: Interpretation of Plots

An example of simulation output is provided to help interpret the plots. In Fig. 1, the peak-of-the-mean performance metric using the lognormal distributions in Table 1 is shown for a poorly contained case. Labels for points A through F are added to this figure for purposes of this discussion and interpretation. The color legend at the top of the plot provides the base 10 logarithm of the ratio of the predicted risk divided by the nominal or true risk. A value of 2 is interpreted in the risk assessment as an over-estimation of the actual risk by a factor of 100. Negative values indicate that the risk from the site has been under-estimated.

Point A represents a simulation with low uncertainty and values for all means adjusted such that the release would be delayed (nonconservative bias). As expected, the nonconservative parameter bias causes the risk to be underestimated. Movement from point A to point B represents an increase in uncertainty assuming the same degree of bias. Along line segment AB there is a decrease in the predicted risk with increasing uncertainty or "risk dilution." That is, having limited information about the model parameters yields a prediction of lower risk for the disposal system even though the true risk has not changed. Line segments FC and ED behave similarly and show risk dilution.

Line segment FC represents increasing uncertainty at constant bias for the “no bias” case. No bias represents equal modeled mean values of the parameters and the nominal mean values. Line segments AB and ED also show increasing uncertainty at constant bias; however, the biases are “nonconservative” and “conservative”, respectively. A nonconservative bias represents the use of assumptions about the means of the parameter distribution that result in generally smaller and later releases, whereas a conservative bias represents the use of assumptions in parameter distribution means that result in generally larger and earlier releases. Movement vertically in Fig. 1, such as from points A to F to E or from points B to C to D, show an increase in the predicted risk. The predicted risk increases because the bias changes from nonconservative to conservative values for the parameter means.

Point F represents “no bias” and “low uncertainty”. The contoured value at the intersection of the vertical bias axis with line segment FC extended from point F is zero. Since the contoured values are the log10 normalized ratio of a risk prediction at a level of bias and uncertainty to the nominal risk, a value of zero indicates the predicted risk equals the nominal risk. This observation is expected since nominal risk is defined as the outcome for no bias and zero uncertainty.

It is important to note that Fig. 1 displays results for the peak-of-the-mean performance metric with lognormal parameter distributions when poorly contained. Not all results exhibit this behavior and show risk dilution.

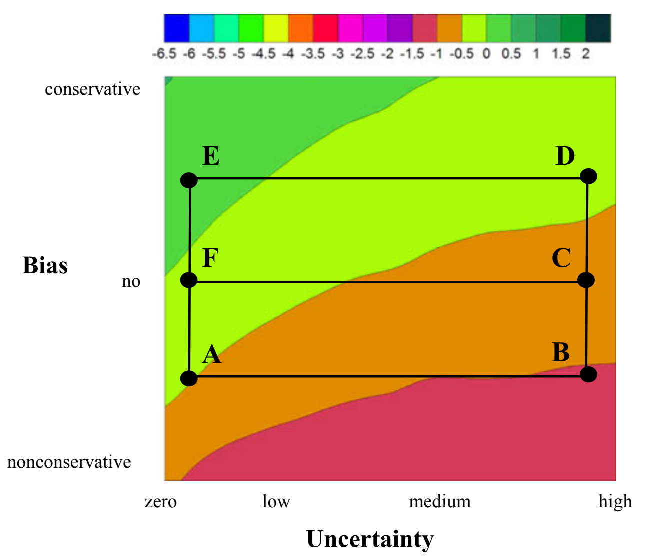

Fig. 1. Example of simulation results for the peak-of-the-mean performance metric using lognormal distributions with bias and uncertainty for all parameters showing the poorly contained case.

IV.B. All Performance Metrics

In Figs. 2(a) and 2(b), the results in Fig. 1 are expanded for points A and B to show the risk for a subset of the first 50 of the 4,000 realizations. Note that the values of the risk are not significant, only the relative values. The time variant risk is plotted as a function of the number of containment times ranging from 0.3 to 25. The mean risk and the peak-of-the-mean, mean-of-the-peaks, cumulative release, and peaks of the 50th and 95th quantile performance metrics for those 50 realizations are also presented. The relationship between time variant risk for each realization, the mean risk, and the performance metrics is illustrated in Figs. 2(a) and 2(b). The relationship among the performance metrics is also shown. Figs. 2(a) and 2(b) utilize the same scales for the horizontal axis, which facilitates comparing the results.

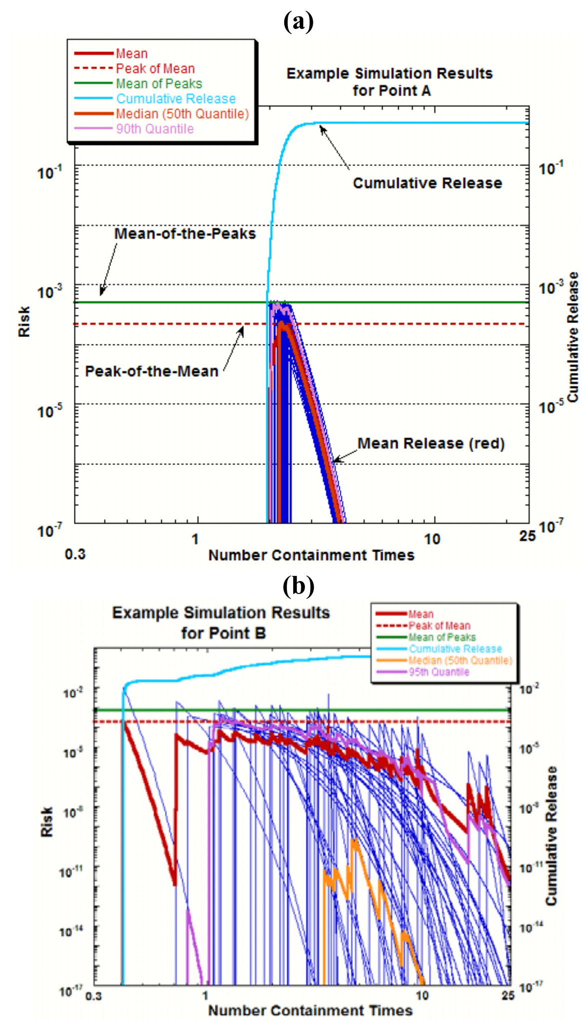

Fig. 2. Results for (a) point A and (b) point B from 50 realizations in Fig. 1 showing the mean release, peak-of-the-mean, mean-of-the-peaks, cumulative release, and 50th (median) and 95th quantiles.

The difference between Point A and Point B is the uncertainty. Point A models "low" uncertainty, whereas Point B models a "high" uncertainty. The biases for Points A and B are the same and represent a "nonconservative" bias. In both figures (although it is more apparent in Fig. 2(a)), releases begin at about two containment times. This time corresponds to the "no bias" mean time of release (i.e., 1.0 containment times) multiplied by the bias factor of 1.66.

Risks are significantly more variable for Point B, where uncertainty is "high", than for Point A, where there is "low" uncertainty, as evidenced by the saw-tooth pattern for the Point B mean risk. The peak-of-the-mean for Point B is entirely determined by one realization with an early release rate. Although it is difficult to observe in Fig. 2(a), because of the relatively narrow ranges of release rates, a number of realizations contribute to the peak-of-the-mean for Point A. Comparing Figs. 2(a) with 2(b) illustrate how increasing uncertainty increases the separation between individual peak risk. This increased separation yields a lower peak-of-the-mean risk that is mostly determined by the peak for the largest individual realization since the other peaks are not superimposed. This example shows how increased uncertainty, which is often characterized as a "conservative" assumption, leads to a decrease in the predicted risk or "risk dilution".

The mean-of-the-peaks in Figs. 2(a) and 2(b) is greater than the peak-of-the-mean because the time that the peak occurs is irrelevant for this metric. Risks plotted in Fig. 2(b) display this dominance. The difference between the mean-of-the-peaks and the peak-of-the-mean is greater for Point B than for Point A because the former metric is insensitive to the time of the peaks, while the latter is sensitive. Note that if the peak releases all occurred at the same time, the mean-of-the-peaks and the peak-of-the-mean would be equal.

The cumulative release utilized the same scale as the release rates. Comparing the cumulative release metrics in Figs. 2(a) and 2(b) reveals a stability that is not dominated by release rates from individual realizations (i.e., there is no saw-tooth pattern in the individual release rates) even though the uncertainty changes from "low" to "high". This is in contrast to the peak-of-the-mean metric which is dominated in this case by a single realization and to some extent to the mean-of-the-peaks metric shown in Fig. 2(b) that appears to be determined by about five relatively large realizations. These results suggest that the cumulative release metric is the most stable of these performance metrics.

IV.C. Risk Predictions for Each Risk Metric

Simulation results are presented in Fig. 3 as separate rows for the peak-of-the-mean, mean-of-the-peaks, cumulative release, and peaks of the 50th quantile and 95th quantile performance metrics. The three columns represent different values for the degree of containment. Within each plot, the bias and uncertainty are changed to reflect the analyst's understanding of the appropriate parameter values for the disposal system as labeled on the lower left plot.

The results in these plots demonstrate risk predictions relative to nominal (actual) risk. The ideal situation would be where the predicted risk was independent of uncertainty and matched the bias. Each column of plots has a different value for nominal risk because the columns represent a different degree of containment. Poorly contained systems occur when the contaminant either does not degrade (e.g., a heavy metal) or degrades very slowly. The peak-of-the mean results in Fig. 3 exhibit all of the following: (1) risk dilution (i.e., a positive slope in the contour); (2) an increase in the predicted risk with increasing uncertainty (i.e., a negative slope in the contour); and (3) no change in the risk prediction with different degrees of uncertainty (i.e., zero slope in the contour, the preferred behavior). These results indicate the instability of the peak-of-the-mean performance metric at different levels of containment.

The mean-of-the-peaks results are comparatively more accurate than peak-of-the-mean results and do not show risk dilution. At lower levels of uncertainty the mean-of-the-peaks are flat (do not change with uncertainty) and accurately reflect conservative and nonconservative biases in the parameters. At higher uncertainty the peak-of-the-mean results develop a negative slope, meaning the metric tends to over-estimate risk when uncertainty is high. This tendency is consistent with the preferences of most analysts (i.e., make accurate predictions whenever possible but if uncertainties are great, over-estimate the risk).

At most locations the cumulative release metric provides more accurate predictions than either peak-of-the-mean or mean-of-the-peaks. However, for poorly contained systems, risk dilution is predicted at high uncertainty.

V. CONCLUSIONS

This work characterizes behavior of the proposed performance metric based on a peak of the quantile (50th quantile or median) in relation to other performance measures of peak-of-the-mean, mean-of-the-peaks, cumulative release, and peak of the 95th quantile.

The analysis utilizes a highly simplified model with lumped parameters for each of the major components of confinement, release, and transport. The following observations can be drawn from this work:

- Both the peak-of-the-mean and peak median tend to underestimate risk and be subject to risk dilution

- The peak median is subject to greater risk dilution than the peak-of-the-mean
- The mean-of-the-peaks or a higher quantile (peak of the 95th quantile) reduces risk dilution and underestimates the true risk
- When uncertainty is present, current methods of risk assessment may underpredict risk even when conservative parameters are chosen.
- Metrics currently not in vogue, such as mean of the peaks and peak of 95th or higher quantiles provide more accurate risk predictions, usually without causing risk to be overestimated.

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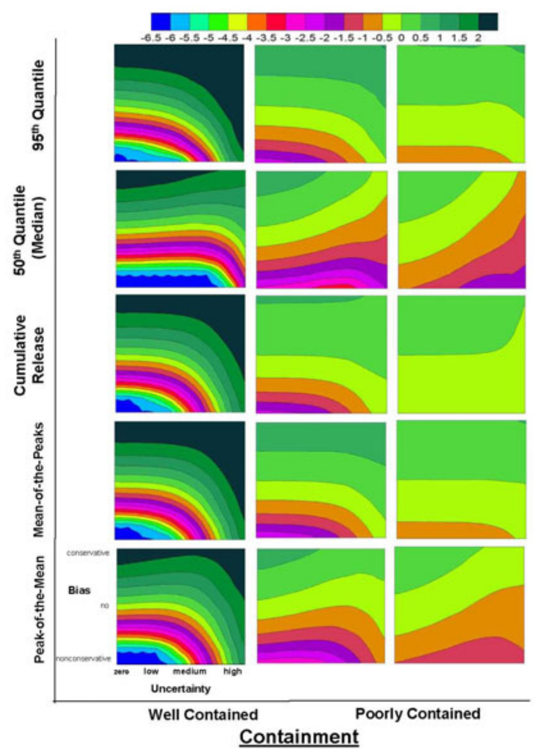

Fig 3. Simulation results showing the peak-of-the-mean, mean-of-the-peaks, cumulative release, and peaks of the 50th (median) and 95th quantiles with varying bias and uncertainty over a range of containments.