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Framework for risk-informed decisions beyond point estimates: statistically rigorous Monte Carlo methods for heavy-gas dispersion uncertainty analysis

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Accurate modelling of toxic dispersion for denser-than-air gases is inherently complex, where atmospheric variability intersects with dense-gas dynamics. The SLAB model offers an optimal balance of physical fidelity, coupling mass, momentum, energy, and species conservation equations, with computational efficiency. Prior uncertainty analyses within Quantitative Risk Analysis often rely on simpler dispersion models or lack rigorous statistical validation tests for Monte Carlo-based uncertainty propagation, sacrificing accuracy and reliability in high-stakes assessments.

This contribution presents a computationally robust Uncertainty Analysis (UA) framework tailored to Quantitative Risk Analysis for a catastrophic ammonia tank rupture scenario, emphasizing input uncertainties rising from practitioner assumptions and site-specific variability. Leveraging Monte Carlo methods for nonlinear, high-uncertainty propagation, our approach addresses a key gap in dispersion risk modelling UA: the rare application of rigorous convergence tests. We implement the Law of Large Numbers-guided Maximum-to-Sum plots to verify stability of output moments, namely the mean and the variance, ensuring dependable estimates even under fat-tailed distributions, adding essential scientific rigor to Monte Carlo applications in risk analysis and mitigating sampling-driven variability that can lead to unreliable results. The methodology features a sampling and uncertainty propagation scheme that integrates several stability classes, capturing atmospheric variability beyond discrete scenarios.

The resulting analysis guarantees consistency of Monte Carlo outputs and delivers statistically robust toxic concentration uncertainty estimates. This framework enables insightful interpretation for risk thresholds and regulatory decisions, reinforcing risk-informed decisions beyond the traditional single-point estimates.

Keywords: Dense-gas Dispersion, Quantitative Risk Analysis (QRA), Monte Carlo, Uncertainty, Convergence Analysis.

1. Introduction

Quantitative Risk Analysis (QRA) is a key methodology in process safety, as it provides a systematic and quantitative evaluation of risks associated with engineering activities. However, it is also known for its associated uncertainties, from the aleatory characteristics of variables affecting accident development, e.g., weather conditions, to the reliability of the models employed and the numerous assumptions needed to run the analysis.

These uncertainties challenge the common practice of representing QRA outcomes as single-point estimates. The limitations of such representations have been repeatedly discussed in the literature (e.g., Abrahamsson, 2002; Rae et al., 2014). A single numerical value, while appearing definitive and providing a – false – sense of accuracy, hides the inherent uncertainties in the analysis and can lead to inadequate process safety-related decision-making. This is further supported by the substantial variability in QRA results reported in several historically conducted benchmark studies, for example, by Fabbri and Contini (2009). In light of the variability of QRA results observed across these studies, it is natural to consider the implications of using single-point estimates as absolute truth for the result of a risk analysis. The repercussions of an underestimation of the risks associated with industrial or chemical facilities are quite evident, given that it might lead to insufficient implementation of safety measures or affect risk acceptance decisions, resulting in under-protection of the population, workers, and the environment. However, an over-conservative estimation of risk can also be detrimental owed to poor decision-making due to limited resources (Abrahamsson, 2002) or drive excessive expenditure due to unnecessary protective actions (Abdo et al., 2017).

Among the different components of QRA, consequence modelling plays a key role in shaping overall risk estimates and is a major source of uncertainty. In particular, dispersion modelling directly influences predicted exposure levels and therefore the estimated severity and extent of accident consequences.

In this context, heavy-gas dispersion modeling is one of the key phases in QRA calculations for evaluating the potential consequences of a loss of containment (LOC). As part of consequence modeling in QRA, it enables the estimation of concentration profiles of hazardous substances in air. These concentrations can have harmful effects due to the flammability and/or toxic characteristics of the released substances. Knowledge of airborne concentrations thus serves as an indicator of the potential damage a LOC can cause.

The phenomena governing dense cloud dispersion are more intricate than those represented by conventional Gaussian models for neutrally buoyant gases, leading to the development of numerous models with varying levels of completeness and complexity (Markiewicz, 2012).

To address dispersion modelling uncertainties, different approaches within the fields of risk assessment and environmental sciences have been explored, including interval analysis, fuzzy arithmetic, and probabilistic methods, among others. Comparative studies of Uncertainty Analysis (UA) methods in QRA and dispersion modelling (Abdo et al., 2017; Abrahamsson, 2002) have reported that Monte Carlo (MC) methods – also termed in literature as probabilistic approach – are the most commonly used and widely accepted as reliable. These, based on the principles of the Law of Large Numbers (LLN), stand out as a suitable framework for capturing epistemic (knowledge-related), and most particularly, aleatory (inherent variability) uncertainty and dealing with complex problems (Sin and Espuña, 2020). However, their computational expense stands as a major limitation and has prompted exploration of more efficient alternatives.

Despite their proven effectiveness, MC-based UAs have predominantly been applied to Gaussian dispersion models (e.g., Hanna 2007; Abdo et al., 2017; Abrahamsson 2002), with limited exploration in accidental scenarios involving heavy-gas dispersion, likely due to the higher computational demands these models require. These studies typically explore uncertainties in meteorological data, e.g., wind speed, and the surrounding area characteristics, e.g., surface roughness uncertainty. A frequent limitation in these studies is that uncertainties are often explored separately for each atmospheric stability class. Furthermore, existing studies typically do not employ convergence analysis to verify statistical rigor, omitting an essential step for the validity of the MC methods applied.

The main goal of this work is to provide a robust MC-based UA framework making use of convergence analysis for statistical rigor verification aimed at its use within QRA. Hence, it addresses typical QRA practitioners' assumptions and uncertainties. Additionally, it incorporates the simultaneous analysis of several stability classes for denser-than-air dispersion. To the best of the authors' knowledge, no UA analysis on the SLAB heavy-gas dispersion model using MC methods with convergence analysis has been carried out to date.

An exemplary case study is implemented with the aim of showcasing the significance of the proposed framework. The case study, based on a pressurized tank of ammonia, and the SLAB heavy-gas model are described in Section 2. Followingly, the core aspects of the proposed framework are explained. These include the characterization of the input uncertainties, estimating corresponding probability distributions for each of the inputs through available data or engineering knowledge, the propagation of the characterized uncertainties through the MC methods and the use of convergence analysis as a necessary inspection of methods validity. Last, results for the UA are reported, including the characterization of the obtained distribution for the uncertain output of interest – airborne ammonia concentration – and its relevance and implications for QRA-related models are outlined.

2. Heavy-gas dispersion modeling

2.1. *Catastrophic ammonia tank rupture scenario*

Ammonia is one of the fundamental constituents in the chemical industry, and its storage is, therefore, a conventional practice across different sectors from agriculture to the pharmaceutical industry and – more recently – as a fuel and hydrogen carrier within emerging low-carbon energy systems. The UA framework is thus showcased with a hypothetical case study based on a vertical pressurized ammonia tank of 500 m^3 total volume, in which the instantaneous release of the full contents of the tank occurs. The facility and tank are assumed to be located in the vicinity of Copenhagen, and site-specific weather variability due to the weather will thus be characterized for this particular region.

Ammonia hazards include its high toxicity and flammability. In this particular case study, the main hazard to be studied is its toxic effects on people, since its consequences are usually more severe than those related to its flammability.

The conditions of ammonia inside the tank are determined based on the local ambient temperature and the filling degree. The vapor saturation pressure is calculated using the Antoine equation, and the total mass of ammonia contained in the tank, m_{tank}, subsequently determined considering the volumetric filling degree, the total tank volume, the liquid density and the calculated gas density assuming ideal gas behavior. This characterization of the tank state and, hence, of the source term – the mass inside the tank instantaneously released – provides the necessary input for subsequent flash evaporation and dispersion models.

The flash evaporation of ammonia due to rapid depressurization forms an aerosol assuming no pool formation. The applied model for flash evaporation assumes adiabatic partial flash-vaporization of the liquid, lowering the temperature to the normal boiling point, where the fraction of the vaporized liquid is defined by:

$$f_v = \frac{m_v}{m_{tank}} = \frac{C_p \cdot (T_0 - T_b)}{\Delta H_v} \tag{1}$$

Being m_v the vapor mass, m_{tank} the total mass in the tank being released, C_p the heat capacity of the liquid, T_0 the temperature of the liquid before depressurization, i.e., the ambient temperature, T_b the normal boiling point of ammonia and ΔH_v the heat of vaporization (Crowl, 2019). The model in Eq. (1) assumes constant physical properties of the substance over the whole temperature range. The initial dimensions of the resulting denser-than-air cloud are approximated, assuming a hemispherical shape following industry consequence modelling standards (RIVM, 2005), to calculate the base area, AS, of the cloud and then calculating its height, HS, assuming it is a vertical cylinder as required for the puff dispersion in the heavy-gas model.

The formed cloud is constituted by an aerosol, and for this reason, it will behave as a denser-than-air cloud, despite having a low molecular weight. This behavior is represented by the SLAB model (Ermak, 1990). Values for the properties of ammonia are taken from the NIST Chemistry WebBook (National Institute of Standards and Technology, 2025).

2.2. *The SLAB model for heavy-gas dispersion*

The SLAB model is a one-dimensional, shallow-layer model classified by Markiewicz (2012) as an intermediate-complexity tool. Serving as the foundation for the Joint Research Centre's ADAM (Accident Damage Analysis Module) software, this system of coupled Ordinary Differential Equations (ODEs) is capable of simulating primarily dense and but also buoyant gas releases. Unlike simpler neutrally buoyant models, SLAB utilizes mass, momentum, energy, and species conservation equations to account for complex phenomena. These include turbulence damping, ambient velocity field alterations, ground heating, air entrainment, and the thermodynamic impacts of two-phase releases involving liquid droplet formation and evaporation (Ermak, 1990). The SLAB model offers a balanced middle ground between the advantages and disadvantages of simple integral models and the highly complex Computational Fluid Dynamics (CFD) models for heavy-gas modelling. It is less empirical and more robust than integral models, with the advantage of providing reduced run-time in comparison to CFD models, while allowing for realistic representation of the behavior of denser-than-air gas releases.

3. Uncertainty analysis methodology

3.1. *Input uncertainty characterization*

As already mentioned, many assumptions need to be made so as to provide input to the QRA calculations. These can be of diverse nature and origin. The dominant source of uncertainty analyzed in UA of dispersion models is the stochastic character of atmospheric conditions. In this regard, the uncertainties for the different considered weather-related inputs in this work, namely ambient temperature, wind speed, cloud cover – with discrete values between zero and ten –, and relative humidity, are characterized by using recorded data of meteorological conditions in a weather station located in the vicinity of Copenhagen (Danish Meteorological Institute, 2025). Data for 2024 is extracted, collected, and analyzed to fit adequate distributions to the given data. The most appropriate fits to the distributions are selected according to the nature of the input and the tendency of the data, e.g., skewed or symmetrical, and the parameters defined using available distribution-fitting tools. The resulting characterization of input distributions can be seen in Table 1. The data, and hence the simulations, are limited to day conditions, with the aim of analyzing several Pasquill stability classes, A to D, while maintaining physically feasible and realistic weather conditions.

Facility characteristics, such as the tank filling degree and the surface roughness, are also estimated for QRA. While the accepted practice in QRA is to assume the maximum filling degree as a result of the worse-case scenario approach, in practice, there is no certainty on the exact filling degree of a tank that is operationally fluctuating due to substance loading and unloading. Ideally, the uncertainty in the filling degree should be characterized by fitting operational data to a distribution. Given the hypothetical nature of the case study in this work, the filling degree

Table 1. List and characterization of uncertain inputs. LB and UB stand for Lower Bound and Upper Bound for uniform distributions, and Greek letters refer to distribution-specific parameters.

Input	Distribution	Fitted parameters
Ambient temperature	Normal	μ = 12.994 (°C); σ = 6.639 (°C)
Tank filling degree	Beta	α = 6; β = 3; [$\cdot$100 (%)]
Wind speed	Weibull	λ = 5.870 (m/s); k = 2.311
Cloud cover	Discrete	P(X=0) = 0.3; P(X=1) = 0.06; P(X=2) = P(X=3) = 0.16; P(X=4) = 0.04; P(X=5) = P(X=6) = 0.03; P(X=7) = P(X=8) = 0.019; P(X=9) = 0.15; P(X=10) = 0.32 (-)
Relative humidity	Normal	μ = 74.115 (%); σ = 14.549 (%);
Ground roughness	Uniform	LB = 0.0002 (m); UB = 3.0 (m)
Liquid heat capacity	Uniform	LB = 75.993 (J/mol$\cdot$K); UB = 82.125 (J/mol$\cdot$K)
Vapor heat capacity	Uniform	LB = 38.896 (J/mol$\cdot$K); UB = 55.394 (J/mol$\cdot$K)
Heat of vaporization	Uniform	LB = 22.7 (kJ/mol); UB = 23.5 (kJ/mol)

uncertainty is modeled using a left-skewed beta distribution – where the value of first shape parameter, α, is higher than that of the second shape parameter, β –, reflecting operational realities where tanks are typically maintained above 50% capacity to maximize storage efficiency. This uncertainty, oftentimes overlooked, can have an impact on the calculated risk because of its direct relation to the released mass. With regards to surface roughness, it is common practice to assume one roughness for all the areas surrounding the studied facility. This is an oversimplification of the environment, where, depending on the wind direction, the characteristics of the terrain where the dispersion of the toxic substance takes place might change. To account for these situations in a theoretical exercise, the full feasible range of surface roughness according to Casal (2017) is considered in the UA.

Last, uncertainties related to the substance properties are also incorporated into the analysis. Though thoroughly studied, the accuracy with which we can estimate the exact value of some specific properties in an accidental scenario is limited. For example, as previously stated, the model used for flash evaporation assumes that the substance possesses constant physical properties. This entails that, for properties such as the liquid heat capacity that exhibits temperature-dependent variability, a reference value must be selected, i.e., yet another assumption needs to be made in order to complete the modelling of physical effects within QRA. The same applies in the case of the vapor heat capacity, which is required as input to the heavy-gas dispersion model. These represent additional sources of uncertainty, which are incorporated into the current analysis by using ranges of the heat capacities for each phase corresponding to the scenario's minimum and maximum temperatures, -34.15 °C to 29.65 °C, as retrieved from the NIST Chemistry WebBook (2025).

Aside from these temperature-dependent associated uncertainties, other substance properties can be inherently uncertain due to fundamental human and scientific limitations to estimate certain values with precision. In some cases, there is a lack of consensus among values reported in literature, and even when consensus exists, the reported values are typically presented with an associated error margin. For this reason, the heat of vaporization is also included as a source of uncertainty in the study utilizing reported values from NIST.

3.2. *Uncertainty propagation methods*

Input-to-output uncertainty propagation is made by means of the Monte Carlo methods. N = 10,000 MC samples are drawn from the different defined uncertain input distributions, making use of the stratified sampling strategy Latin Hypercube Sampling (LHS) with truncation to enhance input coverage and confine sampling to the empirical domain defined by the data, ensuring methods feasibility. Simulations following the scheme provided in Fig.1 and making use of the above-explained models, provide as a final uncertain output the one-hour time-averaged airborne ground level concentration of ammonia at 200 m downwind of the release point. This particular output is selected because it can be directly used as a risk indicator and compared to standard thresholds for toxic exposure, such as the Emergency Response Planning Guidelines (ERPGs).

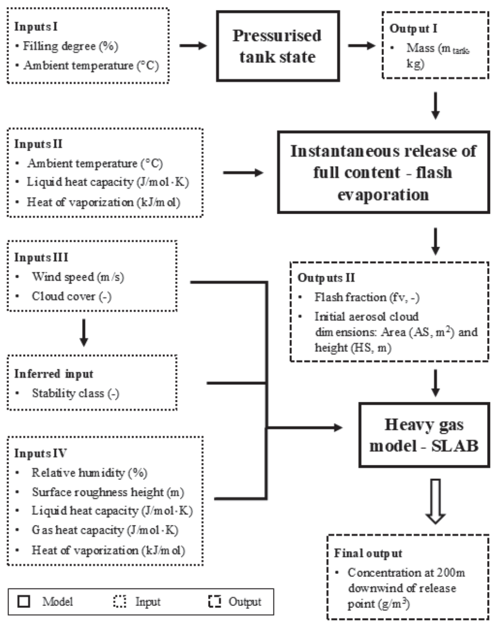

Fig. 1. Monte-Carlo simulations scheme.

Simulations were run for approximately eight hours on a PC with an Intel(R) Xeon(R) w7-2595X (26 cores, 52 threads, 2.81 GHz), 256,0 GB 4800 MT/s RAM, and 1,9 TB NVMe SSD, running MATLAB R2022b in Windows 11.

3.3. *Convergence analysis: incorporating statistical rigor*

Verification of the stability of the moments of an output distribution is essential to guarantee the reliability of the UA results. The MC methods possess inherent random characteristics, and convergence tests are pivotal for mitigating their effects on the characterization of the UA results.

In practice, if convergence is not ensured through an appropriate number of N, two different sets of MC simulations can yield different output sample characteristics. For instance, repeating the same experiment with different random number seeds for sampling can produce different means for the same output distribution studied. This is particularly critical for fat-tailed distributions, e.g., lognormal. Hence, the convergence analysis methods presented next ensure compliance with the fundamentals of the LLN in the usage of MC methods.

Two main indicators are used for this purpose: the MC error and the Maximum-to-Sum (M/S) plots method. The MC error serves as a preliminary indicator of the convergence of the MC methods, showing whether the number of MC samples, N, in a particular MC setup is sufficient or not. The implementation in Eq. 2, which uses the sample variance s approximates the population variance σ is further normalized through the sample population mean to convert it to a percentage that can be more clearly evaluated against an error acceptability threshold, which is recommended to be below one percent.

$$MC_{error} = \frac{\sigma(f)}{\sqrt{N}} \approx \frac{s(f)}{\sqrt{N}} \quad (2)$$

The M/S plots are graphical tools that complement the use of the MC error. The method, based on the Law of Large Numbers (LLN), examines the contribution of extreme sample values on a distribution's four statistical moments – namely, mean, variance, skewness, and kurtosis. It defines that, as shown in Eq. 3, for each of these moments, p, the ratio, R, between the maximum value, M, and the sum of the values, S, in a sample will converge to zero as the number of random variables in the sample, n, increases.

$$R_n^p = \frac{M_n^p}{S_n^p} \rightarrow 0 \; for \; n \rightarrow \infty \quad (3)$$

Making use of this approach, statistical consistency of the UA can be secured, more importantly, when fat-tailed distributions are involved in the MC analysis (Sin, 2024).

4. Results and discussion

4.1. *Uncertainty analysis results*

The output distribution obtained through the UA is illustrated in Fig. 2, including the probability density function (PDF) and survival function – defined as the inverse of the cumulative density function ($1 - CDF$). The interpretation of the survival function is valuable for the understanding of the degree of (un)certainty with which we are estimating a value. For example, to answer the question: With which degree of certainty can we affirm that owing to this event a specific threshold will be surpassed $P(C > c)$?

The results indicate a mildly fat-tailed distribution; while the majority of values are concentrated within the range of zero to five, the presence of strong outliers indicates a departure from standard normality. This characteristic is further reflected in the positive skewness of the distribution, as shown by the estimation of a higher sample mean, $\bar{y}$, and median, $\tilde{y}$, in Table 2.

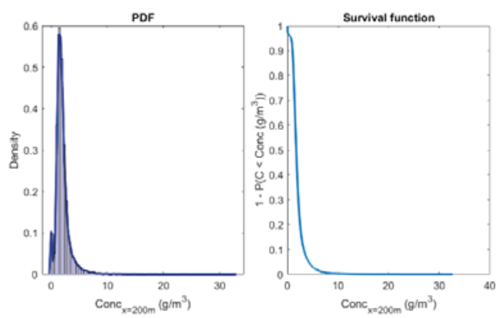

Fig. 2. Probability density function (PDF, left) and survival function ($1 - CDF$, right) of the obtained sample for concentration output.

Table 2. Output distribution characterization

Mean, $\bar{y}$ (g/m^3)	Median, $\tilde{y}$ (g/m^3)	Standard deviation, s (g/m^3)	95th percentile (g/m^3)	MC error (%)
1.9767	1.7198	1.3209	4.1759	0.6682

In this analysis, the $\tilde{y}$ is interpreted as the "best estimate" – resembling the single-point estimate it is commonly utilized –, while the 95th percentile provides a conservative perspective by means of a one-sided 95% confidence interval for the risk indicator. This upper confidence interval can provide a solid reference value for compliance criteria, for example, if a concentration should not exceed a certain value, the 95th percentile should not be higher than this specific value. The ERPG-3 threshold is 1500 ppmv (approximately 1.09 g/m^3 using average conditions for the scenario), which notably falls below both the mean and the median. The probability in this case of surpassing this particular threshold is $P(C > 1.09\ g/m^3) = 86.37\%$ This value confirms that, within the modeled scenario, a one-hour exposure for any individual at the studied location is highly likely to result in life-threatening effects. In this particular case, both the mean and the 95th percentile prominently exceed standard thresholds.

4.2. *Convergence analysis results*

In order to validate the statistical consistency of the results, a convergence analysis was conducted on the first two moments (mean and variance). These are the basic metrics for characterizing distributions and, further, provide a robust foundation for derived sensitivity analyses.

As illustrated in Fig. 3, outputs derived from simpler models demonstrate relatively rapid convergence, stabilizing at approximately 100 MC simulations. In contrast, Fig. 4 shows that more complex models – specifically those incorporating heavy-gas dynamics and the use of nonlinear, ODEs-based, models – exhibit significantly slower convergence, needing around 10,000 MC simulations to stabilize. This behavior is linked to the model's complexity; as models become more exhaustive, they might yield more outliers, resulting in mildly fat-tailed distributions that are highly sensitive to sampling-driven variability.

Demonstrating convergence is vital because it confirms that the obtained sample is an adequate representation of the true population. For smaller sample sizes, the behavior of the desired output might be inadvertently misrepresented, as the mean, median and percentiles – on which safety decisions rely – can fluctuate from one MC simulations run to another. In the present case study, as already mentioned, the risk-compliance criterion – surpassing ERPG-3 level – is clearly unacceptable. However, in situations where the threshold lies closer to the central tendency measures, the inaccurate estimation of these statistics can critically influence decision-making, particularly when dealing with fat-tailed distributions.

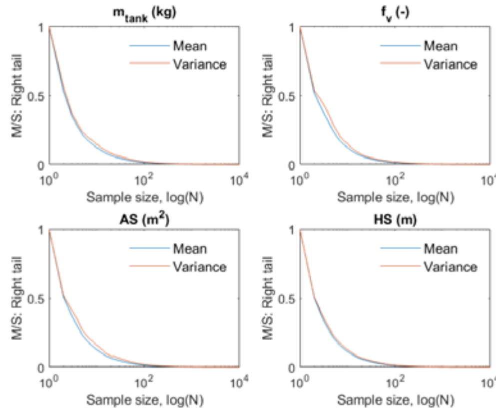

Fig. 3. Output convergence analysis through the M/S plots method for outputs before the heavy-gas model.

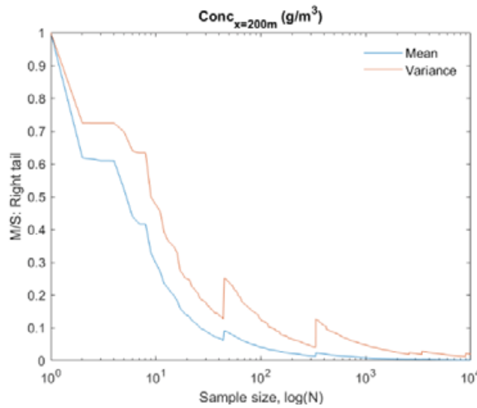

Fig. 4. Output convergence analysis through the M/S plots method for concentration obtained using the heavy gas model.

The inclusion of M/S plots as part of the framework for UA ensures statistical robustness of the MC methods. Confirming the convergence of the basic moments of a distribution, the mean and the variance, guarantees a reliable understanding of the output uncertainty, as well as helping to decide the number of MC samples needed for the analysis. A comprehensive representation of the output uncertainty is guaranteed and concluded with the use of the mean, median and percentiles to provide insights with regards to different levels of conservativeness within risk – or risk indicators – calculations. Moreover, considering these provides a more informative basis for interpreting concentration outcomes particularly with respect to low-probability, high-impact events that can constitute prominent outliers in an output distribution. This approach to perform UA of risk-related calculations, should lead to more dependable safety and risk management decisions, especially in relation to emergency planning and investment in safety measures. Nevertheless, it is important to consider that achieving convergence of the MC methods for obtaining a complete picture of risk and its associated uncertainties, can significantly increase the computational expense requiring for more complex models – such as the ones used within QRA calculations – 10,000 MC simulations, as seen in this case, to mitigate the effects of randomness.

5. Conclusion

This research showcases the need of incorporating convergence analysis to ensure statistical rigor Uncertainty Analysis of – complex – models utilized in QRA. The proposed uncertainty framework centers on stability of Monte Carlo methods, shifting the focus from single-point best estimates to a more robust, uncertainty-informed perspective.

While achieving this level of precision can be computationally demanding, often requiring high number of simulations for complex models, it provides a defensible foundation for risk management. By validating the first two moments of the distribution, practitioners can support high-stakes decisions with reliable data, ensuring that safety measures and economic investments are based on a comprehensive understanding of the risk picture associated with a facility rather than simplified point estimates.

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