Parsing the Chemical Risk Assessment Process for the Laboratory

Ralph Stuart
Chemical Hygiene Officer, Keene State College

Keene State College
Wisdom to make a difference.

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Why Risk Assessment?

• My grandfather graduated from high school in 1919, before the periodic table was used as a teaching tool; he spent 30 years in the Niagara Falls chemical industry as a research lab tech. He brought home CCl₄ to do laundry with.

• My father graduated with an agricultural degree from Cornell in 1951; he spent 5 years working in Cornell's labs and orchards testing pesticides in the 1950's.

• I graduated with an engineering degree from Cornell in 1979; in the 1980's I spent 5 years as an academic lab tech conducting environmental chemical analyses.
The Chemical Safety Tradition: Rules Based Safety

• Caveat emptor: Chemistry textbooks and laboratory manuals provide a overview of generic rules, usually followed by "see the MSDS for further instructions".
The Continuing Evolution of Science

Lab science in the 21st Century is an emerging complex system which highly values converging knowledge.

Changing Science, Changing Learning Styles

Science Paradigms

- Thousand years ago: science was empirical describing natural phenomena
- Last few hundred years: theoretical branch using models, generalizations
- Last few decades: a computational branch simulating complex phenomena
- Today: data exploration (eScience)
  - Data captured by instruments or generated by simulator
  - Processed by software
  - Information/knowledge stored in computer
  - Scientist analyzes database/files using data management and statistics

FIGURE 4-2. The web of faculty interactions created by Bio-X. The network of faculty interactions across Stanford has expanded since the establishment of the Bio-X program. The resulting network reportedly appeals to technology com-
The Limits of the Chemical Safety Tradition

• Reports by the National Research Council, the Chemical Safety Board and the NFPA after specific laboratory safety incidents found the rules-based approach to chemical safety education and information inadequate.
A Cultural Watershed: The 2011 Report from CSB

Concerns about Research Lab Safety
Another Emerging Issue: Safety in the Chemistry Classroom

Demonstration methanol fires in high schools and public settings:

1. New York City, January 2014
2. Reno, Nevada, September 2014
3. Denver, Colorado, September 2014
4. Raymond, Illinois, October, 2014
5. Chicago, November, 2014
7. Washington, DC, October 30, 2015

18 incidents alcohol-fueled fires from educational demos injured at least 72 people since 2011
Managing chemical hazards in the lab integrating 5 strategies into a system:
1. Hazard Reduction
2. Engineering Controls
3. Training and Oversight
4. Personal Protective Equipment
5. Emergency Planning and Environmental Protection

Organizing such a system requires conscious thought and documented planning. This skill involves education rather than training.
Emerging Risk Assessment Educational Tools

• The logic for developing the system is described in emerging tools available since 2010.
  – The **Globally Harmonized System**
  – The RAMP paradigm from **Laboratory Safety for Chemistry Students** (Hill and Finster)
  – *Identifying and Evaluating Hazards in Research Laboratories* from the ACS
Using Information in the Lab Risk Assessment Process

- To support safe science while protecting research, safety information must be scalable, transferable and sustainable.
- These goals entail describing the safety use case using ontology and curation tools and applying the logic developed established by the CH&S community to the use of these tools.
Laboratory Use Cases to Consider

• **Teaching laboratory setting:** short term use of specific chemical concentrations in procedures with expected outcomes; close oversight of inexperienced lab workers by experienced personnel can be assumed.

• **Research laboratory setting:** evolving use of chemicals with uncertain process outcomes for lengths of time determined by results of work; diverse group of lab workers with loose supervision by experienced personnel.

• **Service laboratory setting:** long term use of specific chemicals in similar processes with reproducible outcomes on an long term basis.
Sample Lab Safety Questions

- Does the use of this chemical require the use of a fume hood or other local ventilation system?
- What PPE is appropriate for the use of this chemical?
- What waste disposal protocols are required to legally dispose of this chemical?
- Are unusual emergency response protocols necessary for work involving this chemical?
- Are the specific chemical reactivity hazards associated with the use of this chemical that all users should be aware of?
The Current Context of Chemical Safety Information

- **Caveat emptor**: Chemistry textbooks and laboratory manuals provide a overview of generic rules, followed by "see the MSDS".
- For example, Wikipedia provides links to random MSDS sources with no evidence of why that source is selected; some sources are kaput, many are dated.
The Structure of Chemical Safety Information

Increasingly well-defined; also increasing voluminous

Chemical Safety Information Source Hierarchy

- 1970's: Raw Data in Disparate Sources
- 1980's: Merck Index, Brethericks
- 1990's: Suppliers' Legal Requirements
- 2000's: GHS Definitions
- 2010's: NRC Examples

Type of Source

Basis for Data Provided

Increasingly well-defined; also increasing voluminous
Less Structured Chemical Safety Information

Scientific Audiences (Principal Investigators)
- Flashpoint
- LD50's
- Odor threshold

Bench Chemists (lab staff)
- Flinn's List of the “40 Devils”
- Not Voodoo “Rookie Mistakes”
- Word of Mouth

Lab Lore and Lessons Learned

PubChem data collection and data views

Wikipedia ChemBoxes

Institutional Policy Statements and Procedures
- Emergency Response Plans
- Waste Disposal Programs
- Ventilation Support
- General training Support

Process Oriented

Chemical Based

The General Public (Students)
- GHS statements
- NFPA diamonds
- Miscellaneous notes in the wiki article

External Audiences (Funders and Regulators)
Looking for Structure in the Electronic Data

- How large is the PubChem chem safety information universe?
- How high quality is it (including consistency & provenance information)?

Key safety information fields:
- GHS class designation(s) and signal word
- NFPA diamond information

PubChem data collection and data views

Wikipedia ChemBoxes

Millions of chemicals; 3500 with GHS info

How much overlap is there between the two?

How large is the Wikipedia chem safety information universe?
- How high quality is it?
Project Overview

Objective is to analyze how many chemicals in the PubChem LCSS have GHS and NFPA data in the Wikipedia Chembox

Download list of Chemicals from PubChem Containing LCSS

Use Excel to filter the download of information to only PubChem CIDs

Use Google Sheets to pull NFPA 704 data from Wiki Chembox for Wiki Names

Use Google Sheets to convert InChI Keys to Wiki Names

Use Google Sheets to analyze data

Use Google Sheets to pull GHS Hazard Statements from Wiki Chembox for Wiki Names

Use Google Sheets to pull NFPA 704 data from Wiki Chembox for Wiki Names

Use PubChem Identifier Exchange to convert List of CIDs to InChI Keys

Future Goals to compare Safety Information of Wikipedia to PubChem
The Early Statistics

- PubChem has an LCSS view for about 3500 (2000 more to come soon) chemicals; Wikipedia has Chemboxes for about 10,000 chemicals
- Of those in the PubChem LCSS collection, about 30% have an entry in Wikipedia
- 4% of the Pubchem collection has GHS information; 12% of the PubChem collection have NFPA diamond information

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<th>Not in Wikipedia</th>
<th>In Wikipedia</th>
<th>GHS Hazard Statement</th>
<th>NFPA 704</th>
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<td>29.78%</td>
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Conclusions

• Risk assessment is an information process and provides a significant educational opportunity for concurrently teaching safety and information literacy.

• Safety information is currently not well organized for lab use

• Understanding how to organize safety information requires envisioning who and how this information will be used.

• Leveraging this opportunity will require collaboration between EHS, chemical information professionals and chemical educators.