

DATA-DRIVEN SPATIAL RISK ASSESSMENT OF INDOOR GAS DISPERSION USING KRIGING REGRESSION AND MONTE CARLO UNCERTAINTY ANALYSIS

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Fraunhofer



MOTIVATION AND OBJECTIVE

WHY PROPANE RISK ASSESSEMENT MATTERS

THE PROBLEM

Propane is increasingly used in heat pumps as low-GWP refrigerant--but it's highly flammable.

Leaks in confined or semi-enclosed spaces can result in explosive gas air mixtures, posing severe safety hazards.

Early detection and accurate risk quantification are vital for preventing accidents



CHALLENGES IN QUANTITATIVE RISK ASSESSEMENT (QRA):



Sparse sensor coverage limits spatial resolution



Deterministic models overlook environmental variability



Extrapolating risk beyond sensor range

Project Objective

1



3D Field Reconstruction

Reconstructs 3D concentration fields using **Kriging interpolation** to fill gaps between sparse sensors.

2



Uncertainty Quantification

Quantifies measurement and model uncertainty via **Monte Carlo simulation** for robust risk metrics.

3







Ignition Risk Evaluation

Evaluates overall system safety and ignition probability via **Fault Tree Analysis (FTA)**.

STATE OF THE ART

State of the Art

ASPECT	COMMON INDUSTRY QRA	OUR APPROACH
Concentration Field Estimation	CFD-based	 Kriging interpolation
Uncertainty Treatment	Scenario-based	 Monte Carlo on sensor & model uncertainty
Flammable Volume Estimation	CFD post-processing	 Thresholding on probabilistic 3D field
Safe Distance Estimation	Manual from CFD spread	 Radial extent from LFL field

EXPERIMENTAL SETUP

Campaign 1 – Simple Concept

KEY PARAMETERS

Air exchange ratio (AER)

Refrigerant charge

Leakage flow

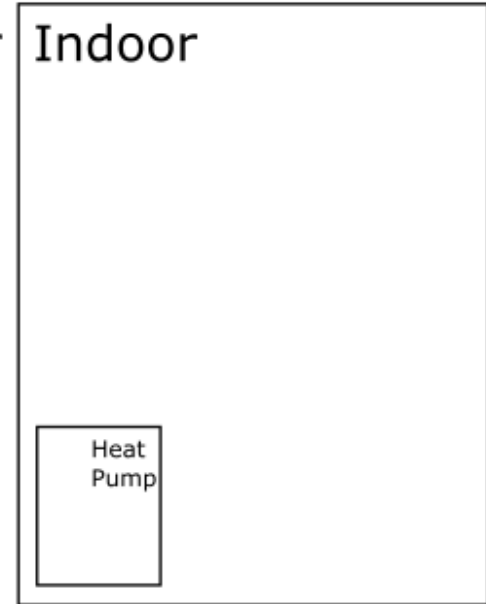
Slot width

OTHER PARAMETERS (CONSTANT)

Held constant or not varied:

Bleed hole Wind speed Ideal mixing Tightness Chimney head

Outdoor Indoor



Setup: Simple closed room with a heat pump inside. No active ventilation or exhaust systems.

Campaign 2 – Internal

KEY PARAMETERS

Air exchange ratio (AER)

Refrigerant charge

Leakage flow

Air flow fan (mixing)

Bleed hole

OTHER PARAMETERS

Held constant or not varied:

Wind speed

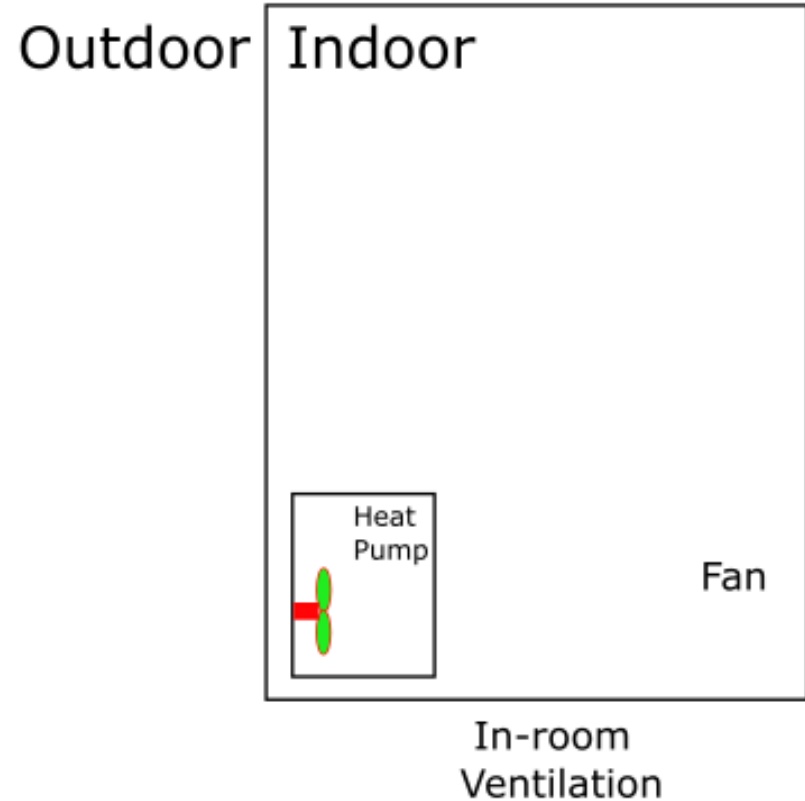
Ideal mixing

Tightness

Chimney head

Slot width

Setup: Same room as Campaign 1, but with an **internal mixing fan** placed inside the room near the heat pump to promote air circulation.



Campaign 3 – External

KEY PARAMETERS

Air exchange ratio (AER)

Air flow fan (external)

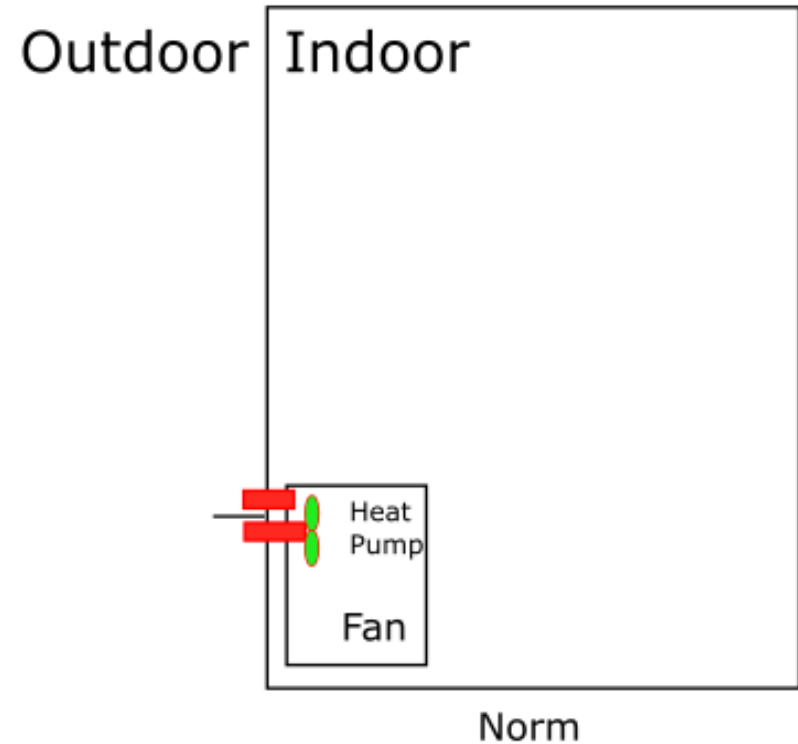
Leakage flow

Slot width

OTHER PARAMETERS

Refrigerant Charge Bleed hole Wind speed Ideal mixing Tightness

Chimney head



Setup: External ventilation fan connected through the wall, drawing air from outside into room. Represents the normative installation approach.

Campaign 4 – Chimney

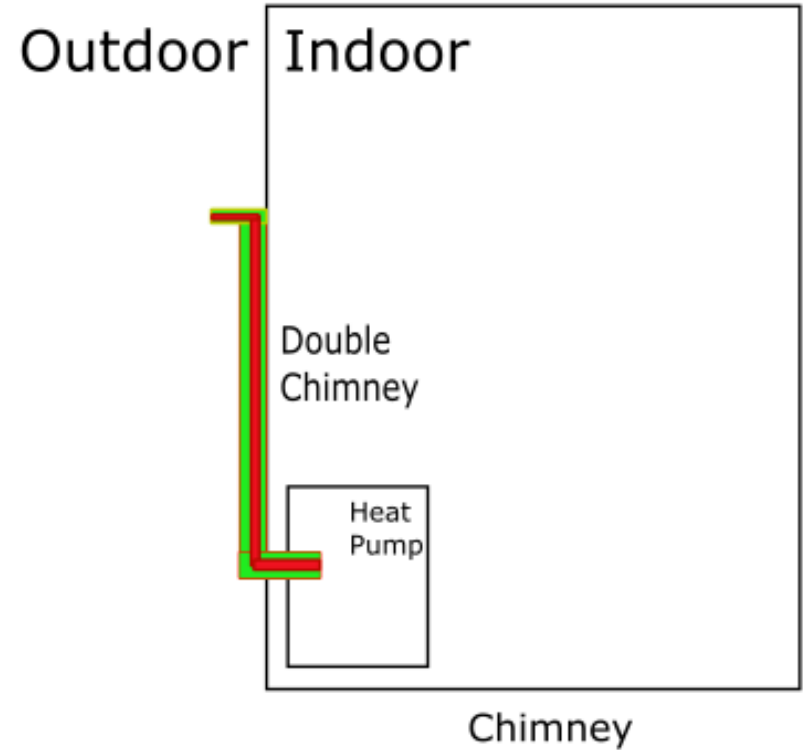
KEY PARAMETERS

Air exchange ratio	Leakage flow
Bleed hole	Wind speed
Ideal mixing	Tightness
Chimney head	Wind scenario

OTHER PARAMETERS

Refrigerant charge Slot width Air flow fan Venturi scrubber Drain check valve

Setup: Heat pump connected to a double chimney pipe extending through the wall. Tests passive ventilation effectiveness under varying wind/tightness.



Campaign 5 – Drainage

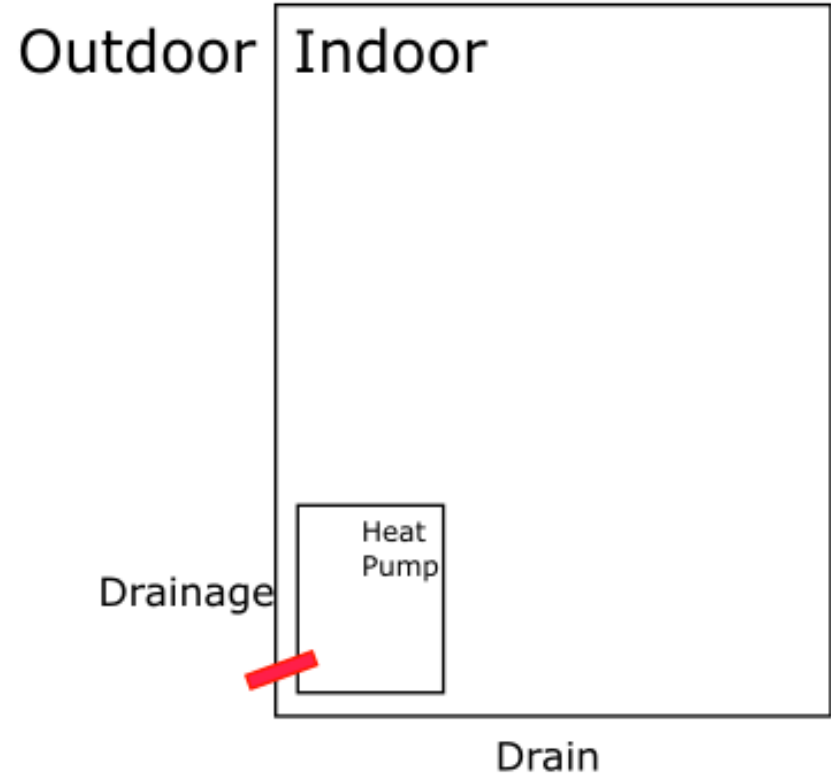
KEY PARAMETERS

Leakage flow	Wind speed
Ideal mixing	Tightness
Chimney head	Wind scenario
Venturi scrubber	Drain check valve

OTHER PARAMETERS

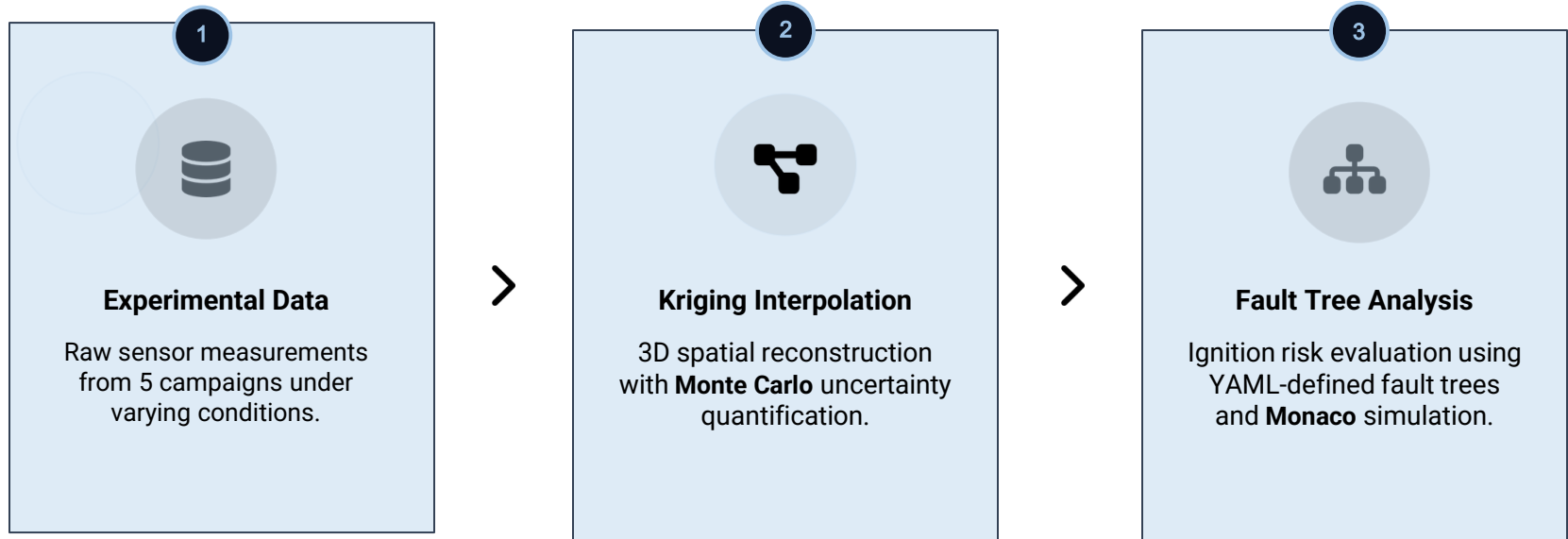
Air exchange ratio Refrigerant charge Slot width Fans (Mixing/Ext) Bleed hole

Setup: Heat pump with a drainage pipe going down through the floor. Tests the effectiveness of drainage-based gas removal under various wind and mixing conditions.



METHODOLOGY

Analysis Pipeline



Experimental Data

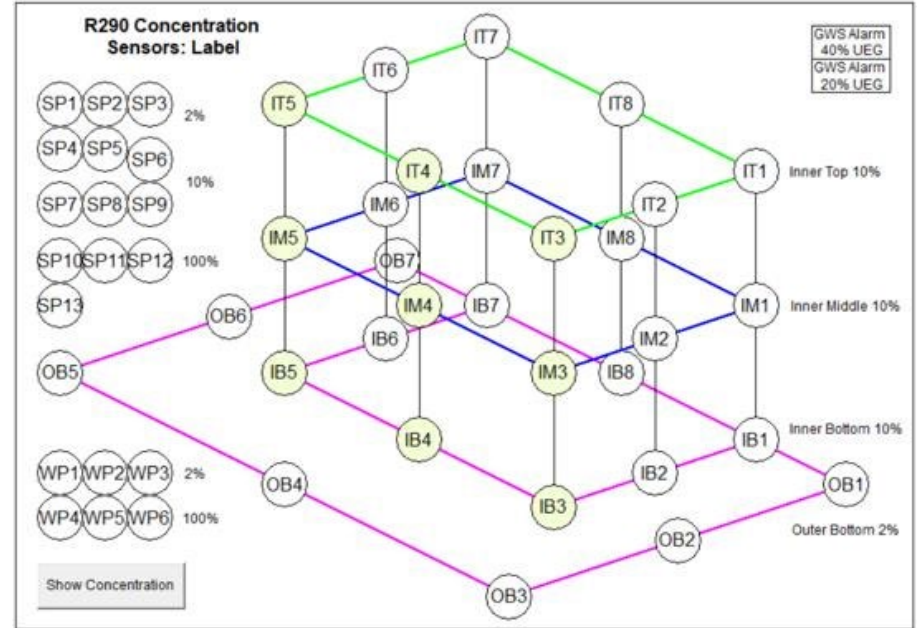
3D Sensor Grid

Deployed across the room at multiple vertical levels to capture spatial stratification.

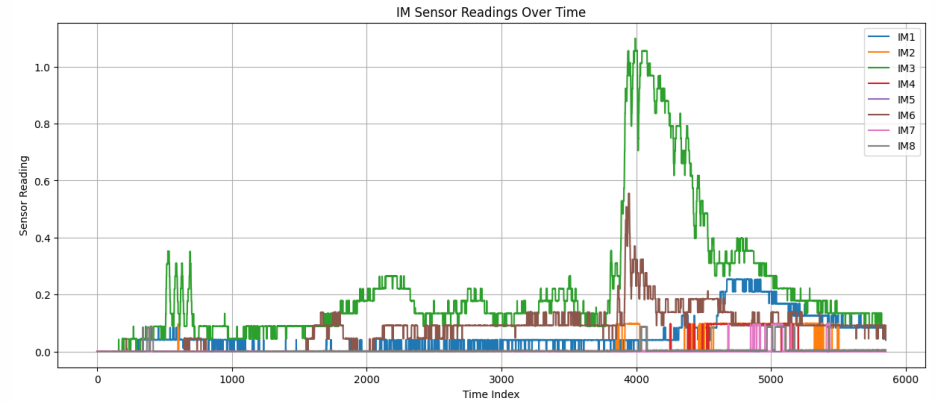
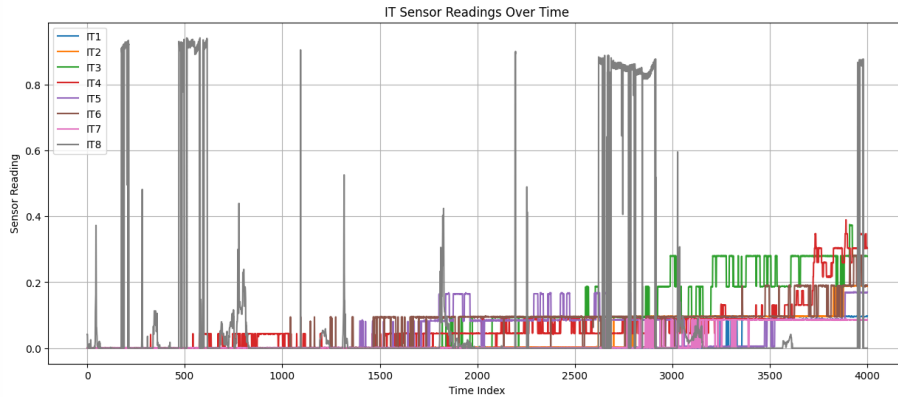
Leakage Campaigns

Varying AER, leak rate, charge, fan use. Outputting time-resolved concentration datasets.

Level	Height	Sensors
IT Inner Top	~34% H	IT1 – IT8
IM Inner Mid	~18% H	IM1 – IM8
IB Inner Bot	~0.2% H	IB1 – IB8
OB Outer Bot	~0.2% H	OB1 – OB7

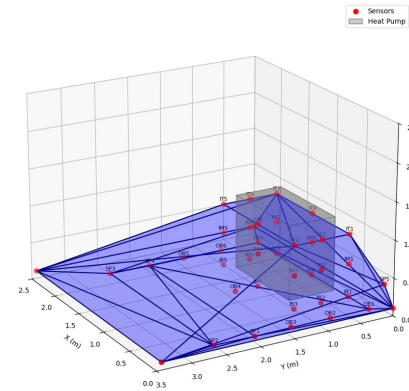
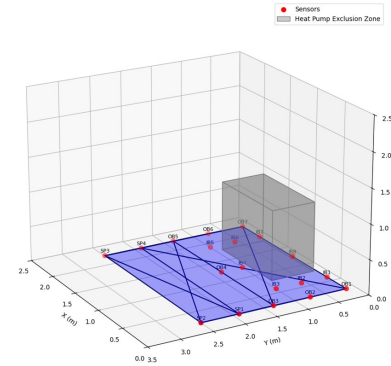
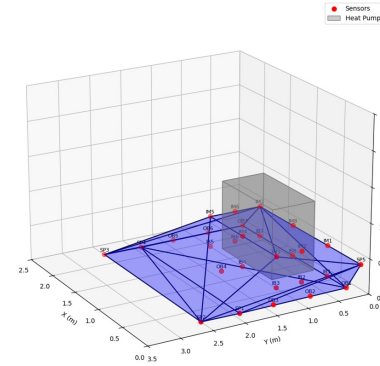


Raw Sensor Data



Smart Interpolation via Kriging

- Interpolation is restricted to the **convex hull** of sensor locations strictly no extrapolation beyond the measured sensor boundary.
- Kriging** estimates unknown concentration values using spatial correlation and weighted sensor data.
- A **Heat Pump Exclusion Zone** is applied to avoid invalid interpolation inside the equipment volume.



Monte Carlo Simulation



1. PERTURB INPUTS

Randomly perturb sensor inputs within realistic noise bounds to simulate measurement uncertainty.



2. INTERPOLATE

Reconstruct 3D concentration fields using Kriging interpolation for each perturbed dataset.



3. QUANTIFY RISK METRICS

Calculate the flammable mixture volume and Minimal safe distance from the leak source

Results Overview

EXPERIMENTAL SCOPE

C1 Closed Room (Baseline)

C2 Internal Mixing (Fan)

C3 External Ventilation (Norm)

C4 Chimney (Passive)

C5 Drainage (Floor)

KEY EVALUATION METRICS

Flammable Volume (V)

Total volume of gas cloud within the flammability limits (LFL – UFL). Indicates the potential severity of an ignition event.

Safe Distance (d)



Minimum distance from the leak source where the concentration drops below the Lower Flammability Limit (LFL).

Probabilistic Approach: All results are reported with 95% confidence intervals derived from Monte Carlo simulations to account for sensor uncertainty.

RESULTS

Campaign 1 Results – Closed Room

KEY OBSERVATIONS

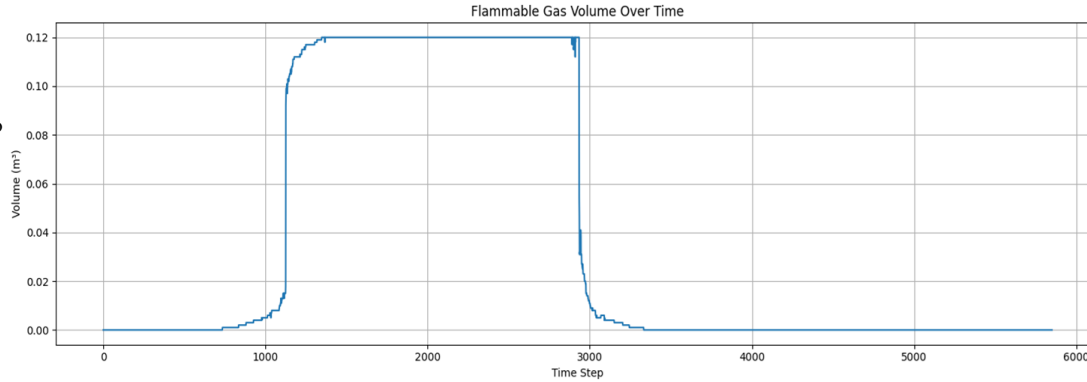
-  **High Accumulation:** Without ventilation, gas accumulates rapidly and persists for extended periods.
-  **Strong Stratification:** Propane (R290) is heavier than air, leading to significantly higher concentrations at floor level.

METRIC	RESULT / VALUE
Max Flammable Volume	~0.12 m ³
Max Safe Distance	> 1.5 m
Stratification Factor	Strong (Bottom > Top)

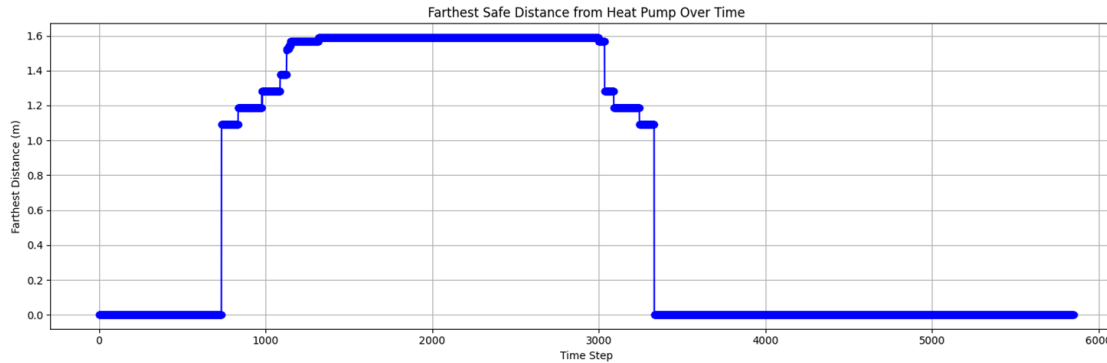
Note: Values represent the worst-case scenario observed across multiple leakage mass flow (3.3 g/s).

Campaign 1 – Time-Series Charts

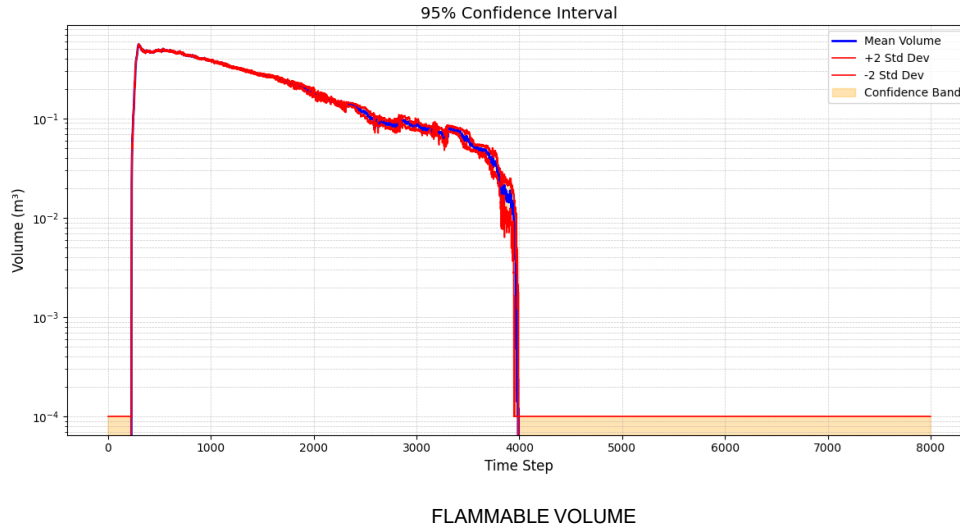
Flammable Volume
Closed Room Scenario



Safe Distance
Distance from Leak
Source



Monte Carlo – 95% Confidence Interval



UNCERTAINTY QUANTIFICATION

The shaded region represents the **95% Confidence Interval** derived from 10,000 Monte Carlo iterations.

SAFETY IMPLICATIONS

Risk assessment must rely on the **Upper Bound** (conservative estimate) rather than the mean, as sensor sparsity can lead to underestimation of the true cloud size.

LOG-SCALE INSIGHT

Uncertainty spans orders of magnitude, especially during the initial leak phase.

Conclusion

METHODOLOGY



Robust Reconstruction: Kriging interpolation successfully reconstructs 3D gas concentration fields from sparse sensor data, overcoming spatial limitations.



Probabilistic Risk: Monte Carlo simulations quantify uncertainty, providing 95% confidence intervals essential for safety-critical decision making.

KEY FINDINGS



Mitigation Hierarchy: External ventilation remains the most effective strategy. Floor drainage offers a viable passive backup for heavy gases like R290.



Mixing Trade-off: Internal mixing eliminates stratification but can temporarily increase the flammable volume by diluting rich cores.

"A scalable, data-driven framework for Quantitative Risk Assessment of indoor heat pump installations."

Beyond This Thesis

Open to Opportunities in AI & Intelligent Systems



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OPEN TO OPPORTUNITIES

- Applied AI & Machine Learning
- Scientific Machine Learning
- AI for Physical Systems
- Data Science & Digital Twins
- Research Engineer / AI Engineer roles
- PhD positions in AI & Intelligent Systems

"Passionate about building reliable AI systems that turn sparse and uncertain data into actionable decisions."

Acknowledgments



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