

Chemical Hazards Information System

AI-Powered Decision-Support System for Laboratory Chemical Hazard Assessment

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

THE PROBLEM: COGNITIVE OVERLOAD



Time Intensive: Manual reviews take hours per experiment, delaying research.



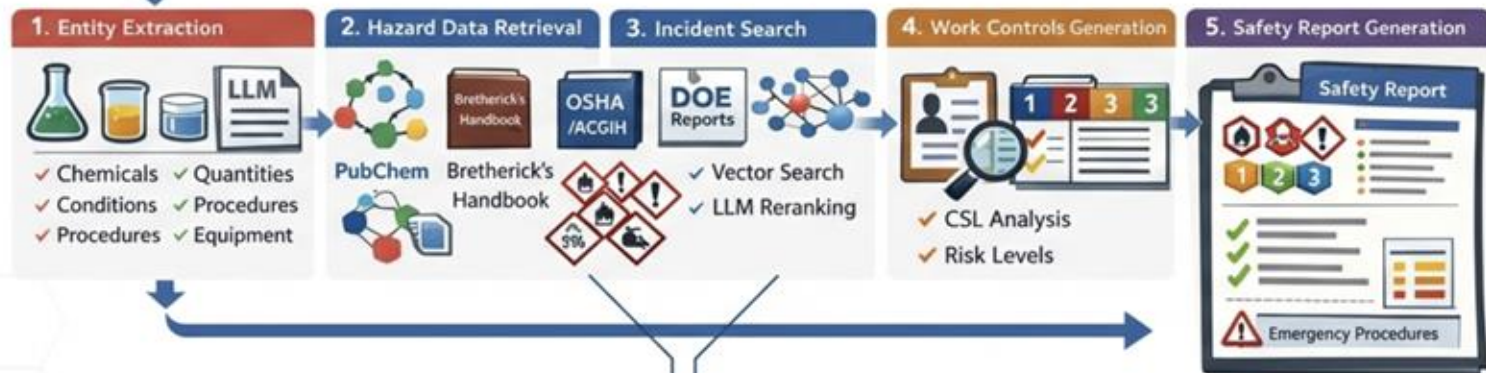
Human Error: Safety data is scattered across SDS, reactivity databases, and archives.



Information Overload: Narrow margins for error; oversights lead to injuries or environmental harm.

Solution: Unified Intelligence System

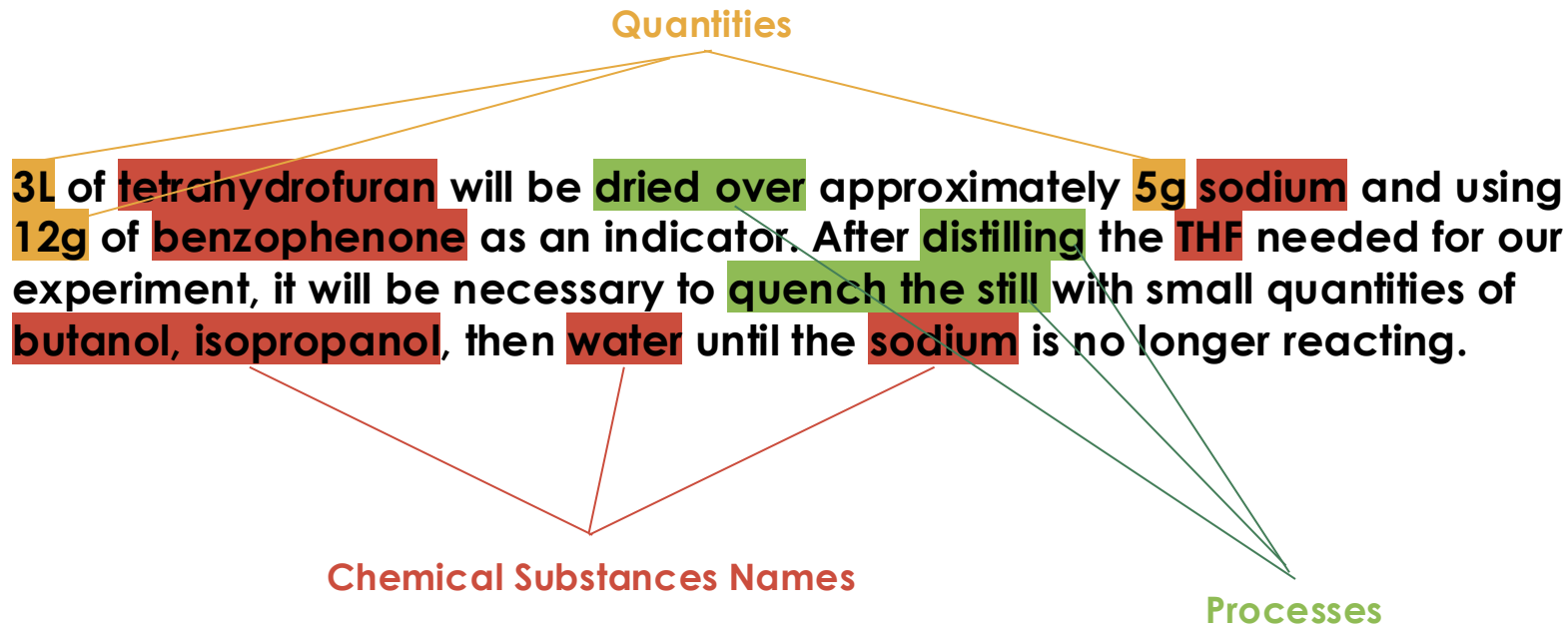
Input: Natural Language
Experiment Description



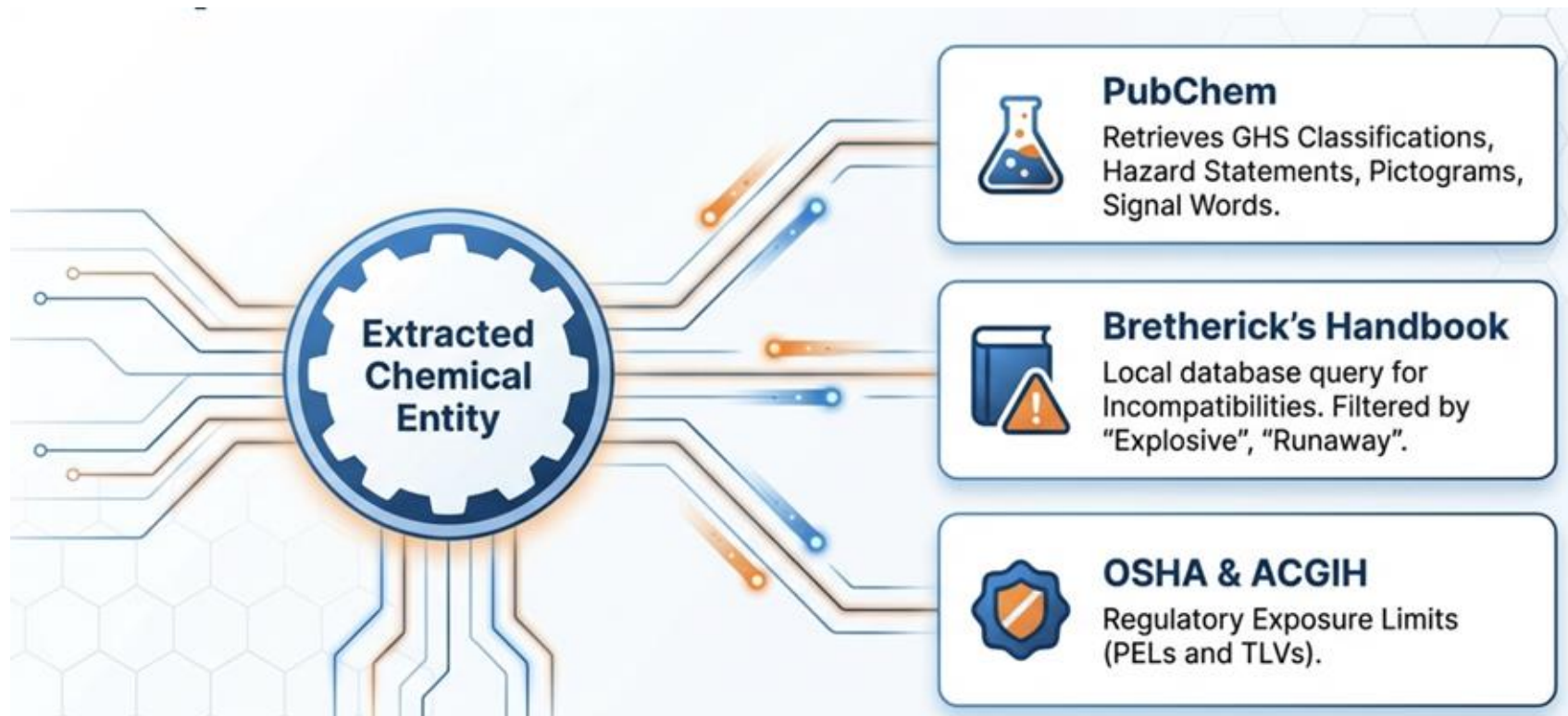
Output: Comprehensive
Decision Support Report

Core: Hybrid Retrieval
& Multi-Source RAG

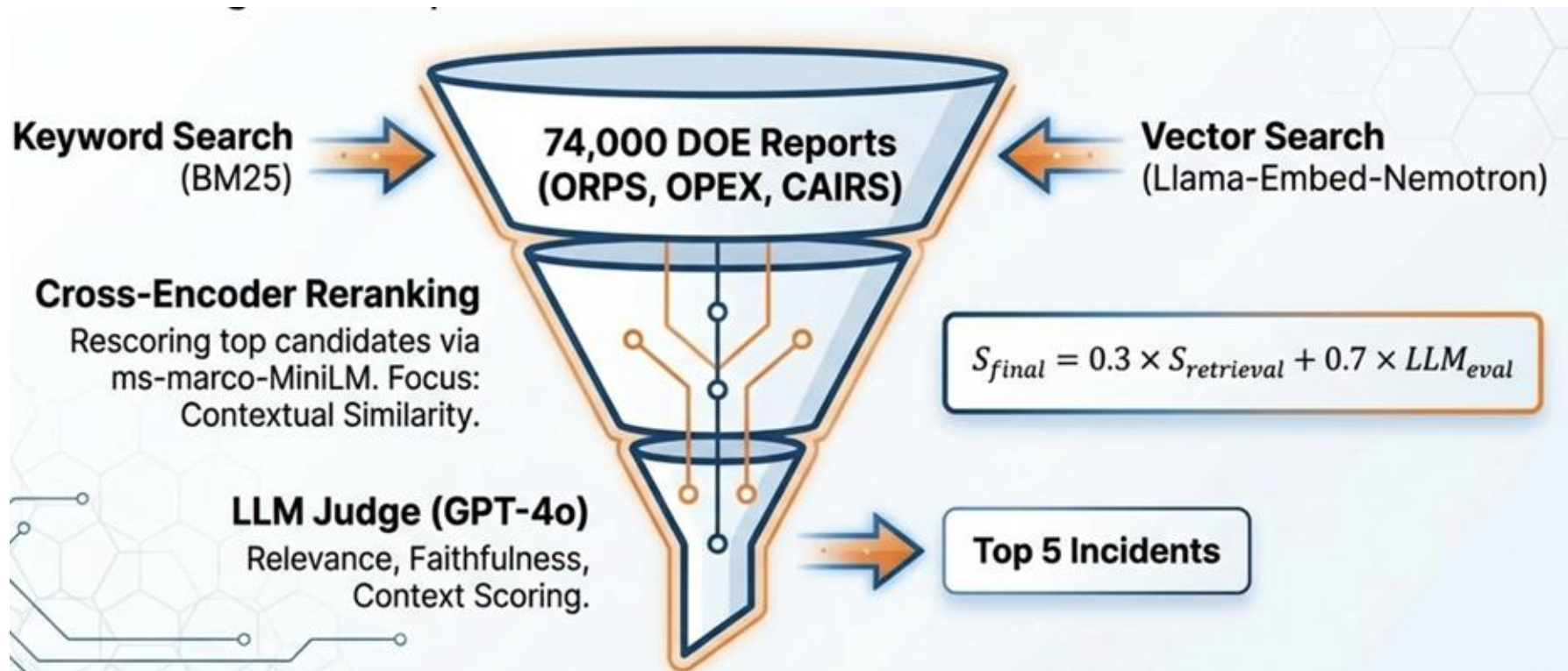
Step 1: Structured Entity Extraction



Step 2: Multi-Source Data Retrieval



Step 3: Hybrid Incident Search



Step 4: ABHA Suggestions

IR Risk Level	IR Work Step	IR Hazards	IR Work Controls	IR Critical (Y/N)
Medium	Preparation of drying setup	Chemical exposure to tetrahydrofuran Fire hazard from sodium Chemical exposure to benzophenone	Wear gloves and goggles Use a fume hood Wear gloves and goggles	Y
High	Drying tetrahydrofuran with sodium and benzophenone	Exothermic reaction with sodium Flammable vapors from tetrahydrofuran Chemical exposure to benzophenone	Use a dry ice and acetone bath to control temperature Perform under argon purge Wear gloves and goggles	Y
High	Distillation of dried tetrahydrofuran	Thermal hazard from heating mantle Flammable vapors from tetrahydrofuran Pressure buildup	Monitor temperature closely Ensure proper ventilation Use a pressure relief valve	Y
High	Quenching of sodium residue	Violent reaction with water Flammable vapors from alcohols Thermal hazard from exothermic reaction	Add quenching agents slowly and in small quantities Perform under argon purge Use a dry ice and acetone bath	Y
Medium	Monitoring and maintaining argon purge	Inert gas asphyxiation Equipment malfunction	Ensure proper ventilation Regularly check equipment for leaks	N
Medium	Cleanup and disposal	Chemical waste disposal Residual chemical exposure	Follow chemical waste disposal guidelines Wear gloves and goggles	N

The Final Output: Comprehensive Safety Report

1. Scope/Description

3L of tetrahydrofuran will be added over approximately 1g sodium and using 12g of bromophenol as an indicator. After distilling the THF needed for our experiment, it will be necessary to quench the stir with small quantities of isohexanol, isopropanol, then water until the sodium is no longer reacting. Both distillation and quenching will be performed under an argon purge. A dry ice and acetone bath will be used to control the heat from the quench. Equipment used will include a 4L round bottom flask, condenser, and heating mantle.

2. Materials/Equipment List

Extracted Materials/Equipment:

- 4L round bottom flask
- condenser
- heating mantle
- dry ice and acetone bath

3. Chemicals List

1. tetrahydrofuran

General Information

• Quantity: 3 L

• CAS Number: 109-99-9

Safety Data Sheet (SDS)

[View SDS](#)

Exposure Limits (TLV)

• TWA (8-hour): 50 ppm

• Notations: Skin, H3

• STEL (15-min): 100 ppm

• TLV Basis: CRT (H, CNS, Impair), Kidney dam.

Hazard Information (SHS)

▲ GHS Pictograms:



• Signal Word: Danger

• Flammability Class: 1B

• Flammability: Highly Flammable

Hazard Statements (H-Codes):

• H225: Highly flammable liquid and vapor

• H319: Causes serious eye irritation

• H335: May cause respiratory irritation

• H351: Suspected of causing cancer

2. sodium

General Information

• Quantity: 5 g

• CAS Number: 7632-90-5

Safety Data Sheet (SDS)

[View SDS](#)

Exposure Limits (TLV)

• TWA (8-hour): 5 mg/m³

• Notations: A4

• STEL (15-min):

• TLV Basis: Skin, eye, & URT (ir)

Hazard Information (SHS)

▲ GHS Pictograms:



Flammable
H



Corrosive

• Signal Word: Danger

• Flammability Class: None

Hazard Statements (H-Codes):

• H260: In contact with water releases flammable gases which may ignite spontaneously

• H314: Causes severe skin burns and eye damage

FUTURE WORKS



Equipment Analysis

Advanced monitoring and predictive maintenance for lab instruments



Hazards Prediction for New Chemicals

AI-driven toxicity and reactivity forecasting for novel compounds.



Waste Management Integration

Seamless system for tracking and optimizing chemical waste disposal.