



PROBABILISTIC ASSESSMENT OF TIME TO REACH THE LOWER EXPLOSIVE LIMIT FOLLOWING ACCIDENTAL METHANE LEAKS

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Abstract: *Accidental methane leaks in enclosed or semi-enclosed spaces may generate hazardous atmospheres within short time intervals, particularly when ventilation is weak or uncertain. Deterministic calculations are commonly used to estimate the time required to reach the lower explosive limit (LEL), but such approaches do not account for uncertainty in rupture geometry, discharge characteristics, gas pressure, or ventilation conditions. This paper develops a probabilistic framework for assessing methane accumulation based on a deterministic zero-dimensional mass-balance model extended through Monte Carlo uncertainty propagation using Latin Hypercube Sampling. Uncertainty is introduced in the effective area factor, discharge coefficient, pipe pressure, wind speed, and pressure coefficient difference, and the resulting distributions of time to reach the LEL, steady-state concentration, and critical ventilation thresholds are evaluated. Two representative residential scenarios are analysed: a kitchen of 18 m³ with a 3/4" hose and a kitchen of 18 m³ with a 1/2" hose, both at 25 mbar. For the 3/4" scenario, the predicted 90% interval for the time to reach the LEL is 50.3–102.3 s, compared with a deterministic estimate of 60.4 s. For the 1/2" scenario, the corresponding interval is 71.9–146.0 s, compared with a deterministic estimate of 86.4 s. Sensitivity analysis shows that the effective area factor dominates the airtight case, whereas wind speed and pressure coefficient difference dominate the ventilated case. The concept of a deterministic critical ventilation threshold is further generalized into probabilistic ventilation thresholds linked to specified confidence levels. For Scenario S1, achieving 95% confidence that the steady-state concentration remains below the LEL requires ACH=71.6 h⁻¹, compared with a deterministic threshold of 59.6 h⁻¹. The proposed framework provides a more realistic basis for forensic interpretation, detector placement, ventilation design, and risk-informed gas safety assessment than deterministic methods alone.*

1. Introduction

1.1 Background and Motivation

Methane is widely used as a domestic and industrial fuel, but accidental leaks in enclosed spaces can rapidly create hazardous atmospheres. Of particular concern is the time required for the methane concentration to reach the lower explosive limit (LEL), defined as the minimum fuel concentration in air below which flame propagation cannot be sustained. For methane under normal conditions, the LEL is approximately 5% by volume in air. Above this threshold, ignition becomes possible provided that oxygen is sufficient and an ignition source is present. At higher concentrations, the mixture eventually becomes too rich to burn; for methane in air, the corresponding upper explosive limit (UEL) is approximately 15% by volume.

A deterministic 0D (well-mixed) mass-balance model provides a simple and useful first estimate of methane accumulation in an enclosure. Such a model yields closed-form expressions for the time required to reach the LEL as a function of key parameters, including leak flow rate, room volume, and ventilation rate. For representative residential kitchen scenarios, deterministic calculations indicate that the LEL may be reached within approximately 1–2 minutes, while ordinary natural ventilation may be insufficient to prevent hazardous accumulation under unfavourable conditions.

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However, deterministic models, while useful for screening and order-of-magnitude estimates, have a fundamental limitation: they treat input parameters as fixed, known values. In reality, these parameters are subject to significant uncertainty and variability. In accidental leak scenarios, the actual rupture geometry is rarely known exactly, so the effective leak area may differ substantially from the nominal hose cross-section. The discharge coefficient depends on the shape and roughness of the rupture opening. Pipe pressure may vary around its nominal value. In naturally ventilated spaces, wind speed and the pressure coefficient difference across openings also vary in time and depend on local environmental and building conditions. As a result, the time to reach the LEL is not a single deterministic quantity, but a random variable influenced by multiple uncertain inputs.

This uncertainty has direct implications for engineering assessment and risk management. A single deterministic prediction may create false confidence, especially when decisions depend on conservative estimates of detection time or required ventilation. For example, treating a value such as $t_{LEL}=60.4$ as an exact prediction obscures the possibility that the LEL may be reached substantially earlier or later, depending on the combination of uncertain parameters. A probabilistic treatment is therefore needed to quantify not only the expected outcome, but also the spread, tails, and sensitivity of the response.

In this context, probabilistic methods provide a more realistic basis for gas safety analysis than single-point deterministic calculations. By assigning probability distributions to uncertain inputs and propagating them through the mass-balance model, it becomes possible to estimate distributions of the time to reach the LEL, confidence intervals for key statistics, the probability of LEL exceedance as a function of time, and the probability that ventilation remains sufficient to prevent hazardous accumulation. This motivates the probabilistic framework developed in the present paper.

Figure 1 illustrates schematically the flammability range of methane in air, highlighting the lower explosive limit (LEL) at 5% by volume and the upper explosive limit (UEL) at 15% by volume.

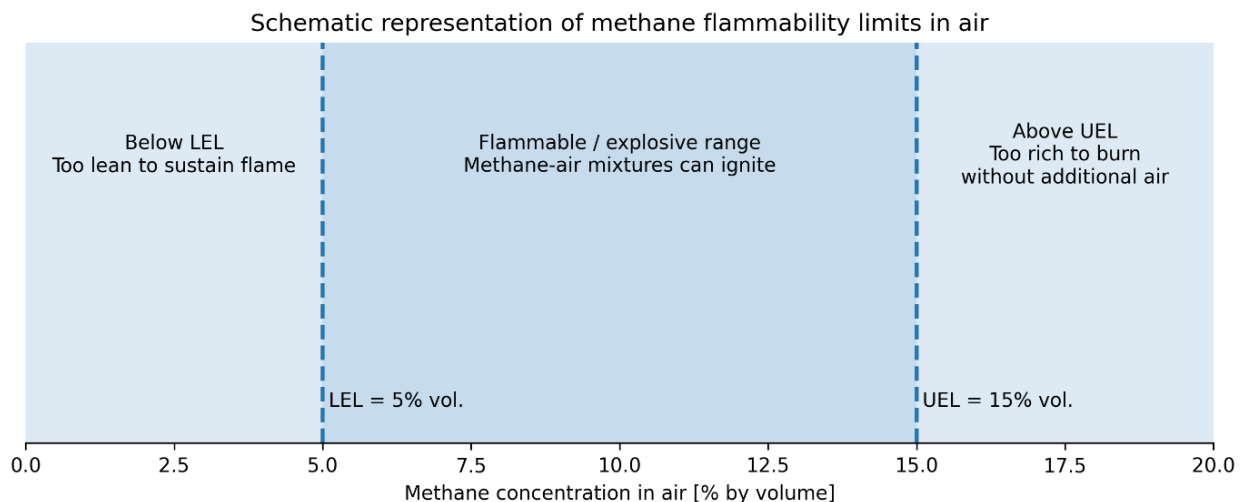


Fig. 1. Schematic representation of methane flammability limits in air. Methane-air mixtures below the lower explosive limit (LEL = 5% by volume) are too lean to sustain flame propagation, whereas mixtures above the upper explosive limit (UEL = 15% by volume) are too rich to burn without further mixing with air. The interval between 5% and 15% by volume defines the flammable (explosive) range.

1.2 The Need for Probabilistic Assessment

Probabilistic risk assessment (PRA) provides a rigorous framework for explicitly quantifying and propagating uncertainty in engineering models [1, 2]. Instead of producing a single deterministic output, PRA yields a probability distribution that characterizes the range of plausible outcomes together with their associated likelihoods. This is particularly important in safety-critical applications, where decisions must account not only for central estimates, but also for variability, tail behaviour, and confidence levels.

In the present context, a probabilistic approach is warranted because several of the key inputs governing methane accumulation are inherently uncertain. These include the effective leak area, discharge coefficient, pipe pressure, wind speed, and pressure coefficient difference across ventilation openings. Even when the governing mass-balance model is relatively simple, uncertainty in these inputs can propagate nonlinearly into the outputs and significantly affect the predicted time to reach the lower explosive limit (LEL), the steady-state concentration, and the required ventilation rate.

A probabilistic treatment is especially valuable when:

- input parameters are imperfectly known or only partially characterized;
- natural variability is significant;
- safety-critical decisions depend on tail behaviour rather than average values;
- one wishes to identify which uncertain parameters contribute most strongly to output variability.

Among the available probabilistic methods, Monte Carlo simulation is one of the most widely used because of its flexibility, robustness, and applicability to nonlinear models [3, 4]. By repeatedly sampling the uncertain inputs from their prescribed probability distributions and evaluating the model over a large number of realizations, one may construct empirical distributions of the outputs of interest.

This approach offers several advantages over a purely deterministic analysis. It allows the analyst to estimate percentiles, confidence intervals, and exceedance probabilities, rather than relying on a single nominal prediction. It also provides a natural basis for global sensitivity analysis and for risk-informed design criteria, such as probabilistic ventilation thresholds corresponding to specified confidence levels. For these reasons, a probabilistic framework is adopted in the present study.

1.3 Objectives and Scope

This paper develops a probabilistic framework, based on Monte Carlo simulation, for a deterministic 0D model of methane accumulation and time to reach the lower explosive limit (LEL). The specific objectives are as follows:

1. To identify the key uncertain parameters in the 0D LEL model and assign appropriate probability distributions based on literature data, field evidence, and engineering judgment.
2. To propagate these uncertainties through the model using Monte Carlo simulation, thereby generating probability distributions for the principal output quantities of interest, namely:
 - the time to reach LEL, t_{LEL} ;
 - the steady-state methane concentration, C_{∞} ;
 - the probability of LEL exceedance as a function of time;
 - the probability of non-attainment of LEL in steady state.
3. To analyse two representative case studies (Scenarios S1 and S2) probabilistically, presenting the results in terms of percentiles and confidence intervals rather than single deterministic values.
4. To perform sensitivity analysis in order to identify the parameters that contribute most strongly to output uncertainty, using Partial Rank Correlation Coefficients (PRCC) and, where appropriate, Sobol indices.
5. To redefine the critical ventilation threshold, ACH_{crit} , in probabilistic terms, for example as the air change rate required to ensure a specified probability of remaining below the LEL.
6. To derive practical implications for gas safety engineering, including detector placement, ventilation design, and risk-informed assessment.

1.4 Relation to Previous Work

Deterministic 0D mass-balance models are widely used as rapid screening tools for indoor contaminant accumulation and gas leak assessment. In the present paper, the governing equations, leak-flow model, and ventilation formulation are summarized explicitly so that the probabilistic analysis remains self-contained and reproducible. The notation and scenario definitions are kept consistent throughout the paper in order to facilitate comparison between deterministic estimates and probabilistic results.

The principal contribution of the present work is not the introduction of a new mass-balance equation, but the probabilistic extension of the deterministic framework through uncertainty propagation, confidence intervals, sensitivity analysis, and probabilistic critical ventilation thresholds. The appendices provide supplementary material on distribution selection, convergence analysis, and additional case studies that support and complement this probabilistic formulation.

2. Mathematical framework

2.1 Recap of the Deterministic 0D Model

The deterministic 0D model considered in this paper is based on the mass-balance equation for the methane concentration $C(t)$ in a room of volume $V[m^3]$:

$$V \frac{dC}{dt} = Q_{in} - Q_{out}C(t), C(0) = 0 \quad (1)$$

where:

- $Q_{in}[m^3/s]$ is the volumetric methane inflow rate;
- $Q_{out}[m^3/s]$ is the ventilation or exhaust flow rate.

Here, $C(t)$ is treated as a dimensionless volumetric concentration (volume fraction), consistent with the 0D well-mixed approximation.

For constant Q_{in} and Q_{out} , the analytical solution is:

$$C(t) = \frac{Q_{in}}{Q_{out}} (1 - e^{-Q_{out}t/V}) \quad (2)$$

The corresponding steady-state concentration is:

$$C_{\infty} = \frac{Q_{in}}{Q_{out}} \quad (3)$$

The time required to reach the lower explosive limit, $C_{LEL} = 0.05$ (5% by volume), is obtained by setting $C(t) = C_{LEL}$, which gives:

$$t_{LEL} = -\frac{V}{Q_{out}} \ln \left(1 - \frac{C_{LEL}}{C_{\infty}} \right) = -\frac{V}{Q_{out}} \ln \left(1 - \frac{C_{LEL} Q_{out}}{Q_{in}} \right) \quad (4)$$

This expression is valid only if $C_{\infty} > C_{LEL}$. If $C_{\infty} \leq C_{LEL}$, the lower explosive limit is never reached in the 0D well-mixed sense.

For an airtight room, $Q_{out} = 0$, and the governing equation reduces to:

$$V \frac{dC}{dt} = Q_{in} \quad (5)$$

which yields:

$$C(t) = \frac{Q_{in}}{V} t \quad (6)$$

Hence, the time to reach the LEL becomes:

$$t_{LEL} = \frac{V C_{LEL}}{Q_{in}} \quad (7)$$

2.2 Leak Flow Rate Model

For residential installations with typical operating pressures of 20–30 mbar, the leak flow may be approximated as incompressible [5]. In the present formulation, the methane inflow rate Q_{in} is expressed as a volumetric flow rate referenced to ambient conditions:

$$Q_{in} = \frac{\dot{m}}{\rho_a} \quad (8)$$

where $\dot{m}$ [kg/s] is the methane mass flow rate, given by the standard orifice-flow expression

Thus, Q_{in} represents the methane volumetric inflow rate expressed at ambient conditions, which is consistent with the concentration-based room mass-balance model used in the present study.

$$\dot{m} = C_d A_{eff} \sqrt{2\rho_g \Delta p} \quad (9)$$

In these expressions:

- C_d [-] is the discharge coefficient;
- A_{eff} [m²] is the effective leak area;
- Δp [Pa] is the gauge pressure in the pipe relative to ambient pressure;
- ρ_g [kg/m³] is the methane density at upstream conditions;
- ρ_a [kg/m³] is the methane density evaluated at ambient pressure and temperature.

In the present formulation,

$$\Delta p = p_{pipe} - p_0 = p_a + \Delta p \quad (10)$$

where p_0 is the absolute upstream pressure and p_a is the ambient pressure.

The upstream methane density is calculated from the ideal gas law as

$$\rho_g = \frac{p_0}{R_{CH_4} T} \quad (11)$$

where $R_{CH_4} \approx 518.3$ J/(kg · K) is the specific gas constant of methane and T [K] is the absolute temperature.

The methane density at ambient conditions is

$$\rho_a = \frac{p_a}{R_{CH_4} T} \quad (12)$$

The effective leak area is related to the nominal internal cross-sectional area of the hose or pipe through an effective area factor η_A :

$$A_{eff} = \eta_A A_{nom} = \eta_A \frac{\pi D_i^2}{4} \quad (13)$$

where D_i [m] is the internal diameter.

2.3 Ventilation Model

For wind-driven cross-ventilation through two openings (e.g., a window and a door), the ventilation flow rate is approximated as [6]:

$$Q_{out} = C_{d,vent} A_{eq} U \sqrt{\Delta C_p} \quad (14)$$

where:

- $C_{d,vent}[-]$ is the discharge coefficient associated with the ventilation openings;
- $A_{eq}[m^2]$ is the equivalent opening area;
- $U[m/s]$ is the wind speed;
- $\Delta C_p[-]$ is the pressure coefficient difference across the openings.

The equivalent opening area is given by

$$A_{eq} = \frac{A_w A_d}{\sqrt{A_w^2 + A_d^2}} \quad (15)$$

where $A_w[m^2]$ is the window area and $A_d[m^2]$ is the door area.

The corresponding air change rate is

$$ACH = \frac{3600 Q_{out}}{V} \quad (16)$$

where ACH is expressed in h^{-1} .

This formulation represents a simplified wind-driven ventilation model and is appropriate for the present 0D screening analysis. More detailed airflow behaviour, including buoyancy effects, transient wind fluctuations, and internal flow stratification, would require higher-fidelity multizone or CFD treatment.

2.4 Identification of Uncertain Parameters and Their Probability Distributions

The deterministic model presented in Sections 2.1–2.3 treats the input parameters as fixed values. In practice, however, several of the key parameters are affected by uncertainty arising from measurement error, natural variability, or incomplete knowledge of the leak and ventilation conditions. For a probabilistic assessment, these uncertain inputs must be represented by appropriate probability distributions.

Based on the literature [5, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17], available engineering evidence, and engineering judgment, the following parameters are identified as the primary sources of uncertainty in the present model.

Effective Area Factor η_A

The effective area factor η_A accounts for the difference between the nominal cross-sectional area of the hose or pipe and the actual flow area at the rupture. This is one of the most uncertain input parameters, since rupture geometries may vary widely depending on the failure mode. Typical cases include:

- complete guillotine rupture: $\eta_A \approx 1.0$;
- partial tear: $\eta_A \in [0.3, 0.8]$;
- crack or pinhole: $\eta_A \in [0.01, 0.3]$;
- partially obstructed fitting: $\eta_A \in [0.1, 0.6]$.

For a generic rupture scenario without specific knowledge of the failure mode, a broad probability distribution is appropriate.

A lognormal distribution is a reasonable choice for a strictly positive parameter that may vary substantially over a wide range [18]. A bounded uniform distribution may also be used as a simple representation in the absence of stronger prior information [19].

For the base-case analysis, a lognormal distribution truncated at 1.0 is adopted, with median 0.7 and 95th percentile 0.95. This choice reflects the assumption that rupture openings are often relatively large, while still allowing for smaller effective areas.

Parameters adopted in the base case:

- Distribution: lognormal, truncated at 1.0
- Median: 0.7
- 95th percentile: 0.95
- Implied geometric standard deviation: approximately 1.20

Discharge Coefficient C_d

The discharge coefficient C_d accounts for flow contraction, friction losses, and non-ideal orifice behavior. For sharp-edged orifices, C_d is typically in the range 0.6–0.65 [5]. For well-rounded entrances, it may approach unity. For ruptured hoses with irregular edges, values in the range 0.6–0.9 are plausible [20].

In the present study, a truncated normal distribution is adopted. This provides a convenient representation of variability around a central value while preventing unphysical values outside the admissible range.

For the base-case analysis, a normal distribution with mean 0.75 and standard deviation 0.1 is adopted and truncated to the interval [0.5, 0.95].

Parameters adopted in the base case:

- Distribution: normal, truncated
- Mean: 0.75
- Standard deviation: 0.1
- Truncation limits: [0.5, 0.95]

Pipe Pressure p_{pipe}

The supply pressure in residential natural gas networks is typically of the order of 20–25 mbar (2000–2500 Pa gauge). In practice, however, the actual pressure may vary because of:

- regulator tolerances;
- network demand fluctuations;
- measurement uncertainty;
- time-dependent operational variability.

A normal distribution is appropriate when the variability arises from several small, approximately additive effects [21]. For the base-case analysis, the pipe pressure is modelled as normally distributed with mean 2500 Pa and standard deviation 125 Pa, truncated to positive values.

Parameters adopted in the base case:

- Distribution: normal, truncated to positive values
- Mean: 2500 Pa
- Standard deviation: 125 Pa

Wind Speed U

Wind speed is highly variable and depends on site location, season, time of day, exposure, and local topography. For many practical applications, wind speed data can be represented by a Weibull distribution [10, 22]:

$$f_U(u) = \frac{k}{\lambda} \left(\frac{u}{\lambda}\right)^{k-1} \exp \left[-\left(\frac{u}{\lambda}\right)^k \right], u \geq 0 \quad (17)$$

where k is the shape parameter and λ is the scale parameter.

For many temperate climates, $k \approx 2$ and $\lambda \approx 4$ –5 m/s provide a reasonable first approximation [23].

For the base-case analysis, a Weibull distribution with shape parameter $k = 2.0$ and scale parameter $\lambda = 4.0$ m/s is adopted. To avoid unrealistic extremes within the present screening framework, the distribution is truncated to the interval [0.5, 10] m/s. These bounds should be understood as practical modeling limits for the present study rather than universal physical limits.

Parameters adopted in the base case:

- Distribution: Weibull, truncated
- Shape parameter: $k = 2.0$
- Scale parameter: $\lambda = 4.0$ m/s
- Truncation limits: [0.5, 10] m/s

Pressure Coefficient Difference ΔC_p

The pressure coefficient difference ΔC_p depends on building orientation, facade geometry, surrounding obstructions, and wind direction. For cross-ventilation configurations, values typically range from about 0.1 to 0.7 [11, 24].

In the absence of building-specific aerodynamic data, a uniform distribution over this interval provides a simple bounded representation of the uncertainty.

For the base-case analysis, a uniform distribution on [0.1, 0.7] is adopted.

Parameters adopted in the base case:

- Distribution: uniform

- Minimum: 0.1
- Maximum: 0.7

Internal Diameter D_i

For a given nominal hose size (e.g., 1/2" or 3/4"), the actual internal diameter may vary depending on manufacturer specifications and applicable standards. For 1/2" hoses, D_i typically ranges from about 12 mm to 16 mm [25], whereas for 3/4" hoses it typically ranges from about 18 mm to 20 mm.

In a probabilistic framework, D_i may be treated either as:

- a fixed value, if the hose type is known and measured;
- a bounded distribution, if the actual internal diameter is uncertain.

In the present case studies, D_i is assumed fixed at its nominal value so that the influence of the other uncertain parameters can be examined more clearly. In practical applications, however, D_i could also be represented probabilistically if reliable information on its variability is available.

Temperature T

Indoor temperature typically varies over a relatively narrow range, for example from about 18°C to 25°C. The effect of this variation on methane density, and hence on the calculated flow rate, is comparatively small over such a range. For simplicity, temperature is treated as fixed at 293 K in the base-case analysis. If needed, it could be represented by a narrow normal distribution in a refined probabilistic treatment.

Summary of Input Parameters and Assigned Probability Models

Table 1 summarizes the input parameters and their assigned probability models for the base-case analysis.

Table 1. Input parameters and assigned probability models for the base-case analysis

Parameter	Symbol	Probability model	Parameters	Rationale
Effective area factor	η_A	Lognormal (truncated)	Median = 0.7, 95th percentile = 0.95, upper bound = 1.0	Rupture openings are often relatively large, but substantial uncertainty remains
Discharge coefficient	C_d	Normal (truncated)	Mean = 0.75, standard deviation = 0.1, bounds [0.5, 0.95]	Plausible range for irregular rupture openings
Pipe pressure	p_{pipe}	Normal (truncated)	Mean = 2500 Pa, standard deviation = 125 Pa, lower bound = 0	Regulator tolerances and operational fluctuations
Wind speed	U	Weibull (truncated)	$k = 2.0$, $\lambda = 4.0$ m/s, bounds [0.5, 10] m/s	Representative temperate-climate wind distribution
Pressure coefficient difference	ΔC_p	Uniform	Min = 0.1, Max = 0.7	Wide uncertainty in the absence of building-specific aerodynamic data
Internal diameter	D_i	Fixed (per scenario)	S1: 19 mm; S2: 15.88 mm	Treated as known for the present case studies
Temperature	T	Fixed	293 K	Limited variability and comparatively minor influence

2.5 Outputs of Interest

The Monte Carlo simulation generates distributions for the following output quantities of interest:

- **Time to reach the lower explosive limit**, t_{LEL} [s], computed from the analytical solution of the 0D model for each realization, provided that the LEL is reached under the corresponding conditions;
- **Steady-state methane concentration**, C_∞ [-], computed for ventilated cases as the asymptotic concentration predicted by the mass-balance model;
- **LEL exceedance indicator**, a binary flag identifying whether the steady-state concentration exceeds the lower explosive limit, i.e., whether $C_\infty > C_{LEL}$;
- **Transient concentration**, $C(t)$, evaluated at selected times in order to construct probability-of-exceedance curves and cumulative risk metrics.

For realizations in which $C_\infty \leq C_{LEL}$, the lower explosive limit is not reached in the 0D steady-state sense, and t_{LEL} is therefore undefined as a finite time. In the Monte Carlo analysis, such realizations are recorded separately and used to estimate the probability of non-attainment of the LEL.

2.6 Correlation Between Parameters

In principle, some of the uncertain input parameters may be statistically dependent. For example, higher wind speeds may be associated with different pressure coefficient differences, and the effective area factor η_A may be related to the discharge coefficient C_d if the rupture geometry influences both the opening size and the flow contraction behavior.

In the absence of quantified data describing such dependencies, the uncertain parameters are treated as statistically independent in the present study. This should be regarded as a simplifying base-case assumption rather than as evidence that correlations are negligible in reality.

If reliable information on parameter dependence becomes available, the probabilistic framework could be extended to account for correlated inputs, for example through copula-based methods [26].

2.7 Summary of the Probabilistic Model

The probabilistic model developed in the present study consists of three main components:

- **Inputs:** the uncertain parameters listed in Table 1, each represented by an assigned probability distribution;
- **Deterministic core:** the 0D mass-balance model described in Sections 2.1–2.3, which maps the inputs to the corresponding output quantities;
- **Outputs:** probability distributions of the time to reach the lower explosive limit, t_{LEL} , the steady-state concentration, C_∞ , and the associated LEL exceedance or non-attainment indicators.

In compact form, the probabilistic model may be written as

$$(t_{LEL}, C_\infty, I_{LEL}) = f(\eta_A, C_d, p_{pipe}, U, \Delta C_p; V, D_i, T, \theta) \quad (18)$$

where f denotes the deterministic mapping defined by the governing equations in Sections 2.1–2.3, I_{LEL} is an indicator variable describing whether the LEL is reached or exceeded under the specified conditions, and θ represents additional fixed scenario parameters.

3. Monte Carlo methodology

3.1 Overview

Monte Carlo simulation is a computational technique that propagates uncertainty in model inputs through repeated sampling, thereby approximating the probability distribution of the corresponding outputs [3, 4]. In the present study, Monte Carlo simulation is applied to propagate the uncertainties described in Section 2.4 through the deterministic 0D mass-balance model.

The general procedure is as follows:

1. Assign probability distributions to the uncertain input parameters listed in Table 1.
2. Generate N samples from these distributions.
3. For each sampled input vector, evaluate the deterministic model to compute the outputs of interest, such as t_{LEL} , C_∞ , and related indicators.
4. Analyse the resulting ensemble of outputs in order to estimate empirical distributions, percentiles, confidence intervals, exceedance probabilities, and sensitivity measures.

3.2 Sampling Strategy

Simple Random Sampling

The most basic sampling approach is simple random sampling (SRS), in which each realization is drawn independently from the prescribed input distributions. Although straightforward, SRS may require a large number of simulations in order to obtain stable estimates, particularly for tail percentiles [3].

Latin Hypercube Sampling

To improve sampling efficiency, Latin Hypercube Sampling (LHS) is employed. LHS is a stratified sampling method that provides better coverage of the input space than simple random sampling for the same number of realizations [4, 27].

In LHS:

1. The cumulative probability range of each input variable is divided into N intervals of equal probability.
2. One sample is drawn from each interval, without replacement.
3. The sampled values for different variables are randomly combined to form N input vectors.

Compared with SRS, LHS generally reduces the variance of estimated statistics, especially for smooth response functions and for percentile estimation [28]. For the present study, LHS with $N = 100,000$ simulations is adopted, which provides stable estimates of the output percentiles up to approximately P_{99} , as confirmed by the convergence analysis in Section 3.3.

A compact comparison of alternative sampling strategies for Scenario S1 (airtight case), including simple random sampling (SRS), Latin Hypercube Sampling (LHS), and Sobol-based quasi-Monte Carlo (Sobol-QMC), is presented in Appendix D. The comparison shows that all three methods converge toward very similar percentile estimates at large sample sizes, while LHS and Sobol-QMC provide more stable estimates than SRS for the same computational effort.

3.3 Number of Simulations and Convergence

The choice of $N = 100,000$ simulations is based on preliminary convergence testing. Figure 2 shows the evolution of selected percentiles (P_5 , P_{50} , and P_{95}) of t_{LEL} as a function of N for Scenario S1.

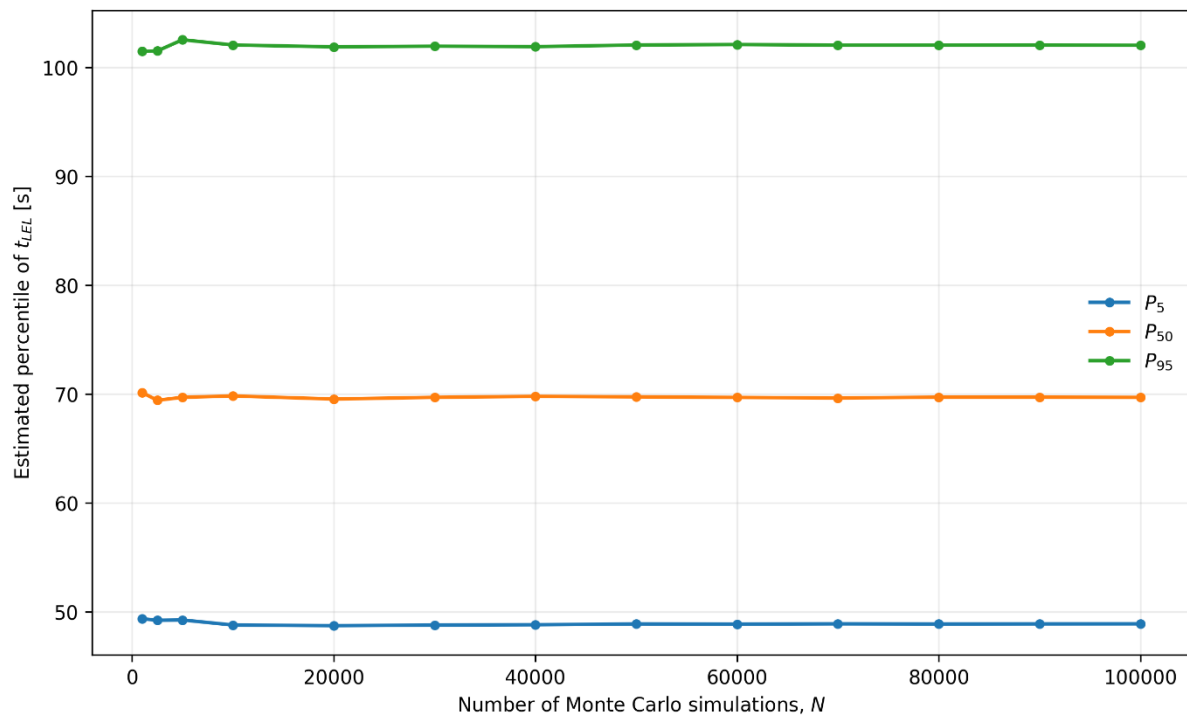


Fig. 2. Convergence of t_{LEL} percentiles with increasing number of Monte Carlo simulations for Scenario S1. The percentile estimates stabilize after approximately 50,000 simulations, with relative changes below 1% between $N = 90,000$ and $N = 100,000$

The convergence criterion adopted in the present study is that the relative change in the estimated P_{95} percentile of t_{LEL} between $N = 90,000$ and $N = 100,000$ should be less than 1%. This criterion is satisfied for Scenario S1 and was therefore considered sufficient for the full analysis.

3.4 Implementation

The Monte Carlo simulation is implemented in Python using the following libraries:

- **NumPy** for numerical arrays and random number generation;
- **SciPy** for probability distributions and statistical utilities;
- **Matplotlib** for visualization;
- **SALib** for Sobol sensitivity analysis [29].

The implementation consists of modules for the leak-flow model, the ventilation model, the 0D mass-balance model, random sampling, post-processing, and sensitivity analysis.

3.5 Output Analysis

For each scenario, the following outputs are computed and analysed.

Empirical Distribution and Percentiles

From the ensemble of simulated values of t_{LEL} (and C_{∞} , where applicable), empirical cumulative distribution functions (ECDFs) are constructed. Key percentiles are then extracted, including:

- P_5 : the value below which 5% of realizations fall;
- P_{50} : the median;
- P_{90} : the value below which 90% of realizations fall;
- P_{95} : the value below which 95% of realizations fall;
- P_{99} : the value below which 99% of realizations fall.

Confidence Intervals

Confidence intervals for the median are estimated using the non-parametric bootstrap method [30]. In the present study, 10,000 bootstrap resamples are generated, and the median is computed for each resample. The 95% confidence interval is then taken as the interval between the 2.5th and 97.5th percentiles of the bootstrap distribution.

Probability of Non-Attainment

For ventilated scenarios, the probability of non-attainment of the lower explosive limit, i.e., the probability that $C_{\infty} \leq C_{LEL}$, is estimated as

$$P_{non-attainment} = \frac{\#\{i: C_{\infty}^{(i)} \leq C_{LEL}\}}{N} \times 100\% \quad (19)$$

where N is the total number of simulations.

This probability may also be evaluated conditionally as a function of wind speed or air change rate (ACH) by analysing subsets of the simulated data.

Probability of LEL Exceedance Over Time

The probability that the lower explosive limit has been reached by time t is estimated from the empirical cumulative distribution function of t_{LEL} :

$$P(t) = \hat{F}_{t_{LEL}}(t) = \frac{1}{N} \sum_{i=1}^N \mathbf{1}_{\{t_{LEL}^{(i)} \leq t\}} \quad (20)$$

where $\mathbf{1}_{\{t_{LEL}^{(i)} \leq t\}}$ is the indicator function, equal to 1 if the condition is satisfied and 0 otherwise.

3.6 Sensitivity Analysis Methods

Partial Rank Correlation Coefficients (PRCC)

PRCC is a global sensitivity measure that quantifies the monotonic relationship between each input parameter and the output after removing the effects of the remaining inputs [27, 28]. The procedure is as follows:

1. Transform the input and output data to ranks;
2. For each input X_j , compute the residuals obtained by regressing its ranks against the ranks of the other inputs;
3. Compute the residuals obtained by regressing the ranked output Y against the same set of ranked remaining inputs;
4. Compute the Pearson correlation coefficient between the two residual series.

PRCC values lie in the interval $[-1, 1]$. The sign indicates the direction of influence, while the magnitude indicates the strength of the monotonic effect. Statistical significance is assessed using the corresponding p-values.

Sobol Indices

Sobol indices are variance-based global sensitivity measures that decompose the variance of the model output into contributions from individual inputs and their interactions [29, 30]. The first-order Sobol index, S_1 , measures the contribution of a single input acting alone, whereas the total Sobol index, S_T , measures the contribution of that input including all interaction effects.

In the present study, Sobol indices are computed using the implementation available in the SALib library [29]. Because variance-based sensitivity analysis is more computationally demanding than PRCC, it is performed on a reduced sample size. The total number of model evaluations depends on the specific Sobol sampling scheme adopted; accordingly, the reduced sample size is selected so as to balance computational cost and statistical stability.

3.7 Software and Code Availability

The Python code developed for this study is available from the corresponding author upon reasonable request. It includes:

- separate modules for the leak-flow, ventilation, and mass-balance sub-models;
- routines for generating random samples from the prescribed probability distributions;
- the main Monte Carlo simulation workflow;
- post-processing routines for figures and tables;
- sensitivity analysis routines based on PRCC and Sobol indices.

3.8 Summary of Methodology

Table 2 summarizes the main methodological choices adopted in the Monte Carlo framework.

Table 2. Summary of Monte Carlo methodology

Aspect	Choice	Rationale
Sampling method	Latin Hypercube Sampling (LHS)	Improved coverage of the input space relative to simple random sampling
Number of simulations	$N = 100,000$	Stable percentile estimates up to the upper tail; convergence verified
Software	Python (NumPy, SciPy, Matplotlib, SALib)	Flexible, transparent, and widely used scientific computing environment
Outputs	t_{LEL} , C_{∞} , $P(t)$, $P_{\text{non-attainment}}$	Comprehensive probabilistic characterization of risk
Sensitivity methods	PRCC, Sobol indices	Complementary correlation-based and variance-based approaches
Confidence intervals	Bootstrap (10,000 resamples)	Non-parametric estimation without strong distributional assumptions

4. Case studies: probabilistic analysis of representative scenarios

In this section, the Monte Carlo methodology described in Section 3 is applied to two representative case studies, denoted S1 and S2. For each scenario, the fixed parameters, uncertain inputs, and probabilistic simulation results are presented. Particular attention is given to the distribution of the time required to reach the lower explosive limit (LEL), the associated confidence intervals, and, where applicable, the probability that the steady-state concentration remains below the LEL.

4.1 Scenario S1: Kitchen 18 m³, 3/4" Hose, $\Delta p = 25\text{mbar}$

Fixed Parameters

The following parameters are treated as fixed in Scenario S1:

- Room volume: $V=18\text{ m}^3$
- Internal diameter (3/4" hose): $D_i = 0.019\text{ m}$
- Nominal cross-sectional area: $[\text{m}^2]$

$$A_{nom} = \frac{\pi D_i^2}{4} = 2.84 \times 10^{-4} \quad (21)$$

- Ambient pressure: $p_a = 101325\text{ Pa}$
- Temperature: $T = 293\text{ K}$
- Methane gas constant: $R_{CH_4}=518.3\text{ J/(kg} \cdot \text{K)}$
- LEL threshold: $C_{LEL} = 0.05(5\% \text{ by volume})$
- Window area: $A_w=0.60\text{ m}^2$
- Door area: $A_d=1.44\text{ m}^2$

Uncertain Parameters and Distributions

The uncertain parameters and their probability models are those defined in Table 1. For convenience, they are reproduced below for Scenario S1.

Table 3. Uncertain parameters for Scenario S1

Parameter	Symbol	Probability model	Parameters
Effective area factor	η_A	Lognormal (truncated)	Median = 0.7, 95th percentile = 0.95, upper bound = 1.0
Discharge coefficient	C_d	Normal (truncated)	$\mu = 0.75$, $\sigma = 0.1$, bounds [0.5, 0.95]
Pipe pressure	p_{pipe}	Normal (truncated)	$\mu=2500$, $\sigma=125$ Pa, lower bound = 0
Wind speed	U	Weibull (truncated)	$k=2.00$, $\lambda=4.00$ m/s, bounds [0.5, 10]m/s
Pressure coefficient difference	ΔC_p	Uniform	Min = 0.1, Max = 0.7

Monte Carlo Simulation Setup

The Monte Carlo simulation for Scenario S1 is performed with the following settings:

- Number of simulations: $N = 100,000$
- Sampling method: Latin Hypercube Sampling (LHS)
- Outputs of interest: t_{LEL} in the airtight case and the probability of non-attainment in the ventilated case
- Bootstrap resampling for the median confidence interval: 10,000 resamples

Results

Distribution of Time to Reach LEL

Figure 3 shows the histogram of t_{LEL} for Scenario S1 in the airtight case. The distribution is right-skewed, reflecting the combined effect of uncertainty in the effective leak area, discharge coefficient, and pipe pressure.

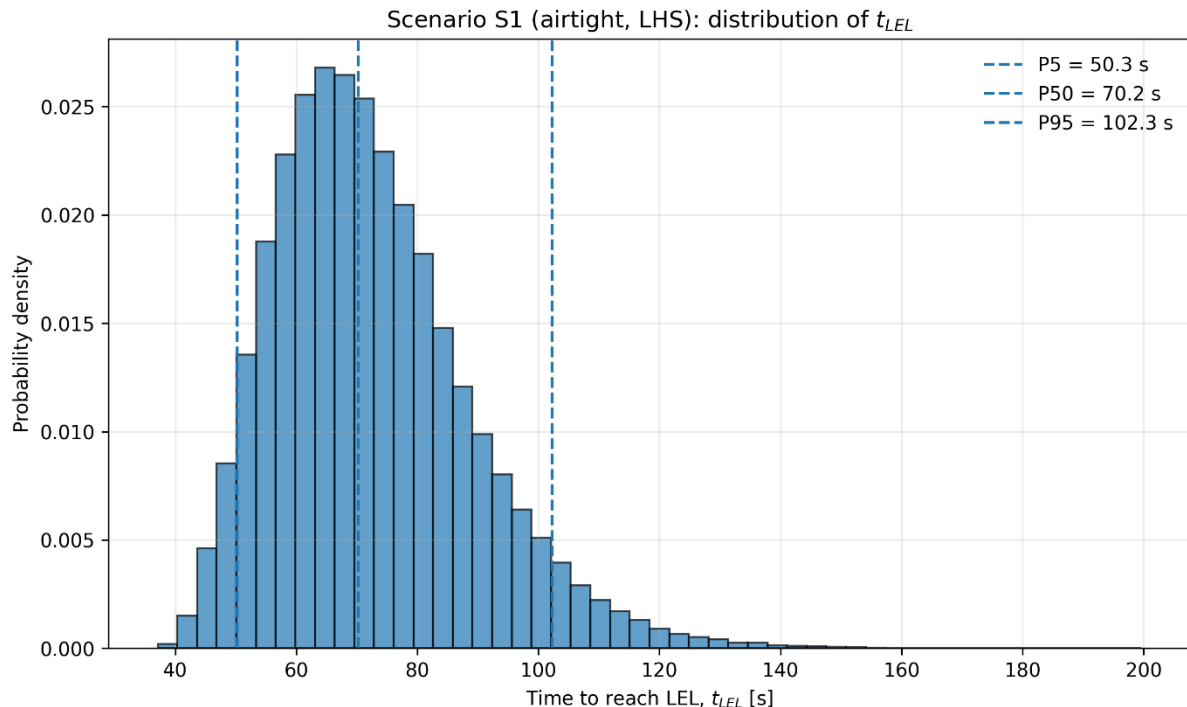


Fig. 3. Histogram of the time to reach the lower explosive limit, t_{LEL} , for Scenario S1 in the airtight case. The dashed lines indicate the 5th percentile (50.3 s), median (70.2 s), and 95th percentile (102.3 s)

Percentiles and Confidence Intervals

Table 4 summarizes the principal percentiles of the t_{LEL} distribution for Scenario S1, together with the bootstrap 95% confidence interval for the median.

Table 4. Percentiles of t_{LEL} for Scenario S1

Percentile	t_{LEL} [s]	Interpretation
P ₅	50.3	5% of realizations give $t_{LEL} \leq 50.3$ s
P ₂₅	60.8	25% of realizations give $t_{LEL} \leq 60.8$ s
P ₅₀ (median)	70.2	50% of realizations give $t_{LEL} \leq 70.2$ s
P ₇₅	81.7	75% of realizations give $t_{LEL} \leq 81.7$ s
P ₉₀	94.1	90% of realizations give $t_{LEL} \leq 94.1$ s
P ₉₅	102.3	95% of realizations give $t_{LEL} \leq 102.3$ s
P ₉₉	120.0	99% of realizations give $t_{LEL} \leq 120.0$ s

The bootstrap 95% confidence interval for the median t_{LEL} =[70.11 s, 70.36 s].

Comparison with the Deterministic Estimate

For the airtight case ($Q_{out} = 0$), the deterministic model gives $t_{LEL} \approx 60.4$ s when evaluated at the nominal parameter values: $\eta_A = 1.0$, $C_d = 0.6$ and $p_{pipe} = 2500$ Pa:

- $\eta_A = 1.0$ (complete rupture)
- $C_d = 0.6$
- $p_{pipe} = 2500$ Pa

The probabilistic median (70.2 s) is higher than this deterministic estimate. This reflects the fact that, in the probabilistic model, the effective area factor η_A is typically below 1.0, which tends to reduce the leak inflow rate and therefore increase the time required to reach the LEL.

The probabilistic analysis also shows that the spread around this central value is substantial:

- the 90% interval (P_5 to P_{95}) extends from approximately 50 s to 102 s;
- in 5% of realizations, the LEL is reached in 50 s or less;
- in 5% of realizations, the LEL is reached only after about 102 s or more.

These results demonstrate that a single deterministic estimate does not adequately characterize the full range of plausible outcomes.

Probability of Non-Attainment of the LEL in the Ventilated Case

For the ventilated case, the same fixed parameters are retained and the ventilation model is activated. For each realization, the steady-state concentration C_∞ is computed. The LEL is considered not attained in the 0D average sense when $C_\infty \leq C_{LEL}$.

To illustrate the role of wind forcing, representative wind-speed scenarios are considered by fixing U at the indicated value while sampling the remaining uncertain inputs from their prescribed distributions. The resulting probabilities of non-attainment are shown in Table 5.

Table 5. Probability of non-attainment of the LEL as a function of wind speed for Scenario S1

Wind speed U [m/s]	Probability that $C_\infty \leq C_{LEL}$ [%]
0.5	0.1
1.0	24.0
2.0	89.2
3.0	99.4
4.0	100.0
5.0	100.0

These results indicate a transition from near-certain attainment of the LEL at low wind speeds to near-certain non-attainment at sufficiently high wind speeds:

- at $U = 0.5$ m/s, the LEL is almost always reached;
- at $U = 1.0$ m/s, only 24% of realizations remain below the LEL;
- at $U = 2.0$ m/s, the probability of non-attainment increases sharply to 89%;
- at $U \geq 3$ m/s, the LEL is almost never reached in the 0D average sense.

This probabilistic view is more informative than a single deterministic threshold. It shows that the transition from likely attainment to likely non-attainment of the LEL is gradual rather than abrupt, and that the relevant probability changes rapidly over the range $U \approx 1$ -3 m/s.

Probability of LEL Exceedance as a Function of Time

Figure 4 shows the cumulative probability that the LEL has been reached by time t , i.e.,

$$P(t) = \Pr(t_{LEL} \leq t) \quad (22)$$

This curve is obtained from the empirical cumulative distribution function of t_{LEL} .

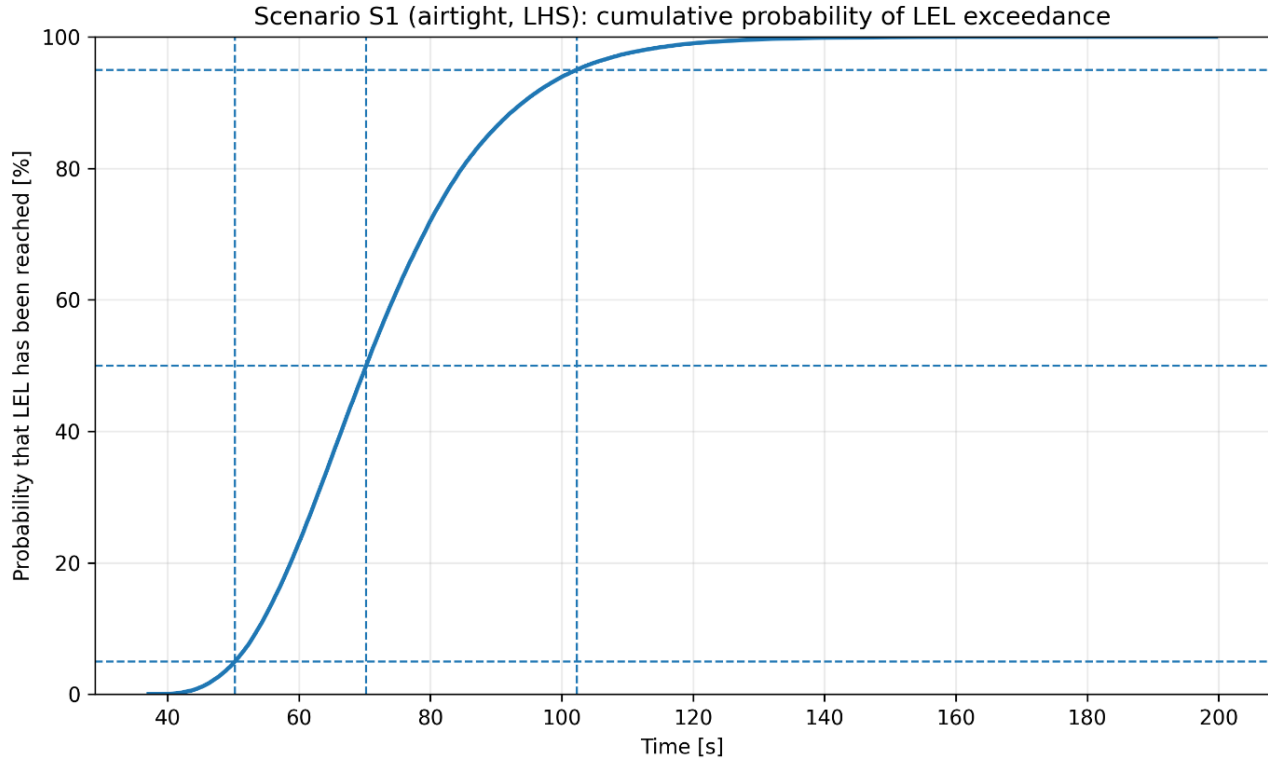


Fig. 4. Cumulative probability that the lower explosive limit has been reached by time t for Scenario S1 in the airtight case. The dashed guides indicate the 5th percentile (50.3 s), median (70.2 s) and 95th percentile (102.3 s) of the t_{LEL} distribution

Such a curve is directly relevant to risk-informed decision-making. If a detection system must ensure, with 95% confidence, that the LEL is not reached before detection occurs, then the allowable response time should not exceed approximately the 5th percentile of the t_{LEL} distribution, i.e., about 50 s. If a 50% confidence level is deemed acceptable, the corresponding response time is approximately the median, i.e., about 70 s.

4.2 Scenario S2: Kitchen 18 m³, 1/2" Hose, $\Delta p = 25\text{mbar}$, Variable C_d

Fixed Parameters

The following parameters are treated as fixed in Scenario S2:

- Room volume: $V=18\text{ m}^3$
- Internal diameter (1/2" hose): $D_i = 0.01588\text{ m}$
- Nominal cross-sectional area: $[m^2]$

$$A_{nom} = \frac{\pi D_i^2}{4} = 1.98 \times 10^{-4}$$

Ambient pressure: $p_a = 101325\text{ Pa}$

- Temperature: $T = 293\text{ K}$
- Methane gas constant: $R_{CH_4}=518.3\text{ J/(kg} \cdot \text{K)}$
- LEL threshold: $C_{LEL} = 0.05(5\% \text{ by volume})$

Uncertain Parameters and Distributions

The uncertain parameters are the same as in Scenario S1, except that D_i is fixed at the 1/2" value. In particular, the discharge coefficient C_d is explicitly treated as uncertain through the truncated normal distribution with $\mu = 0.75$, $\sigma = 0.1$, and bounds $[0.5, 0.95]$.

Results

Distribution of Time to Reach LEL

Figure 5 shows the histogram of t_{LEL} for Scenario S2 in the airtight case. As expected, the distribution remains right-skewed but is shifted toward longer times compared with Scenario S1 because the smaller internal diameter reduces the methane inflow rate.

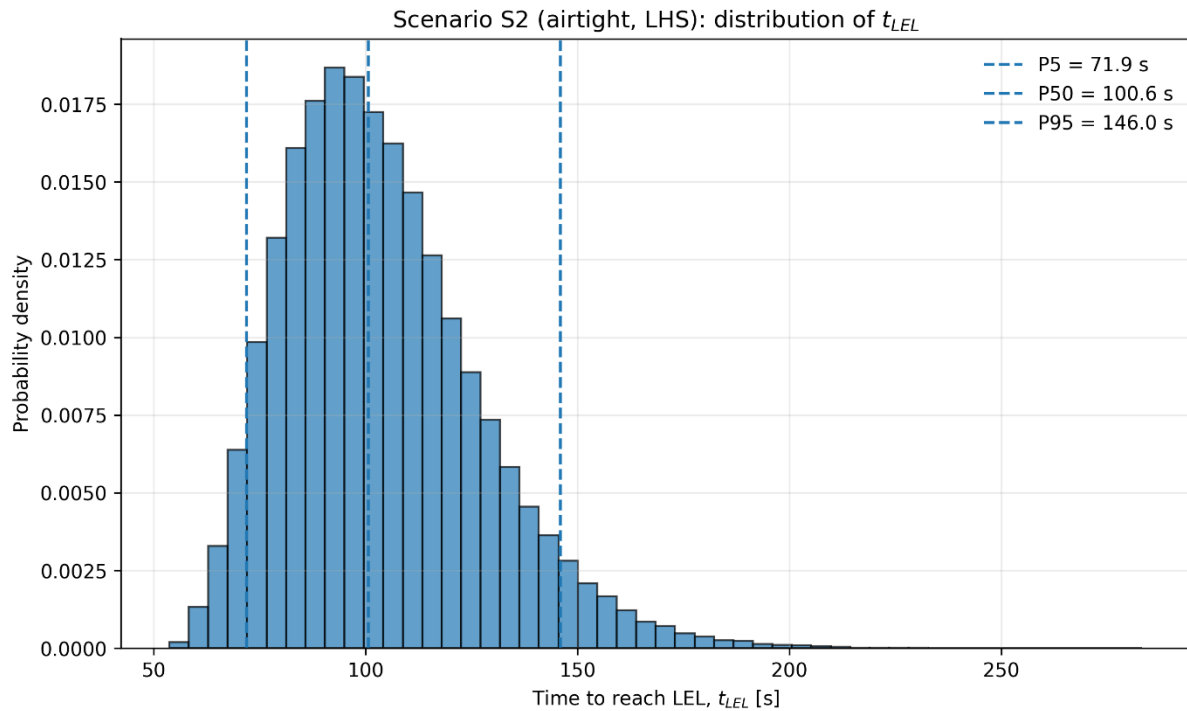


Fig. 5. Histogram of the time to reach the lower explosive limit, t_{LEL} , for Scenario S2 in the airtight case. The dashed lines indicate the 5th percentile (71.9 s), median (100.6 s), and 95th percentile (146.0 s)

Percentiles and Confidence Intervals

Table 6 summarizes the principal percentiles of t_{LEL} for Scenario S2.

Table 6. Percentiles of t_{LEL} for Scenario S2

Percentile	t_{LEL} [s]	Interpretation
P ₅	71.9	5% of realizations give $t_{LEL} \leq 71.9$ s
P ₂₅	86.9	25% of realizations give $t_{LEL} \leq 86.9$ s
P ₅₀ (median)	100.6	50% of realizations give $t_{LEL} \leq 100.6$ s
P ₇₅	117.1	75% of realizations give $t_{LEL} \leq 117.1$ s
P ₉₀	134.4	90% of realizations give $t_{LEL} \leq 134.4$ s
P ₉₅	146.0	95% of realizations give $t_{LEL} \leq 146.0$ s
P ₉₉	171.3	99% of realizations give $t_{LEL} \leq 171.3$ s

The bootstrap 95% confidence interval for the median t_{LEL} is [100.46 s, 100.82 s].

Comparison with Deterministic Values

For Scenario S2, the deterministic model yields different estimates of t_{LEL} depending on the assumed discharge coefficient C_d :

- $C_d = 0.6 \rightarrow t_{LEL} = 86.4$ s
- $C_d = 0.8 \rightarrow t_{LEL} = 64.8$ s
- $C_d = 0.9 \rightarrow t_{LEL} = 57.6$ s

The probabilistic median (100.6) is higher than the deterministic estimate obtained for $C_d = 0.6$, although it is numerically closest to that case. This reflects the fact that, in the probabilistic formulation, the effective area factor η_A is typically below 1.0, which reduces the leak inflow rate and therefore increases the time required to reach the LEL.

More importantly, the probabilistic analysis again reveals substantial variability:

- the 90% interval (P_5 to P_{95}) extends from about 72 s to 146 s;
- in 5% of realizations, the LEL is reached in about 72 s or less;
- in 5% of realizations, the LEL is reached only after approximately 146 s or more.

These results show that, even when deterministic calculations provide useful reference values, the full uncertainty range remains significant and should not be neglected in practical assessments.

Effect of Ventilation

For Scenario S2, the effect of ventilation is examined by evaluating the probability that the steady-state concentration remains below the LEL at selected values of the air change rate (ACH).

Table 7. Probability of non-attainment of the LEL as a function of ACH for Scenario S2

ACH [h^{-1}]	Probability that $C_\infty \leq C_{LEL}$ [%]
0	0.0
1	0.0
3	0.0
5	0.0
10	0.0
15	0.007

The results show that, for the present uncertainty assumptions, the LEL is still almost always reached in the 0D average sense even at $\text{ACH}=15 \text{ h}^{-1}$. This reflects the fact that, for the 1/2" hose scenario, the ventilation rates considered here remain well below the deterministic critical ventilation threshold.

For comparison, the deterministic critical ventilation threshold for Scenario S2 is approximately 41.7 h^{-1} for $C_d = 0.6$, and becomes larger for higher assumed values of C_d . The probabilistic results are therefore consistent with the deterministic estimate: ACH values in the range $1\text{--}15 \text{ h}^{-1}$ are too small to prevent attainment of the LEL in most realizations.

4.3 Summary of Case Study Results

The probabilistic analysis of Scenarios S1 and S2 leads to several main observations.

First, substantial variability exists in the time required to reach the lower explosive limit. For both scenarios, the 90% intervals span broad ranges, indicating that the actual time to reach the LEL may be significantly shorter or longer than suggested by a single deterministic estimate.

Second, in both scenarios the probabilistic median is higher than the deterministic estimate obtained from the nominal parameter values. This reflects the fact that, in the probabilistic formulation, the effective area factor is typically below its nominal upper-limit value, which tends to reduce the methane inflow rate and therefore increase the time to reach the LEL. Deterministic calculations may still provide a useful reference value, but they do not capture the full distribution of possible outcomes.

Third, risk-averse engineering decisions require attention to lower percentiles rather than to the median alone. If the objective is to ensure high-confidence detection before the LEL is reached, design should be based on low-percentile values such as P_5 or P_{10} , rather than on the median alone.

Fourth, ventilation effectiveness is intrinsically probabilistic. In Scenario S1, the results show a transition range over which the probability of non-attainment rises rapidly as ventilation becomes stronger. This demonstrates that ventilation performance is better described in probabilistic terms than by a single deterministic threshold.

Finally, the smaller-diameter hose in Scenario S2 leads to a longer median time to reach the LEL than in Scenario S1, but the spread of the distribution remains substantial. Thus, reduced inflow delays the onset of hazardous conditions, yet uncertainty remains large enough that probabilistic assessment is still necessary. For the ventilation levels examined in Scenario S2, the probability of non-attainment remains negligible, indicating that these ACH values are well below the level required to prevent attainment of the LEL in most realizations.

5. Sensitivity analysis

5.1 Objectives

Sensitivity analysis is used to identify which input parameters contribute most to the uncertainty in the output quantities of interest. This information is valuable for:

- prioritizing data collection and research efforts by focusing on the most influential parameters;
- guiding model simplification, since parameters with negligible influence may be fixed at nominal values;
- improving physical understanding of the mechanisms that drive output variability.

In the present study, global sensitivity analysis is performed primarily using Partial Rank Correlation Coefficients (PRCC), a non-parametric method that quantifies the monotonic relationship between each input parameter and the output after accounting for the effects of the other inputs [27, 28]. PRCC is particularly suitable here because the model response is monotonic with respect to the main uncertain inputs over the ranges considered.

As a complementary variance-based approach, Sobol indices were considered during model development. However, to ensure full consistency with the finalized LHS-based case-study reruns adopted in Chapter 4, the quantitative results reported in this section are based on the verified PRCC analyses. The main conclusions regarding dominant parameters remain physically clear and robust.

5.2 Input Parameters Considered

The sensitivity analysis is based on the uncertain parameters listed in Table 1. However, not all parameters are active in every configuration.

For the airtight case, only the parameters affecting methane inflow are active:

- effective area factor, η_A ;
- discharge coefficient, C_d ;
- pipe pressure, p_{pipe} .

For the ventilated case, both leak-related and ventilation-related uncertainties are active:

- effective area factor, η_A ;
- discharge coefficient, C_d ;
- pipe pressure, p_{pipe} ;
- wind speed, U ;
- pressure coefficient difference, ΔC_p .

The analysis is performed for both Scenario S1 and Scenario S2, and for two outputs:

- time to reach the lower explosive limit, t_{LEL} , in the airtight case;
- steady-state concentration, C_{∞} , in the ventilated case.

5.3 Results

Scenario S1: Airtight Case

Table 8 shows the PRCC values for t_{LEL} in Scenario S1 for the airtight case. Since $Q_{out} = 0$ in this configuration, the ventilation-related parameters U and ΔC_p are not active and are therefore excluded.

Table 8. PRCC values for t_{LEL} – Scenario S1 (airtight)

Parameter	PRCC	p-value	Interpretation
η_A	-0.970	< 0.001	Very strong negative correlation: larger $\eta_A \rightarrow$ shorter t_{LEL}
C_d	-0.943	< 0.001	Very strong negative correlation: larger $C_d \rightarrow$ shorter t_{LEL}
p_{pipe}	-0.488	< 0.001	Moderate negative correlation: higher pressure $\rightarrow$ shorter t_{LEL}

The negative sign indicates that increasing the parameter reduces t_{LEL} , i.e., the lower explosive limit is reached more rapidly. The magnitude of the PRCC indicates the relative strength of the monotonic influence.

Figure 6 shows the PRCC values graphically as a tornado plot.

These results show that uncertainty in the rupture geometry dominates the uncertainty in the time required to reach the LEL in the airtight case. The discharge coefficient is also highly influential, whereas pipe pressure plays a secondary but still physically meaningful role.

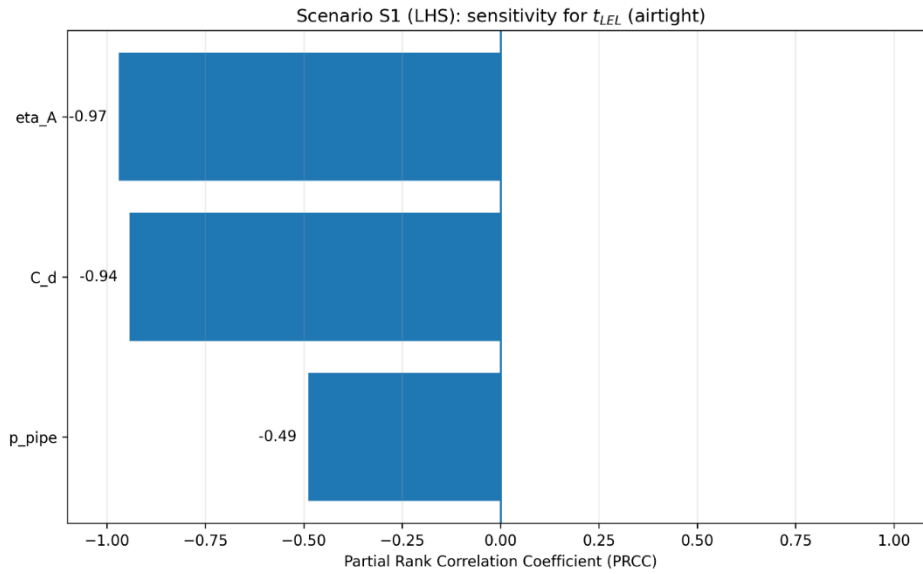


Fig. 6. Tornado plot of PRCC values for t_{LEL} in Scenario S1 (airtight case). The effective area factor η_A is the most influential parameter, followed by the discharge coefficient C_d and pipe pressure p_{pipe} . Negative PRCC values indicate that increasing these parameters reduces the time required to reach the lower explosive limit

Scenario S1: Ventilated Case

For the ventilated case, all five uncertain parameters are active. Table 9 shows the PRCC values for the steady-state concentration C_∞ .

Table 9. PRCC values for C_∞ — Scenario S1 (ventilated)

Parameter	PRCC	p-value	Interpretation
U	-0.970	< 0.001	Very strong negative correlation: higher wind speed $\rightarrow$ lower C_∞
ΔC_p	-0.872	< 0.001	Strong negative correlation: larger pressure coefficient difference $\rightarrow$ lower C_∞
η_A	+0.771	< 0.001	Strong positive correlation: larger effective area $\rightarrow$ higher C_∞
C_d	+0.656	< 0.001	Moderate-to-strong positive correlation: larger discharge coefficient $\rightarrow$ higher C_∞
p_{pipe}	+0.176	< 0.001	Weak positive correlation: higher pipe pressure $\rightarrow$ slightly higher C_∞

The signs are physically consistent with the model structure: parameters that increase methane inflow (η_A, C_d, p_{pipe}) increase C_∞ , whereas parameters that enhance ventilation ($U, \Delta C_p$) decrease C_∞ .

Figure 7 shows the PRCC values graphically.

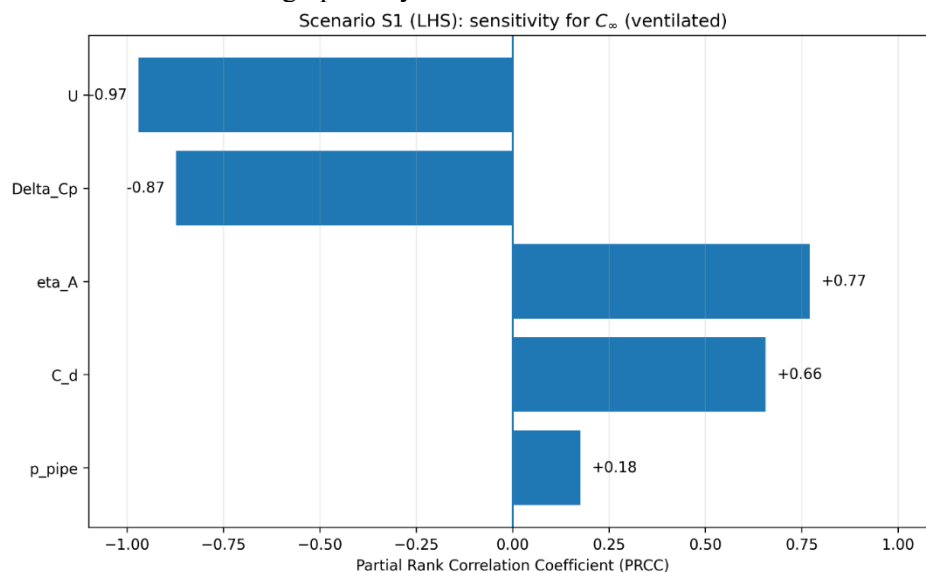


Fig. 7. Tornado plot of PRCC values for C_∞ in Scenario S1 (ventilated case). Wind speed U is the most influential parameter, followed by the pressure coefficient difference ΔC_p , the effective area factor η_A , the discharge coefficient C_d , and pipe pressure p_{pipe} . Positive PRCC values indicate that increasing the parameter raises the steady-state methane concentration, whereas negative PRCC values indicate that increasing the parameter lowers it

These results indicate that, once ventilation is active, uncertainty in ventilation effectiveness dominates the uncertainty in the steady-state methane concentration. Wind speed is the most influential variable, followed by the pressure coefficient difference. Leak-related parameters remain relevant, but their influence becomes secondary compared with the ventilation variables.

Scenario S2

The sensitivity analysis for Scenario S2 yields results qualitatively similar to those obtained for Scenario S1 in the airtight configuration.

In the airtight case, the dominant parameters remain

$$\eta_A > C_d > p_{pipe}. \quad (23)$$

This ranking is physically consistent with the model structure, since the effective leak area and the discharge coefficient directly control the methane inflow rate, while pipe pressure has a weaker secondary effect through the pressure dependence of the leak-flow model.

For the ventilated configuration, the same types of parameters remain active as in Scenario S1. In physical terms, both leak-related and ventilation-related uncertainties contribute to the uncertainty in C_∞ . As in Scenario S1, ventilation-related variables are expected to become dominant whenever ventilation is active, whereas leak-geometry uncertainty remains dominant in the airtight case.

The overall interpretation therefore remains unchanged: uncertainty in the effective leak area is dominant in the airtight configuration, while ventilation-related parameters become increasingly important whenever methane removal by natural ventilation is considered.

5.4 Discussion of Sensitivity Results

The sensitivity analysis reveals several important insights.

Effective area factor η_A is the dominant parameter in the airtight case. In the airtight configuration, η_A contributes the largest share of the uncertainty in the time required to reach the LEL. This highlights the critical importance of characterizing rupture geometry accurately. In post-incident investigations, particular attention should therefore be given to determining the actual flow area, for example through examination of the failed component, measurement of the rupture opening, or forensic reconstruction techniques.

Discharge coefficient C_d is the second most important leak-related parameter. Although less influential than η_A , it still exerts a strong effect on the predicted time to reach the LEL. This suggests that experimental characterization of representative rupture geometries could reduce uncertainty in C_d and improve predictive accuracy.

Pipe pressure p_{pipe} has a weaker but still physically meaningful effect in the airtight case. Its influence is smaller than that of η_A and C_d , which is consistent with the structure of the leak-flow model, where pressure enters less directly than effective area and discharge coefficient.

Ventilation-related parameters dominate the ventilated case. When ventilation is active, the uncertainty in the steady-state methane concentration is governed primarily by the uncertainty in ventilation effectiveness. In the present results, wind speed U is the dominant parameter, followed by the pressure coefficient difference ΔC_p . This indicates that the ability of the room to remove methane is more influential for C_∞ than the secondary uncertainty associated with some leak-side parameters.

Leak-related parameters remain relevant in the ventilated case, but their role becomes secondary. The effective area factor η_A still has a clear positive influence on C_∞ , and the discharge coefficient C_d also contributes, but both are less influential than the dominant ventilation variables. Pipe pressure p_{pipe} has only a weak direct contribution under the present probabilistic assumptions.

Interaction effects are expected to be more important in the ventilated case than in the airtight case. In the airtight configuration, the model response is dominated by a relatively simple inflow mechanism. In the ventilated case, however, the steady-state concentration depends on the competition between methane inflow and ventilation removal, so interaction effects can become more relevant. These findings have several practical implications.

For forensic investigations, priority should be given to estimating the actual effective leak area, since this parameter dominates the uncertainty in the time required to reach the LEL and remains relevant even when ventilation is present.

For detector placement, the most demanding design basis corresponds to combinations of parameters that maximize methane inflow, i.e., large η_A , high C_d , and high p_{pipe} , since these lead to the shortest times to reach the LEL.

For ventilation design, variability in wind conditions and facade pressure effects should be recognized explicitly. The results show that wind speed and pressure coefficient difference can dominate the uncertainty in C_{∞} , which supports the use of probabilistic design approaches rather than reliance on a single deterministic ventilation rate.

Overall, the sensitivity analysis confirms that different physical mechanisms dominate the two configurations considered here: leak-geometry uncertainty dominates the airtight case, whereas ventilation uncertainty dominates the ventilated case.

6. Probabilistic critical ventilation thresholds

6.1 Limitations of the Deterministic ACH_{crit}

Within the deterministic formulation, the critical ventilation threshold, ACH_{crit} , is defined as the air change rate for which the steady-state methane concentration is exactly equal to the lower explosive limit (LEL):

$$ACH_{crit} = \frac{3600 Q_{in}}{V C_{LEL}} \quad (24)$$

For Scenario S1, evaluated at the nominal parameter values $\eta_A = 1.0$, $C_d = 0.6$, and $p_{pipe}=2500\text{Pa}$, the resulting threshold is $ACH_{crit}=59.6$.

However, as the probabilistic analysis shows, this deterministic threshold has important limitations:

- it assumes fixed nominal values for all uncertain parameters;
- it suggests an unrealistically sharp transition, i.e., below ACH_{crit} the LEL is reached, whereas above ACH_{crit} it is not;
- it does not provide the probability of non-attainment of the LEL at a given ventilation rate.

In reality, because both the leak inflow and the ventilation effectiveness are uncertain, the transition from likely attainment to likely non-attainment of the LEL is gradual rather than abrupt.

6.2 Probabilistic Definition

A more informative definition is to express the critical ventilation requirement in probabilistic terms.

The probabilistic critical ventilation threshold, denoted $ACH_{p\%}$, is defined as the air change rate required to ensure that, with $p\%$ confidence, the steady-state concentration remains below the lower explosive limit. Mathematically,

$$ACH_{p\%} = \min \left\{ ACH : Pr (C_{\infty} \leq C_{LEL} \mid ACH) \geq \frac{p}{100} \right\} \quad (25)$$

Typical choices for p are 90%, 95%, and 99%, depending on the required level of safety or reliability.

This definition is more useful for engineering design because it links the ventilation requirement directly to an explicit reliability target.

6.3 Results for Scenario S1

Using the Monte Carlo results for the ventilated case, the probabilistic ventilation thresholds can be obtained as follows:

- for a given value of ACH , evaluate the probability that $C_{\infty} \leq C_{LEL}$;
- construct the resulting probability curve as a function of ACH ;
- interpolate to determine the value of ACH corresponding to a desired confidence level.

Table 10 summarizes the resulting probabilistic critical ventilation thresholds for Scenario S1.

Table 10. Probabilistic critical ventilation thresholds – Scenario S1

Probability level p	$ACH_{p\%}[\text{h}^{-1}]$
50%	51.3
90%	66.9
95%	71.6
99%	80.2

These results may be interpreted as follows:

- To achieve a 50% probability of staying below the LEL, an air change rate of 51.3 h^{-1} is required.
- To achieve a 95% probability of staying below the LEL, an air change rate of 71.6 h^{-1} is required, which is about 20.1% higher than the deterministic threshold $ACH_{crit}=59.6 \text{ h}^{-1}$.

- To achieve a 99% probability of staying below the LEL, an air change rate of 80.2 h^{-1} is required, which is about 34.5% higher than the deterministic value.

These values show that the deterministic threshold does not fully represent the ventilation requirement when uncertainty is taken into account. In the present model, the most hazardous combinations are those that increase methane inflow and reduce ventilation effectiveness, i.e., larger effective area factor η_A , higher discharge coefficient C_d , higher pipe pressure p_{pipe} , and weaker ventilation conditions.

Figure 8 shows the probability of non-attainment as a function of ACH , with both the deterministic threshold and the probabilistic thresholds indicated.

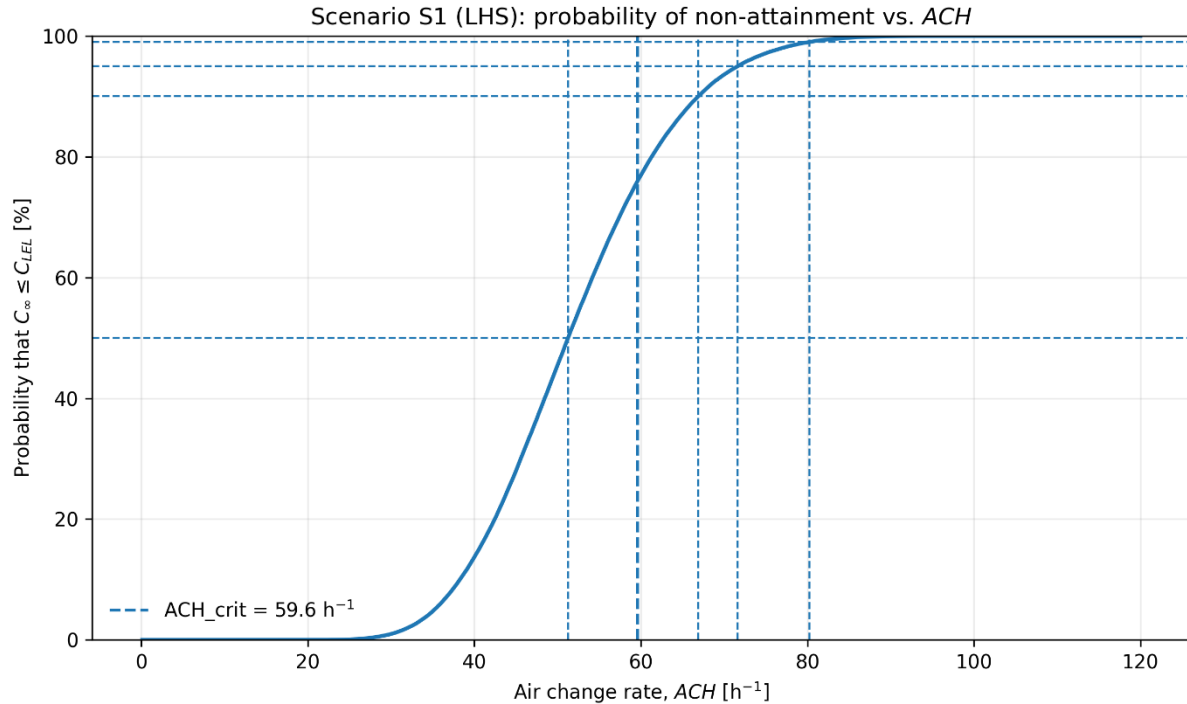


Fig. 8. Probability that $C_\infty \leq C_{LEL}$ (i.e., the LEL is not reached in steady state) as a function of ACH for Scenario S1. The dashed lines indicate the deterministic threshold $ACH_{crit}=59.6 \text{ h}^{-1}$ and the probabilistic thresholds corresponding to 50%, 90%, 95%, and 99% confidence levels

6.4 Results for Scenario S2

Table 11 shows the probabilistic critical ventilation thresholds for Scenario S2.

Table 11. Probabilistic critical ventilation thresholds – Scenario S2

Probability level p	$ACH_{p\%} [\text{h}^{-1}]$
50%	35.8
90%	46.8
95%	50.1
99%	56.1

For comparison, in Scenario S2 the deterministic critical ventilation threshold is approximately 41.7 h^{-1} for $C_d = 0.6$, and increases to about 62.5 h^{-1} for $C_d = 0.9$.

The probabilistic 95% and 99% thresholds lie within this deterministic range, but they remain substantially higher than the nominal deterministic threshold obtained for $C_d = 0.6$. This again shows that deterministic calculations should not be interpreted as a sharp universal boundary between safe and unsafe conditions.

6.5 Implications for Ventilation Design

The probabilistic critical ventilation thresholds have several important implications for design.

Deterministic thresholds may be non-conservative for high-reliability applications. If the design objective is to ensure, with 95% or 99% confidence, that the LEL is not reached, then the required ventilation rate may be significantly higher than the single deterministic threshold ACH_{crit} .

The required design margin depends on the uncertainty in the input parameters. The difference between deterministic and probabilistic thresholds is driven by uncertainty in parameters such as η_A , C_d , p_{pipe} , U , and ΔC_p . Reducing this uncertainty, for example through better characterization of rupture geometry or local ventilation conditions, would reduce the required design margin. Risk-based ventilation design becomes possible.

By specifying an acceptable probability of failure, such as a 5% or 1% chance of reaching the LEL, the designer can select the corresponding probabilistic threshold $ACH_{p\%}$ directly from curves such as Figure 8.

Site-specific data can refine the thresholds. If more accurate information is available regarding local wind conditions, opening geometry, or pressure coefficients, the probabilistic model can be refined accordingly. This may either increase or decrease the required threshold, depending on whether the site conditions are more or less favorable than the generic assumptions used here.

Overall, the probabilistic framework provides a more realistic and decision-relevant basis for ventilation design than a single deterministic threshold, especially in applications where explicit reliability targets are required.

7. Discussion

7.1 Summary of Key Findings

This paper has developed a probabilistic framework for assessing the time required to reach the lower explosive limit (LEL) following accidental methane leaks, based on a deterministic 0D mass-balance model extended through Monte Carlo uncertainty propagation using Latin Hypercube Sampling. Several main findings emerge from the analysis.

First, substantial uncertainty exists in the predicted time to reach the LEL. Even for the relatively simple scenarios considered here, the predicted t_{LEL} spans a wide range depending on the actual realization of the uncertain inputs. For Scenario S1, the 90% interval extends from approximately 50.3 s to 102.3 s, compared with a deterministic estimate of about 60.4 s. For Scenario S2, the corresponding interval extends from approximately 71.9 s to 146.0 s, compared with a deterministic estimate of about 86.4 s. This demonstrates that deterministic calculations, although useful as reference values, do not adequately represent the full range of possible outcomes.

Second, the effective area factor η_A is the dominant source of uncertainty in the airtight case. The sensitivity analysis shows that uncertainty in the actual rupture opening exerts the strongest influence on the time required to reach the LEL. The discharge coefficient C_d is the second most influential leak-related parameter, whereas pipe pressure has a weaker but still physically meaningful effect.

Third, in ventilated cases the dominant sources of uncertainty shift from leak-side parameters to ventilation-related parameters. Wind speed U is the most influential variable, followed by the pressure coefficient difference ΔC_p . This indicates that uncertainty in ventilation effectiveness governs the steady-state methane concentration more strongly than secondary uncertainty in some leak-side parameters.

Fourth, probabilistic ventilation thresholds may differ substantially from deterministic thresholds, particularly when high reliability is required. For Scenario S1, the 95% and 99% probabilistic thresholds are significantly higher than the deterministic ACH_{crit} , indicating that deterministic design may be non-conservative if a high level of confidence is required. For Scenario S2, the probabilistic thresholds remain within the wider deterministic range associated with different assumed values of C_d , but they are still substantially above the nominal deterministic threshold based on $C_d = 0.6$.

Finally, the results show that risk-based design is feasible within a relatively simple modeling framework. By expressing both the time to reach the LEL and the required ventilation in probabilistic terms, the present approach allows safety decisions to be linked directly to an explicit confidence level or acceptable probability of failure.

7.2 Implications for Practice

For Forensic Investigators

The results indicate that forensic investigations should prioritize the characterization of the actual rupture geometry. Because the effective area factor η_A is the dominant source of uncertainty in airtight conditions, efforts should focus on determining the true flow area associated with the failure, for example through direct inspection of the damaged component, measurement of the rupture opening, or image-based reconstruction methods such as photogrammetry.

In addition, forensic reports should avoid presenting a single deterministic estimate of t_{LEL} as if it were exact. A probabilistic interval or percentile-based description provides a more realistic representation of uncertainty and is more informative for legal, technical, and safety-related interpretation.

Where rupture geometry cannot be established reliably, a probabilistic assessment using a broad distribution for η_A should be preferred over a single assumed value.

For Detector Placement

For detector placement and alarm-response design, the most relevant quantities are not the median or deterministic values of t_{LEL} , but the lower percentiles of the distribution. If the design objective is to ensure, with high confidence, that detection occurs before the LEL is reached, then the detector response time should be compared against the P_5 or P_{10} values of t_{LEL} , rather than against the median alone.

This is particularly important in compact rooms or in scenarios with large effective leak areas, where the lower tail of the t_{LEL} distribution may correspond to very rapid methane accumulation.

Where ventilation is present, the probabilistic distribution of C_∞ and the associated probability of non-attainment of the LEL should also be considered when assessing likely accumulation behavior and required response time.

For Ventilation Design

The present results support the use of probabilistic rather than purely deterministic ventilation criteria. Curves such as Figure 8 make it possible to select a ventilation requirement corresponding to a specified reliability target. This is more informative than relying on a single deterministic threshold ACH_{crit} , which provides no direct information about the probability of remaining below the LEL.

The results also show that the required design margin depends on uncertainty in both leak inflow and ventilation parameters. If these uncertainties can be reduced through better characterization of rupture behaviour, local wind conditions, or building-specific pressure coefficients, then the ventilation requirement may be refined accordingly.

In high-risk applications, the probabilistic framework also highlights the value of redundancy. If maintaining a target ACH is critical, backup ventilation capacity or emergency power supply may be justified in order to preserve the intended reliability level under adverse conditions.

For Regulatory Standards

The results suggest that regulatory approaches based solely on deterministic thresholds may not always provide the intended level of safety. A deterministic minimum ventilation rate does not specify the actual probability that the LEL will be avoided under uncertainty.

A more rational approach would be to incorporate probabilistic concepts into standards and guidance documents, for example by linking design requirements to explicit confidence levels or calibrated safety margins. Standards could also encourage the characterization of uncertainty in key parameters, either through prescribed probability models or through safety factors derived from probabilistic analysis.

More broadly, reporting results as percentiles or confidence intervals, rather than as single deterministic values, would improve transparency and support better communication of uncertainty among designers, investigators, regulators, and end users.

7.3 Limitations and Caveats

Although the present probabilistic framework is more informative than a purely deterministic approach, several limitations should be acknowledged.

Assumption of independence.

The uncertain input parameters are treated as statistically independent. In reality, some dependence may exist, for example between wind speed and pressure coefficient difference, or between rupture geometry and discharge coefficient. Ignoring such dependence may either increase or decrease the estimated output variance, depending on the nature of the correlations. Future work could extend the framework to correlated inputs, for example through copula-based formulations.

Choice of probability distributions.

The probability models assigned to the uncertain parameters are based on literature, engineering judgment, and broad physical plausibility, but they are not unique. Alternative choices, such as a different distribution for η_A or different truncation bounds for U , could affect the numerical results. More extensive field data or formal expert elicitation would strengthen the probabilistic specification.

Model-form uncertainty.

The 0D well-mixed model is a simplified representation of methane accumulation in an enclosure. It neglects spatial concentration gradients, stratification, local jets, transient variations in leak rate, and other physical complexities. These model-form uncertainties are not explicitly represented in the present probabilistic framework. For spatially resolved hazard assessment, multizone models or computational fluid dynamics (CFD) may be more appropriate.

Neglect of ignition in the jet.

The model assumes that ignition becomes relevant only when the average room concentration reaches the LEL. In reality, ignition may occur earlier in the rich zone of the leak jet itself. From a hazard-assessment perspective, this is a non-conservative assumption, because it may underestimate the actual ignition risk.

Static ventilation assumption.

The ventilation rate is treated as constant in time for a given realization. In reality, wind conditions fluctuate, openings may change state, and transient flow effects may occur. A time-dependent probabilistic model would provide a more realistic description but would also require substantially greater complexity.

Single-zone assumption.

The present study assumes a single well-mixed zone. For multi-room buildings or spaces with strong internal flow separation, a multizone formulation would be more appropriate. The present framework could, however, be extended in that direction.

7.4 Future Work

Several directions for future work emerge from the present study.

First, additional field and laboratory data are needed to improve the specification of the uncertain inputs, especially rupture geometries, discharge coefficients for failed hoses, and pressure variability in residential gas systems.

Second, the framework could be strengthened through Bayesian calibration against experimental data, such as controlled release experiments, enclosure tests, or tracer-gas ventilation measurements. Such an approach would make it possible to update prior input distributions in a systematic manner.

Third, a dynamic probabilistic model could be developed in order to represent time-varying ventilation, fluctuating wind conditions, and operational events such as opening or closing doors and windows.

Fourth, the framework could be extended to multizone models or simplified CFD-based representations in order to quantify the probability of local methane hotspots rather than only the enclosure-averaged concentration.

Fifth, the probabilistic framework could be used in optimization studies, for example for detector placement under uncertainty or for cost-reliability optimization of ventilation systems.

Finally, the development of simplified engineering tools, surrogate models, or lookup tables based on the present methodology could improve accessibility for practitioners who do not wish to run full Monte Carlo simulations.

8. Conclusions

This paper has developed a probabilistic framework for assessing the time required to reach the lower explosive limit (LEL) following accidental methane leaks, based on a deterministic 0D mass-balance model extended through Monte Carlo uncertainty propagation using Latin Hypercube Sampling.

The main contributions and conclusions may be summarized as follows.

First, a probabilistic formulation has been established for the 0D methane accumulation model by introducing uncertainty in the effective area factor η_A , discharge coefficient C_d , pipe pressure p_{pipe} , wind speed U , and pressure coefficient difference ΔC_p . These uncertain inputs are represented by probability models derived from the literature and from engineering judgment.

Second, Monte Carlo simulation with 100,000 realizations, combined with percentile estimation, bootstrap confidence intervals, and sensitivity analysis, provides a substantially more informative characterization of risk than a single deterministic calculation. Rather than returning only one estimate of t_{LEL} , the probabilistic framework yields full distributions, confidence intervals, exceedance probabilities, and probabilistic ventilation thresholds.

Third, the case studies demonstrate that uncertainty in t_{LEL} is substantial. For Scenario S1, the 90% interval extends from approximately 50.3 s to 102.3 s, compared with a deterministic estimate of about 60.4 s. For Scenario S2, the corresponding interval extends from approximately 71.9 s to 146.0 s, compared with a

deterministic estimate of about 86.4 s. These results show that deterministic estimates may be useful as reference values, but they do not describe the variability that is essential for safety-oriented decision-making.

Fourth, the sensitivity analysis identifies the effective area factor η_A as the dominant source of uncertainty in the airtight case. The discharge coefficient C_d is the second most influential leak-related parameter, while pipe pressure has a weaker effect. In ventilated cases, wind speed U and pressure coefficient difference ΔC_p become the dominant sources of uncertainty in the steady-state concentration. These findings highlight the critical role of both rupture characterization and ventilation conditions in gas safety assessment.

Fifth, the concept of a critical ventilation threshold has been reformulated in probabilistic terms. Instead of a single deterministic ACH_{crit} , the present study defines probabilistic thresholds $ACH_{p\%}$ corresponding to specified confidence levels that the steady-state concentration remains below the LEL. For Scenario S1, achieving 95% confidence requires $ACH=71.6 \text{ h}^{-1}$, compared with a deterministic threshold of $ACH=59.6 \text{ h}^{-1}$. This demonstrates that deterministic ventilation criteria may be insufficient when high reliability is required.

Sixth, the framework provides direct practical value for forensic investigations, detector placement, ventilation design, and the development of more transparent and risk-informed regulatory criteria. In particular, the results support designing for lower percentiles of t_{LEL} when high-confidence detection is required, and using probabilistic ventilation curves when an explicit reliability target must be met.

The present framework remains subject to important limitations, including the assumption of input independence, the choice of probability distributions, the use of a 0D well-mixed model, and the neglect of transient and spatial effects. Nevertheless, it provides a substantially more realistic basis for engineering assessment than deterministic calculations alone.

In conclusion, the probabilistic approach developed here offers a practical and flexible way to move from single-point estimates toward uncertainty-aware gas safety analysis. By explicitly accounting for variability in both leak and ventilation conditions, it supports more robust and defensible decision-making in applications where the consequences of underestimating risk may be severe.

9. Nomenclature

Symbol	Description	Unit
A_d	Door area	m^2
A_{eff}	Effective leak area	m^2
A_{eq}	Equivalent ventilation area	m^2
A_{nom}	Nominal cross-sectional area of hose/pipe	m^2
A_w	Window area	m^2
$C(t)$	Methane concentration at time t	– (volume fraction)
C_d	Discharge coefficient	–
C_{LEL}	Lower explosive limit (0.05)	– (volume fraction)
C_∞	Steady-state methane concentration	– (volume fraction)
D_i	Internal diameter of hose/pipe	m
k	Weibull shape parameter	–
$\dot{m}$	Mass flow rate	kg/s
N	Number of Monte Carlo simulations	–
p	Probability level	%
p_0	Upstream absolute pressure	Pa
p_a	Ambient pressure	Pa
p_{pipe}	Pipe pressure (gauge)	Pa
P_5	5th percentile	s
P_{50}	50th percentile (median)	s
P_{90}	90th percentile	s
P_{95}	95th percentile	s
P_{99}	99th percentile	s
Q_{in}	Volumetric leak flow rate	m^3/s
Q_{out}	Ventilation flow rate	m^3/s
R_{CH_4}	Methane gas constant (518.3)	$\text{J}/(\text{kg}\cdot\text{K})$
S_1	First-order Sobol index	–
ST	Total Sobol index	–

Symbol	Description	Unit
t	Time	s
t _{LEL}	Time to reach lower explosive limit	s
T	Temperature	K
U	Wind speed	m/s
V	Room volume	m ³
β	Pressure ratio (p _a / p ₀)	-
γ	Adiabatic index (1.31 for methane)	-
ΔC _p	Pressure coefficient difference	-
Δp	gauge pressure in the pipe relative to ambient pressure. Δp=p _{pipe} , p ₀ =p _a +Δp	Pa
η _A	Effective area factor	-
λ	Weibull scale parameter	m/s
μ	Mean	varies
ρ _a	Methane density at ambient conditions	kg/m ³
ρ _g	Methane density at upstream conditions	kg/m ³
σ	Standard deviation	varies
τ	Time constant (V / Q _{out})	s

10. Appendices

Appendix A: details of probability distributions

This appendix provides the mathematical formulations and justification for the probability distributions assigned to each uncertain parameter in Table 1. In the present work, the probabilistic case studies are sampled using Latin Hypercube Sampling (LHS), while the marginal distributions remain those defined below.

A.1 Effective Area Factor η_A

The effective area factor η_A is modeled using a lognormal distribution truncated at 1.0. The lognormal distribution is appropriate for positive parameters that can vary by orders of magnitude and is commonly used in uncertainty analysis for geometric quantities [18].

The probability density function (PDF) of the lognormal distribution is:

$$f(\eta_A) = \frac{1}{\eta_A \sigma \sqrt{2\pi}} \exp\left(-\frac{(\ln \eta_A - \mu)^2}{2\sigma^2}\right), \quad \eta_A > 0$$

where μ and σ are the mean and standard deviation of the natural logarithm of η_A.

For the base case, the median is set to 0.7 and the 95th percentile to 0.95, which implies:

$$\begin{aligned} \mu &= \ln(0.7) = -0.3567 \\ \sigma &= \frac{\ln(0.95) - \ln(0.7)}{1.645} \approx 0.186 \end{aligned}$$

The distribution is truncated at η_A = 1.0 to prevent unphysical values greater than the nominal cross-sectional area.

A.2 Discharge Coefficient C_d

The discharge coefficient C_d is modeled using a normal distribution truncated to the interval [0.5, 0.95]. The normal distribution is appropriate for parameters that vary symmetrically around a central value due to multiple small effects [21].

The PDF of the truncated normal distribution is:

$$f(C_d) = \frac{1}{\sigma \sqrt{2\pi}} \frac{\exp\left(-\frac{(C_d - \mu)^2}{2\sigma^2}\right)}{\Phi\left(\frac{b - \mu}{\sigma}\right) - \Phi\left(\frac{a - \mu}{\sigma}\right)}, \quad a \leq C_d \leq b$$

where μ = 0.75, σ = 0.1, a = 0.5, b = 0.95, and Φ is the standard normal cumulative distribution function.

A.3 Pipe Pressure p_{pipe}

Pipe pressure p_{pipe} is modeled using a normal distribution truncated at zero to prevent negative pressures. The mean is set to the nominal value of 2500 Pa (25 mbar) and the standard deviation to 125 Pa (5% coefficient of variation), reflecting typical regulator tolerances and network fluctuations [12].

$$f(p_{pipe}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(p_{pipe}-\mu)^2}{2\sigma^2}\right), p_{pipe} > 0$$

with $\mu = 2500$ Pa, $\sigma = 125$ Pa.

In the LHS implementation, samples are generated by inverse transformation of the truncated cumulative distribution function.

A.4 Wind Speed U

Wind speed U is modeled using a Weibull distribution, which is the standard distribution for wind speed data in meteorology [10, 22]. The PDF is:

$$f(U) = \frac{k}{\lambda} \left(\frac{U}{\lambda}\right)^{k-1} \exp\left(-\left(\frac{U}{\lambda}\right)^k\right), U > 0$$

For temperate climates, the shape parameter $k \approx 2$ and the scale parameter $\lambda \approx 4.0$ m/s for an annual average wind speed of approximately 3.5 m/s [23].

In the present study, the distribution is truncated to [0.5, 10] m/s to exclude unrealistically low values and extremely high values.

A.5 Pressure Coefficient Difference ΔC_p

The pressure coefficient difference ΔC_p is modeled using a uniform distribution over the interval [0.1, 0.7], representing a state of maximum ignorance in the absence of building-specific data [19]. The PDF is:

$$f(\Delta C_p) = \frac{1}{b-a}, a \leq \Delta C_p \leq b$$

with $a = 0.1$ and $b = 0.7$.

A.6 Sampling in the Final Simulations

In the final case-study simulations, the marginal distributions defined above are sampled using Latin Hypercube Sampling (LHS). LHS improves the coverage of the multidimensional input space relative to simple random sampling by stratifying each marginal distribution into equal-probability intervals and drawing one sample from each interval before combining the sampled marginals into complete input vectors.

Appendix B: Monte Carlo convergence analysis

To ensure that the Monte Carlo simulation results are numerically stable, a convergence analysis was performed for Scenario S1 in the airtight case using the finalized Latin Hypercube Sampling setup. The analysis tracks the evolution of the key percentiles of t_{LEL} as a function of the number of Monte Carlo realizations N .

Figure B1 shows the evolution of the 5th percentile, median, and 95th percentile of t_{LEL} with increasing sample size. The results indicate progressive stabilization of the percentile estimates as N increases, with only very small differences between $N = 90,000$ and $N = 100,000$.

Table B1 summarizes the relative change in the main percentiles between $N = 90,000$ and $N = 100,000$.

Table B1. Convergence of t_{LEL} percentiles for Scenario S1 (LHS)

Percentile	t_{LEL} at $N = 90,000$ [s]	t_{LEL} at $N = 100,000$ [s]	Relative change [%]
P_5	50.280	50.256	0.047
P_{50}	70.265	70.235	0.042
P_{95}	102.293	102.290	0.002

All relative changes are below 0.05%, confirming that $N = 100,000$ is sufficient for stable estimates of the key percentiles in Scenario S1.

These results support the use of $N = 100,000$ realizations throughout the main probabilistic analysis.

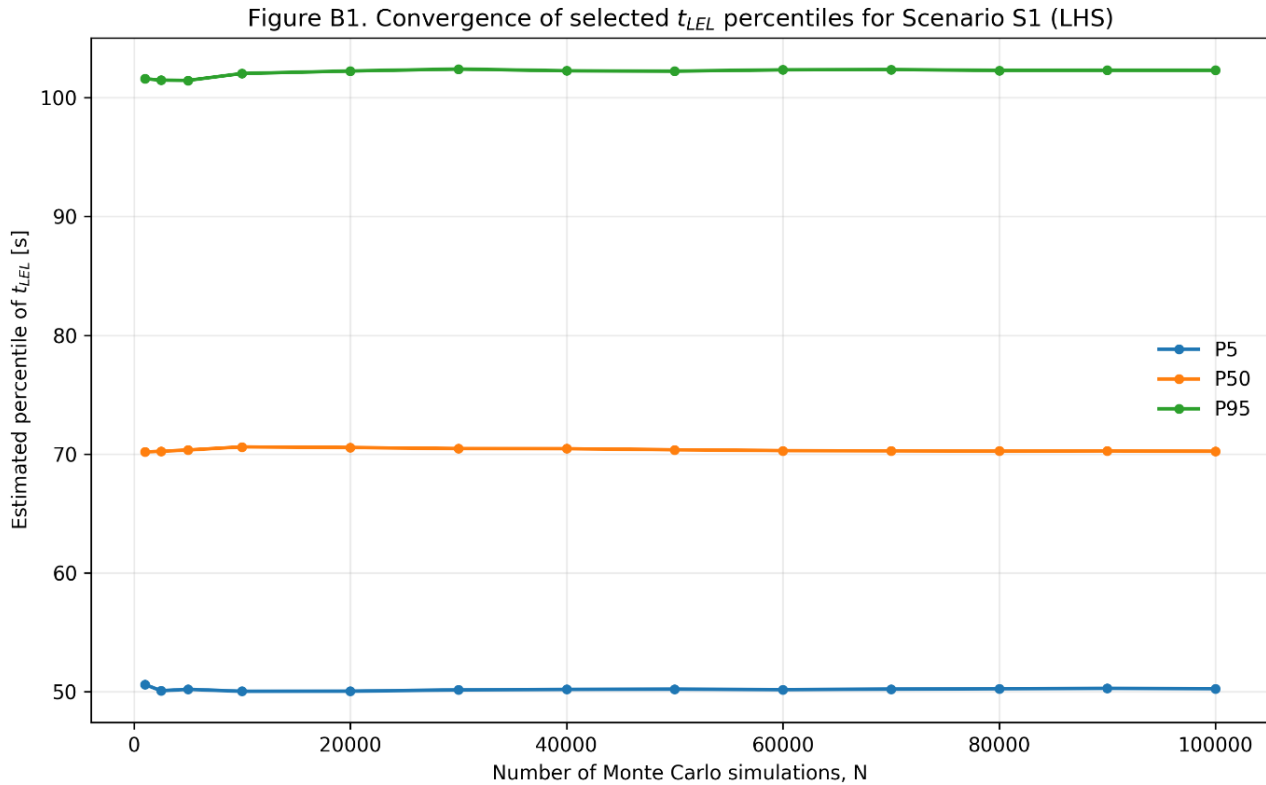


Figure B1. Convergence of selected percentiles of t_{LEL} with increasing number of Monte Carlo simulations for Scenario S1 in the airtight case using Latin Hypercube Sampling. The 5th percentile, median, and 95th percentile stabilize well before $N = 100,000$, indicating that the selected sample size is sufficient for robust percentile estimation

Appendix C: additional results for other scenarios

This appendix presents results for additional scenarios not included in the main text, to illustrate the flexibility of the probabilistic framework. The calculations reported below were updated consistently with the finalized Latin Hypercube Sampling methodology used in the main case studies.

C.1 Scenario S3: Mechanical Ventilation (Fixed ACH)

In this scenario, ventilation is provided by a mechanical system with a fixed air change rate rather than natural ventilation dependent on wind speed. The uncertain parameters are η_A , C_d , and p_{pipe} , while the room volume and the mechanical ventilation rate are treated as fixed. The configuration is otherwise identical to Scenario S1, with $ACH=5 \text{ h}^{-1}$.

Table C1 shows the percentiles of t_{LEL} for Scenario S3.

Table C1. Percentiles of t_{LEL} for Scenario S3 (Mechanical Ventilation, $ACH=5 \text{ h}^{-1}$)

Percentile	$t_{LEL}[\text{s}]$
P_5	52.1
P_{25}	63.5
P_{50}	73.9
P_{75}	86.8
P_{90}	100.7
P_{95}	110.4
P_{99}	131.1

In this scenario, the LEL is reached in all realizations under the adopted uncertainty ranges. Compared with the natural-ventilation case, the mechanical-ventilation case removes uncertainty associated with wind speed and pressure coefficients, while still preserving substantial variability due to leak-side parameters.

C.2 Scenario S4: Larger Room Volume ($V=50 \text{ m}^3$)

This scenario considers a larger room, such as a living room or open-plan kitchen, with volume $V=50 \text{ m}^3$, while keeping all other parameters the same as in Scenario S1.

Table C2 shows the resulting percentiles of t_{LEL} .

Table C2. Percentiles of t_{LEL} for Scenario S4 ($V=50 \text{ m}^3$)

Percentile	$t_{LEL}[\text{s}]$
P_5	139.3
P_{25}	168.8
P_{50}	195.3
P_{75}	227.2
P_{90}	261.2
P_{95}	283.6
P_{99}	332.5

As expected, the larger room volume increases t_{LEL} approximately in proportion to the increase in V . The relative variability remains similar to Scenario S1, but the entire distribution is shifted toward longer times because a larger methane inventory is required to reach the LEL.

C.3 Scenario S5: Higher Pressure ($p_{pipe} = 50 \text{ mbar}$)

This scenario considers a higher supply pressure of 50 mbar (5000 Pa), which may occur in some industrial or commercial installations. The configuration is otherwise identical to Scenario S1, except that the pipe-pressure distribution is recentered at 5000 Pa with a 5% coefficient of variation.

Table C3 shows the resulting percentiles of t_{LEL} .

Table C3. Percentiles of t_{LEL} for Scenario S5 ($p_{pipe} = 50 \text{ mbar}$)

Percentile	$t_{LEL}[\text{s}]$
P_5	35.1
P_{25}	42.4
P_{50}	49.1
P_{75}	57.1
P_{90}	65.7
P_{95}	71.4
P_{99}	84.0

Doubling the nominal pressure reduces t_{LEL} substantially, consistent with the orifice-flow scaling in which the leak inflow rate increases approximately with the square root of the pressure difference. The relative variability remains of the same order as in Scenario S1, but the entire distribution is shifted toward shorter times.

Appendix D: comparison of sampling strategies

This appendix provides a compact comparison of three uncertainty-propagation strategies for Scenario S1 in the airtight case: simple random sampling (SRS), Latin Hypercube Sampling (LHS), and quasi-Monte Carlo sampling based on scrambled Sobol sequences (Sobol-QMC). The purpose of this comparison is to assess whether the principal output statistics are sensitive to the choice of sampling strategy and to compare the numerical stability of the estimators.

All three methods were applied to the same deterministic model and the same input distributions defined in the main text. The quantities compared were the 5th percentile, median, and 95th percentile of the time required to reach the lower explosive limit, t_{LEL} . To allow a fair comparison with Sobol-QMC, the sample sizes were chosen as powers of two: $N = 4,096$, $16,384$, and $65,536$. For each method and each sample size, five independent runs were performed; Table D1 reports the mean estimated percentiles and the standard deviation across runs.

Table D1. Comparison of sampling strategies for Scenario S1 (airtight case)

Method	N	P5 [s]	P50 [s]	P95 [s]	SD(P95) [s]	Mean CPU time [s]
SRS	4,096	50.30	70.31	102.94	0.949	0.0015
SRS	16,384	50.25	70.22	102.45	0.370	0.0031
SRS	65,536	50.24	70.28	102.35	0.138	0.0130
LHS	4,096	50.28	70.13	102.52	0.304	0.0019
LHS	16,384	50.26	70.20	102.33	0.186	0.0042
LHS	65,536	50.23	70.21	102.27	0.153	0.0192
Sobol-QMC	4,096	50.30	70.29	102.17	0.290	0.0017
Sobol-QMC	16,384	50.25	70.29	102.25	0.112	0.0050
Sobol-QMC	65,536	50.23	70.27	102.24	0.019	0.0107

Mean CPU times are reported for the implementation used in the present study and are intended only as approximate comparative indicators.

Figure D1 shows the convergence of the estimated P95 of t_{LEL} with increasing sample size for the three methods. Error bars indicate the standard deviation across five runs.

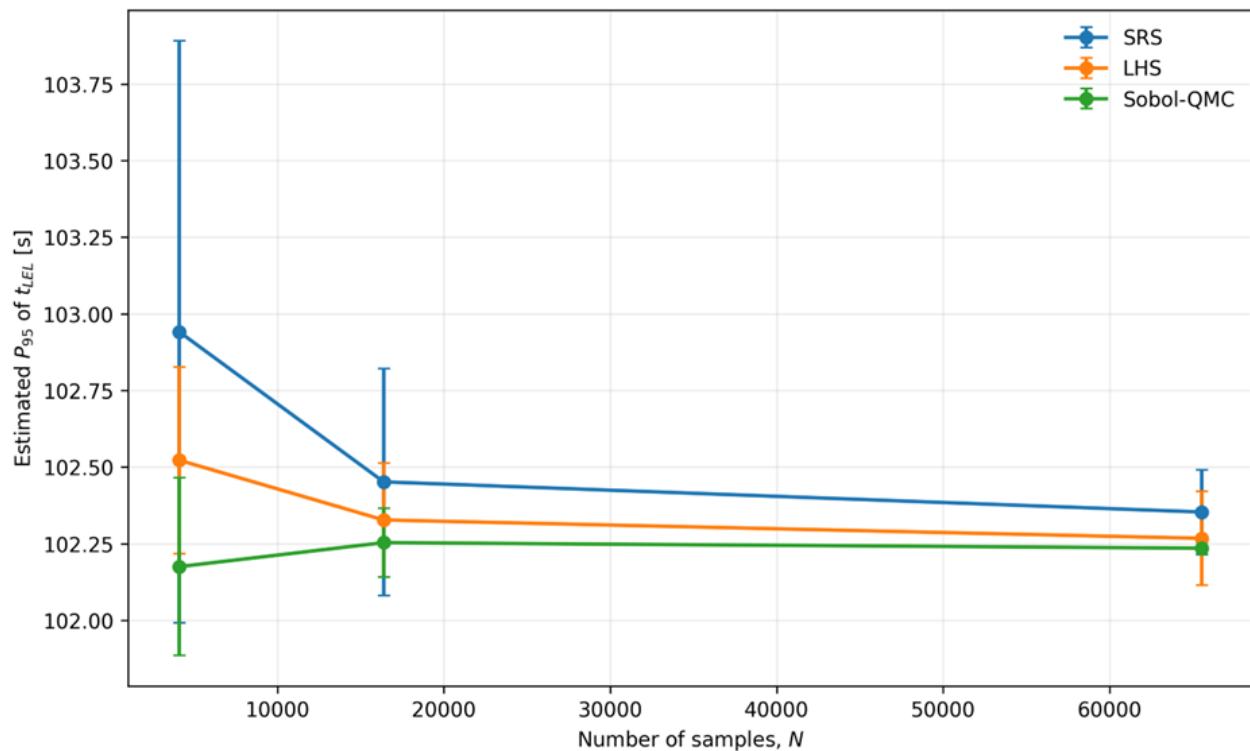


Figure D1. Comparison of sampling strategies for Scenario S1 in the airtight case. Convergence of the estimated P95 of t_{LEL} with increasing sample size for SRS, LHS, and Sobol-QMC. Error bars represent the standard deviation across five independent runs

The comparison shows that all three methods converge toward very similar percentile estimates as the sample size increases, which supports the robustness of the main case-study conclusions. However, for a given sample size, the variance of the estimated P95 is systematically larger for SRS than for the two structured methods. LHS improves the stability of the percentile estimates relative to SRS, while Sobol-QMC provides the smallest inter-run variability at the larger sample sizes considered here.

These results indicate that the main conclusions of the paper do not depend strongly on the particular sampling strategy used, provided that the sample size is sufficiently large. Nevertheless, the comparison also shows that structured designs such as LHS and Sobol-QMC can provide more stable percentile estimates than SRS for the same computational effort, which justifies the use of LHS in the main probabilistic analysis.

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