Keene STATE COLLEGE

Wisdom to make a difference.

Parsing chemical safety information sources

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Virtual Presentation in
"Data Science and the Chemistry Ecosystem"

Venue Acknowledgement

This virtual presentation is made possible by decades of computer science research supported by the federal government which led to the development of the modern Internet and the platforms it supports.

The presentation is based on my professional work supported by salaries from the University of Vermont, Cornell University and Keene State College. ACS IPGs also supported the work that contributed to this presentation.

This story I am sharing encompass the experiences of people I have interacted or heard the stories of with in these roles over the years, but is told from my white male perspective.

A Case Study of the Chemical Safety Information Challenge

- Dr. Karen Wetterhahn was Dartmouth University chemistry professor. Her lab explored heavy metals in the environment, focusing on mercury.
- She died in 1996 of mercury poisoning; she was exposed once to a few drops of dimethylmercury, which penetrated her latex gloves
- OSHA investigated and determined that Dartmouth's Chemical Hygiene Plan and glove selection criteria were inadequate; Dartmouth was fined $9,000

Dr. Karen Wetterhahn

Experimental Design and Exposure

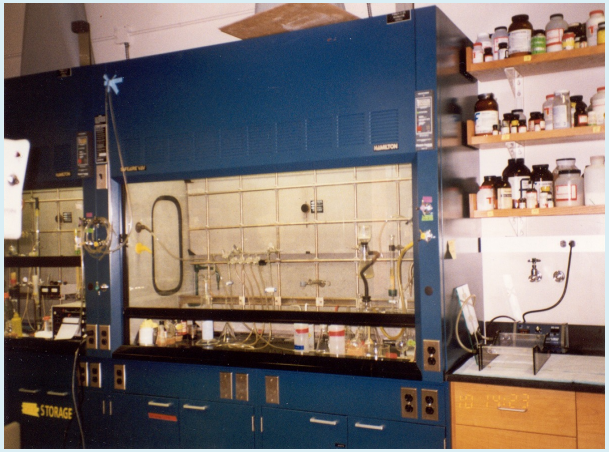
The standard NMR reference for mercury was dimethylmercury (DMM). However, due to its toxicity, Dr. Wetterhahn's lab substituted mercury chloride to make standard concentrations.

The lab switched to DMM after finding the Hg levels in some protein samples were not what the researcher thought they should be.

While transferring liquid DMM, several drops were spilled on the back of Dr. Wetterhahn's gloved hand.

After several days, she started to notice neurological symptoms of Hg exposure and 22 days after initial symptoms she became comatose.

She died 298 days following exposure.

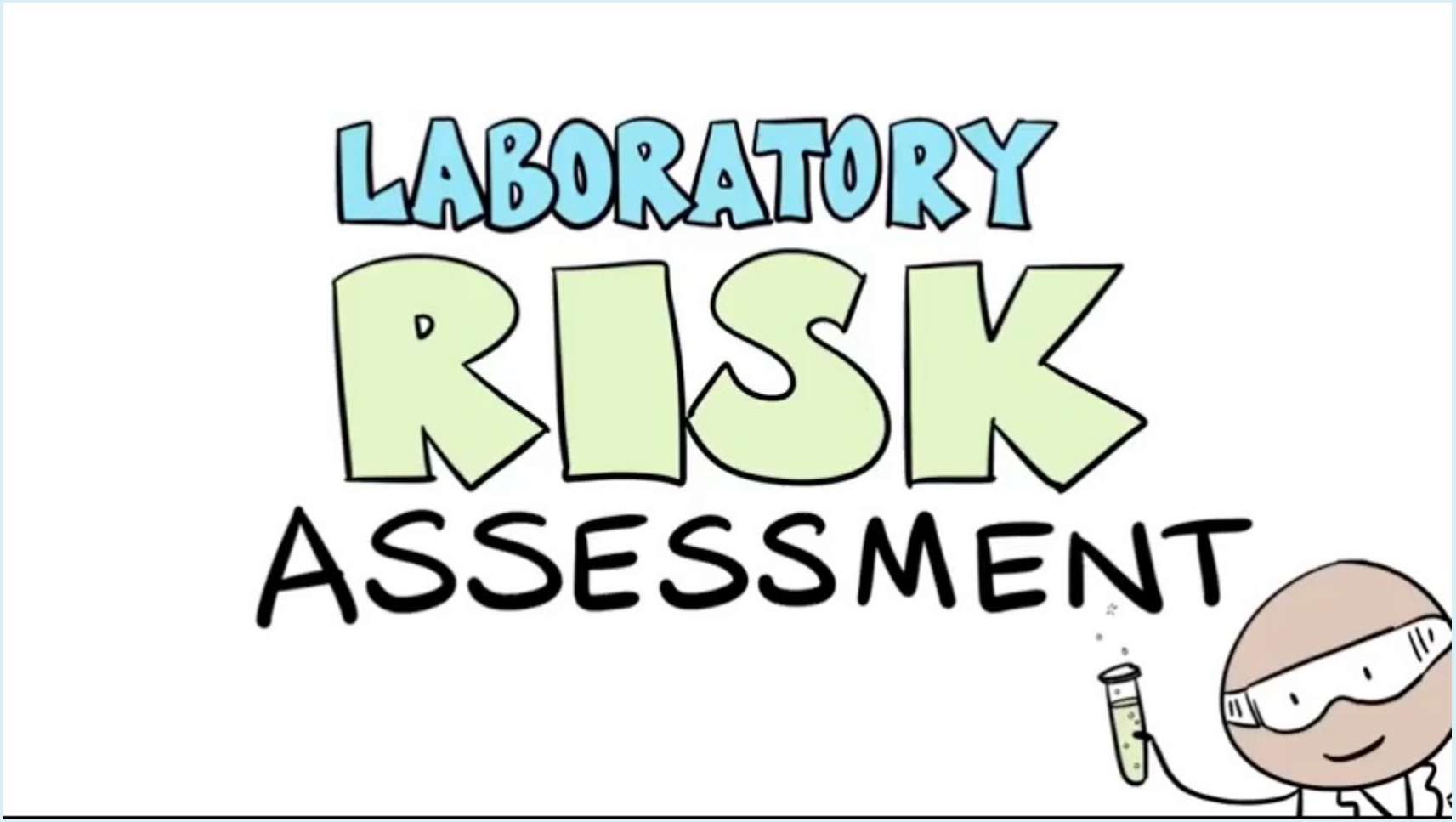


Follow Up Work on Glove Suitability

- It was observed that over the course of 9 months, the contents of the plastic capped NMR tube from the incident evaporated
- Dartmouth hired a lab to test gloves for DMM permeation rates:
  - PVC/latex <15 sec
  - Nitrile 15 sec
  - Neoprene <10 min
  - Butyl < 15 min
  - Viton < 15 min
  - Silver Shield > 240 min

Respiratory Protection: NIOSH/MSHA appr
breathing apparatus.
Ventilation- **Local exhaust:** Fume hood w
smooth even
Mechanical: Not adequate
Special: Glove box vented
Other: Not required
Protective Gloves: Rubber
Eye Protection: ANSI approved safety gl
Other Protective Equipment: Lab coat an
resistant coveralls, eyewash capable of
drench shower and hygienic facilities fo

The RAMP approach to Risk Assessment

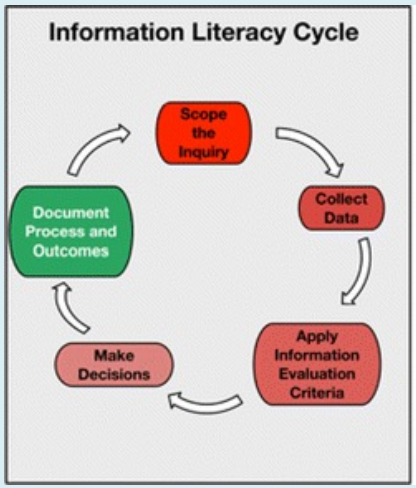


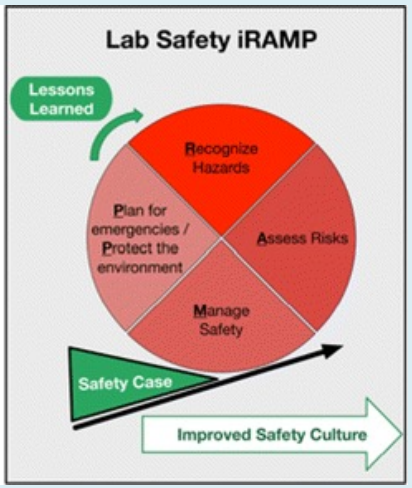
RAMP Chemical Safety Information Tools

Recognize:

The Globally Harmonized System

- Chemical labels
- Safety Data Sheets





Assess:

Field data

- Chemical procedure literature
- Informal communications
- Crowd sourced information / Word of Mouth

Minimize / Manage:

Control bands for ventilation, training and PPE

Plan / Protect:

Institutional emergency planning and emergency response services

Participants in the Chemical Safety Information System

Recognize

- Chemical Information Community
- Provide effective access to core information

Assess

- Chemists
- Understand impact of local conditions on risks identified in the literature

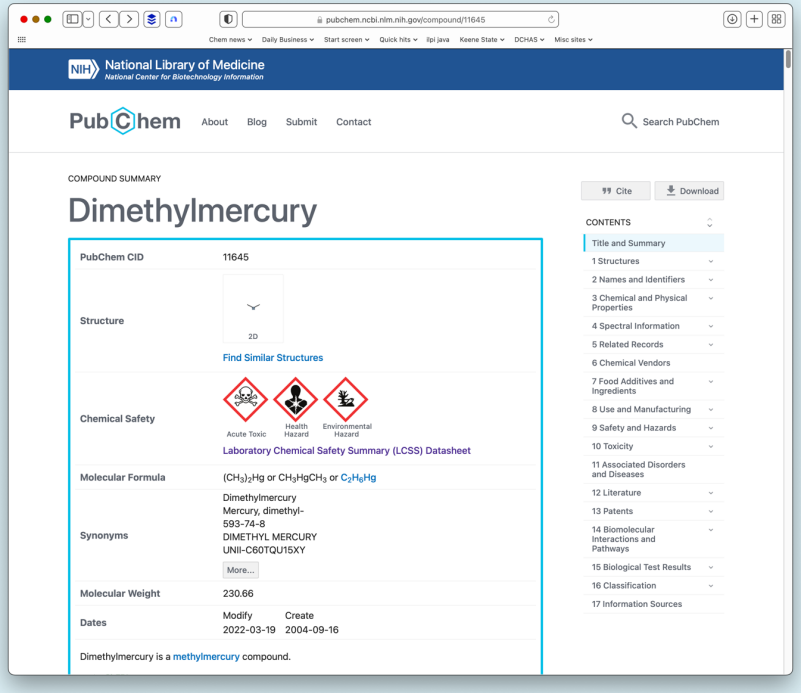
Minimize and Manage

- EHS professionals
- Develop control bands for mitigation measures

Plan and Protect

- Hazmat responders
- Waste disposal services

Information Literacy in the Chemical Safety Information System: a GHS example



Questions related to the Wetterhahn story:

1. Assessment: Which are the most important risks associated with DMM?
2. Minimize: Why was she using DMM in a fume hood?
3. Minimize: Is the personal protective equipment information on the SDS adequate?
4. Emergency Planning: How can when one recognize an exposure has occured?

PubChem Laboratory Chemical Safety Summary for DMM
https://pubchem.ncbi.nlm.nih.gov/compound/11645

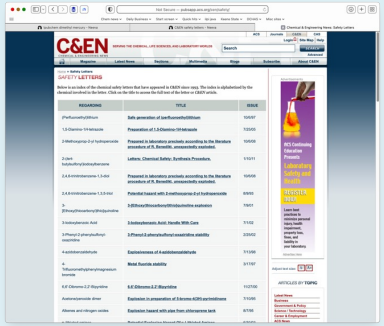
Connecting FAIR and RAMP

Venues for Communicating Safety Information in Curated Publications

ACS Journals – Author Guidelines: Safety Considerations

Authors must emphasize any unexpected, new, and/or significant hazards or risks associated with the reported work. This information should be in the Experimental Section of a full article and included in the main text of a letter. Statement examples can be found in the Safety Statement Style Sheet and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here (https://pubsapp.acs.org/paragonplus/submission/ACS_Guide_to_Scholarly_Communication_1.3_Communicating_Safety_Information.pdf)

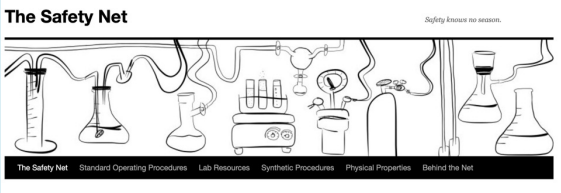
C&EN. Safety Letters

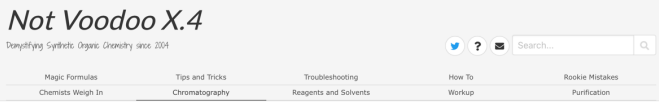


Crowd-Sourced Safety Content: Three Opportunities to Help

- The Safety Net https://safetynet.web.unc.edu/ from Univ of North Carolina
- Not Voodoo X http://www.chem.rochester.edu/notvoodoo/index.php from Univ of Rochester
- CAS Chemical Safety Library(CSL) https://safescience.cas.org/

We are working to curate these resources for both accuracy and usability, at least as much as Wikipedia does. The data they collect is not FAIR, but it can be improved using internal information and cross references. We are also interested in developing strategies for exploring the chemistry literature for safety information.

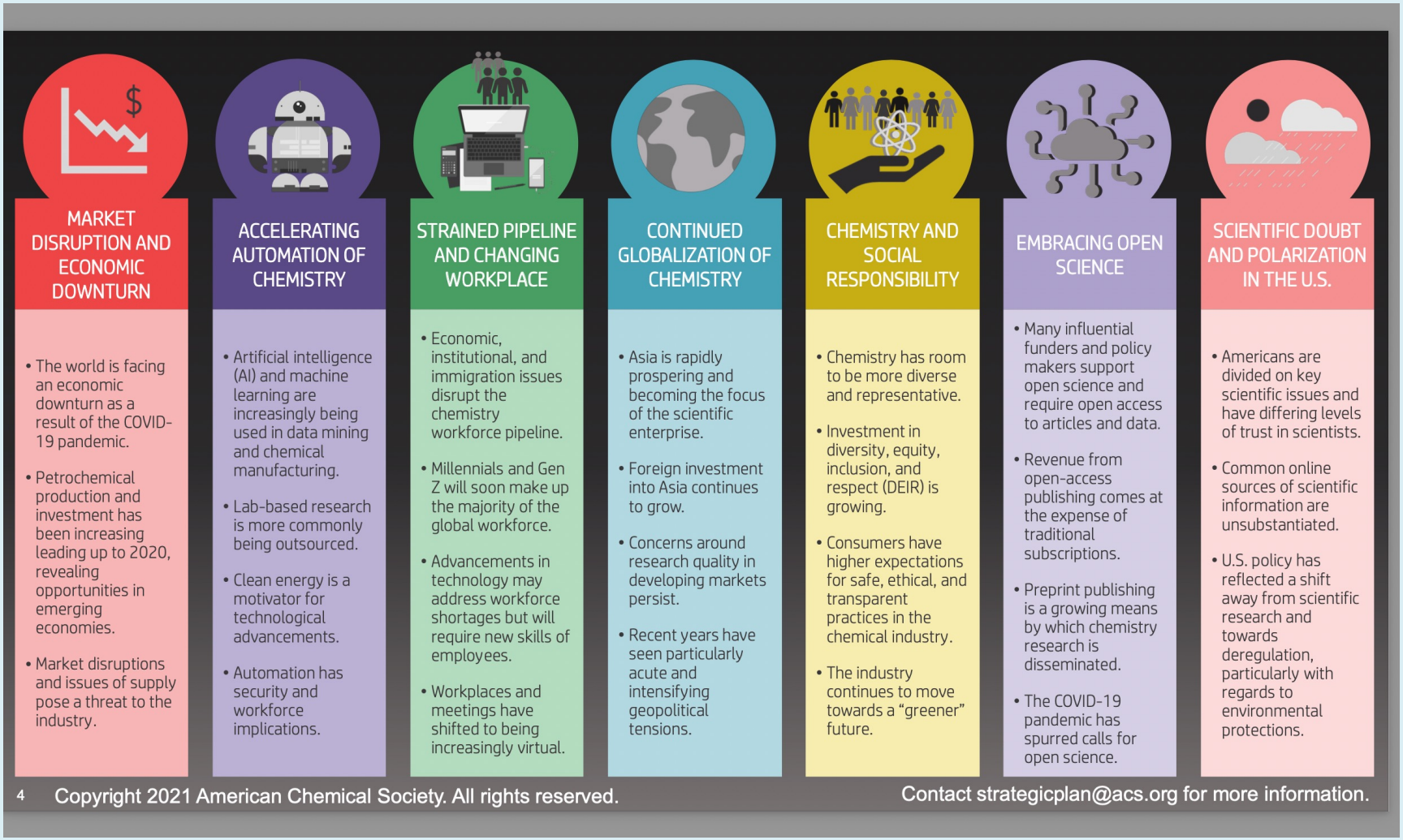




ACS CHANGE DRIVERS

A Planning Tool for Staff and Volunteers

December 2020



Contact strategicplan@acs.org for more information.

Emerging Risks Related to these Changes

1. Market disruptions
2. Social responsibility and interest in Greener Chemistry
3. Lab-based research is being outsourced with computer models replacing lab data.
4. Open science – how can we share risk data in a useful way
5. Strained chemists pipeline – the neglected risks of a mono-culture
6. Continued globalization – technology transfer overlooks risk information transfer

Addressing the challenges will require partnerships within the chemistry community.

CH&S
CONNECTING CHEMISTRY AND SAFETY

Summary:
The Chemical Safety Ecosystem

Safety information is required for many different purposes as products move through the economy.

Safety Data Sheets, transportation labelling and placards, waste code classifications and vendors' technical notes can all refer to the same product but identify different hazards depending on the context of the information.

This presentation will explore the skills chemists and their support staff need to develop to navigate this ecosystem.