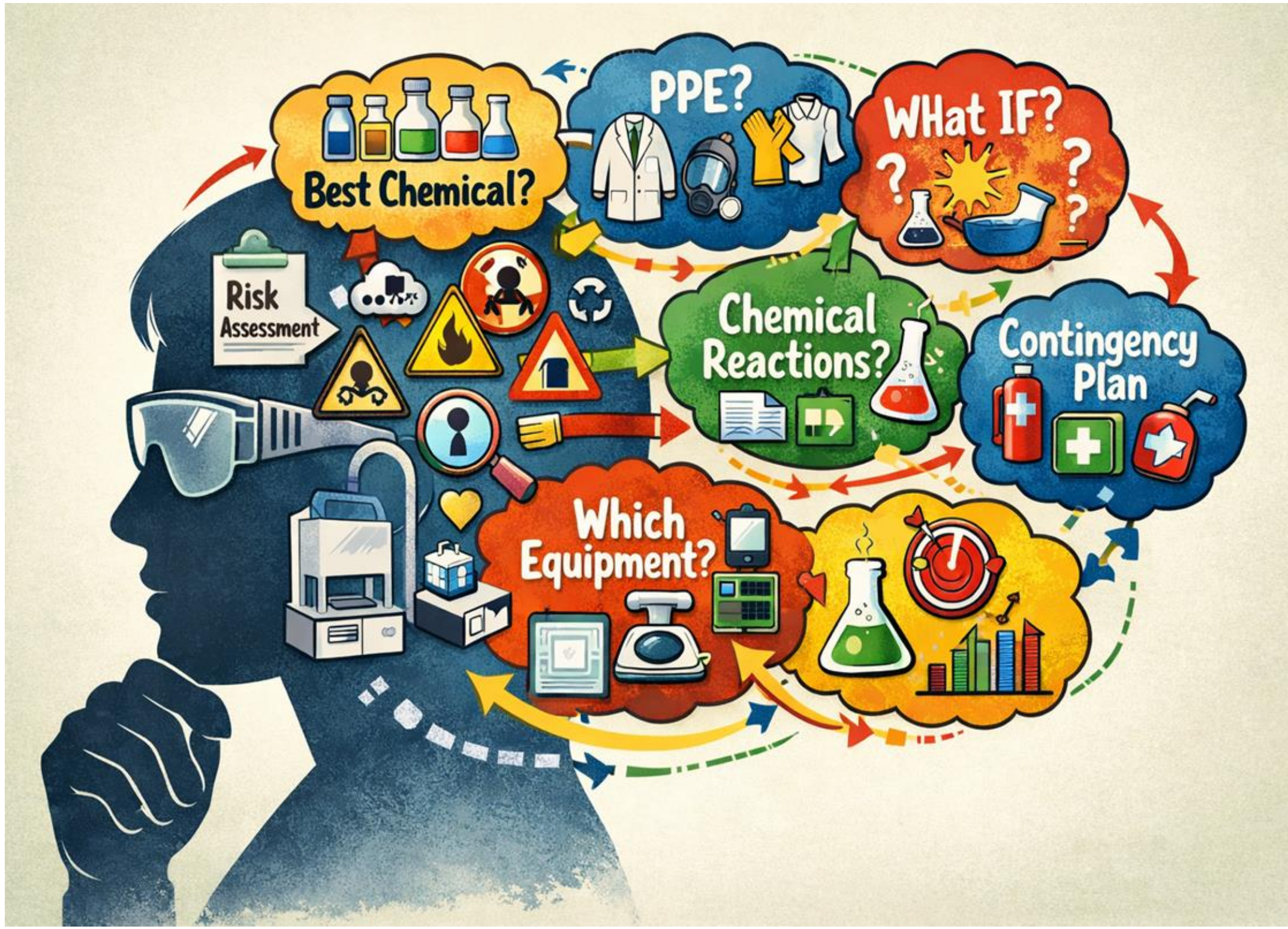


ChemSafe: AI Powered Chemical Hazard Assessment

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Introduction



Problem statement:

Chemical incidents in labs are *preventable* but require comprehensive hazard analysis.

The bottleneck:

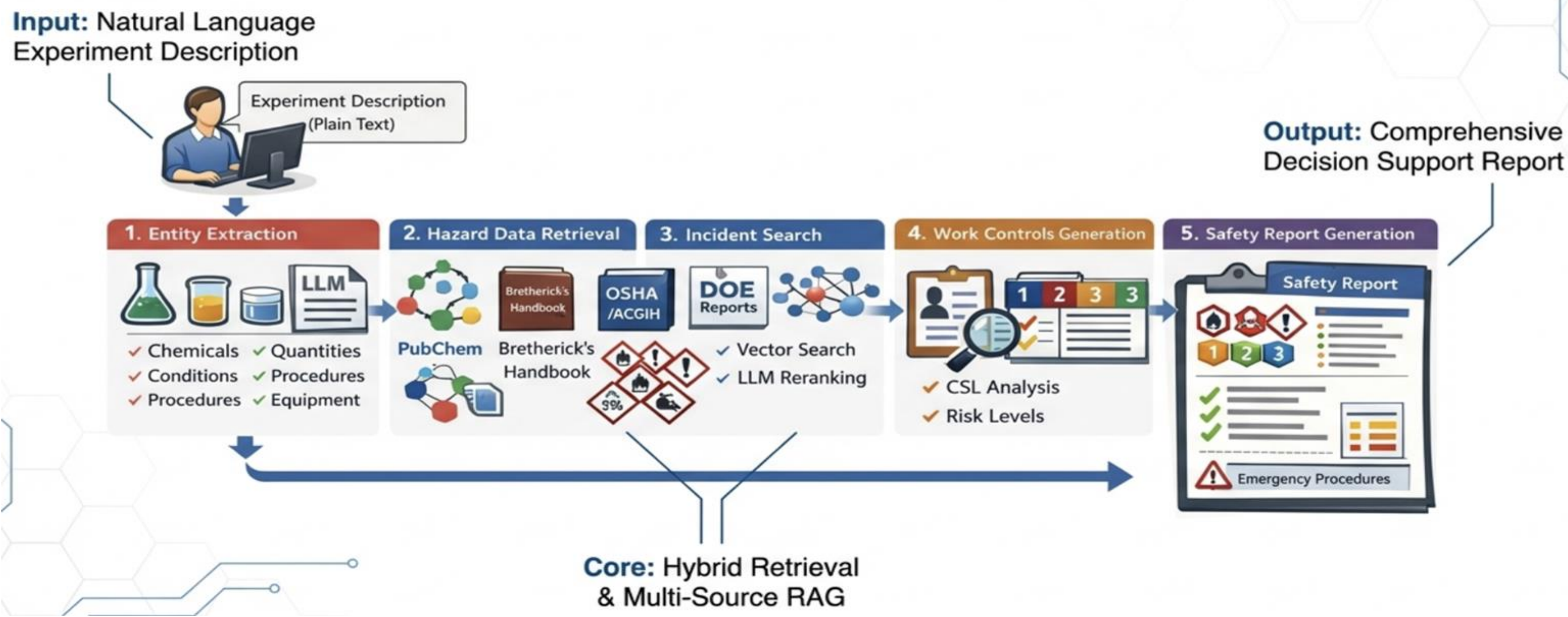
Manual analysis is time intensive and prone to errors.

Our Solution: ChemSafe

An AI-powered decision-support system that automates laboratory chemical hazard assessment by integrating Large Language Models with authoritative safety data sources. It is:

- Fast
- Efficient
- Citation grounded,
- Feedback-driven iteration.

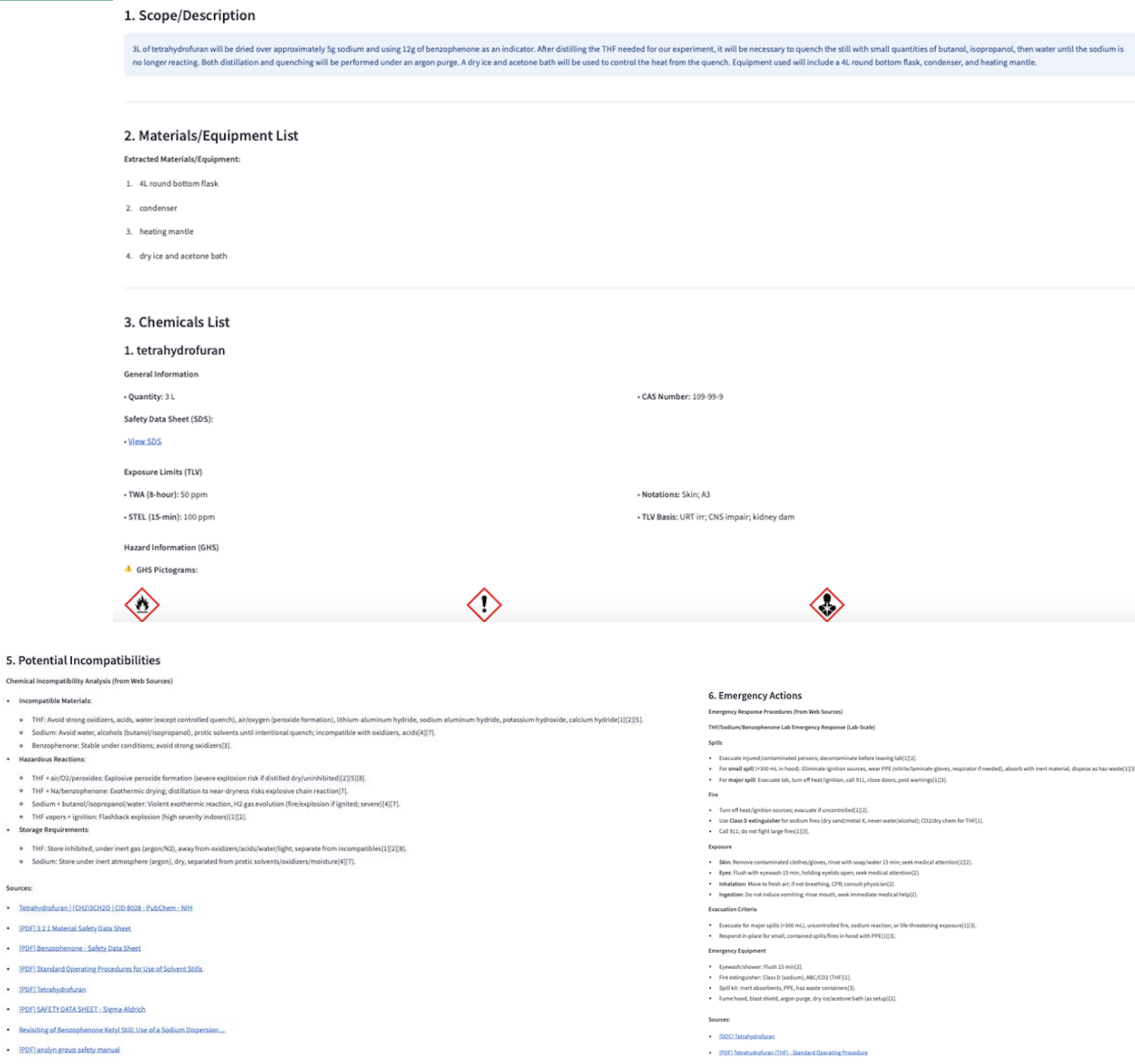
ChemSafe Workflow



System Components

- **Entity Extraction:** The input module; Structured entities are extracted from the input experiment
- **Multi Source Hazard Data Retrieval:** For each chemical, retrieves: GHS classifications from PubChem, chemical incompatibilities from Bretherick's Handbook, and OSHA PELs / ACGIH TLVs.
- **Hybrid Incident Search:** Searches 74,000 reports from 4 DOE databases (ORPS: 45K, OPEX: 18K, CAIRS: 8K, ORNL: 3K) to retrieve most relevant events.
- **Activity Based Work Controls:** Decomposes experiments into discrete work steps; identifies hazards, recommends controls from, assigns risk levels, and flags critical steps.
- **Safety Report Generation:** Integrates all components into a tabbed report: GHS hazards with pictograms, incompatibilities, exposure limits, past incidents, work controls, AI safety analysis, and emergency procedures. Exportable as PDF.

Results



Conclusion

ChemSafe provides a comprehensive framework that addresses laboratory chemical safety from multiple angles: integrating fragmented hazard data from authoritative sources to eliminate information gaps, leveraging hybrid retrieval with LLM-based evaluation to surface relevant historical lessons that prevent repeated mistakes, and automating critical safety documentation to ensure hazards are systematically identified rather than overlooked.

Acknowledgement

This research used resources of the Oak Ridge Leadership Computing Facility (OLCF), which is a DOE Office of Science User Facility at ORNL supported by the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.