



The Safety Use Case for Chemical Safety Information

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The Pithy Quote

Date: Sun, 10 Jul 2005 15:44:41 -0400

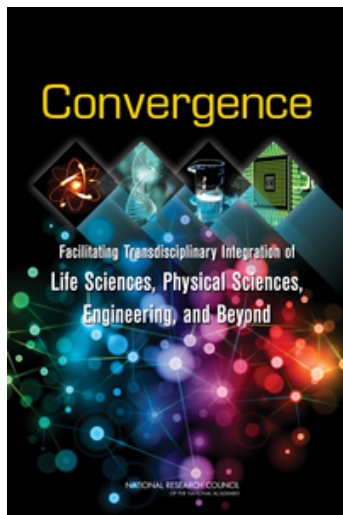
*PS: Alas, in these modern times, these young folks just don't know their **descriptive chemistry** like us old guys do. I predict disaster and catastrophe - as we old guys die off, the world will be left with chemists who don't know descriptive chemistry. Alas and Alak! (or whatever)*

- Jay Young

My version of this statement is that 21st Century Chemistry Education focuses on **discovery processes**, using specific chemical techniques **and information management**. This does not necessarily translate into transferable bench-top skills; of particular concern is safety skills.

The Continuing Evolution of Science

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



Changing Science 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)
unify theory, experiment, and simulation
 - 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



$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - \kappa \frac{c^2}{a^2}$$

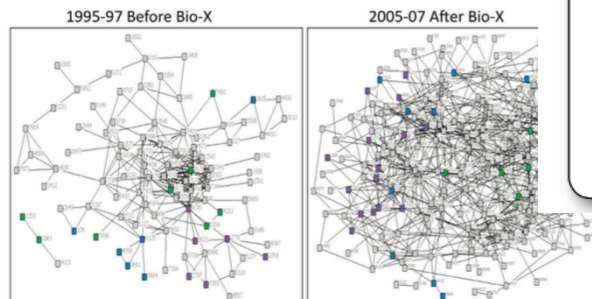
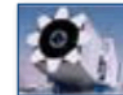
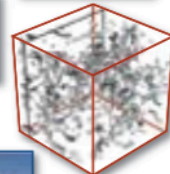


FIGURE 4-2 The web of faculty interactions created by Bio-X. The network of faculty interactions across Stanford has expanded since the establishment of the Bio-X program. The resulting network reportedly appeals to technology com-

The Current Context of Chemical Safety Information

- **Caveat emptor:** Chemistry textbooks and laboratory manuals provide an overview of generic rules, followed by "see the MSDS".
- Wikipedia provides links to random MSDS sources with no evidence of why that source is selected; some sources are kaput, many are dated
- Reports by the **National Research Council**, the **ACS**, **NFPA** after specific laboratory safety incidents found this approach to chemical safety education and information inadequate.

Material Safety

the handling of this
cautions. It is high
Safety Datasheet (M
nd follow its directio

SAFE SCIENCE
Promoting a Culture of Safety in Academic Chemical Research

NATIONAL RESEARCH COUNCIL OF THE NATIONAL ACADEMIES

CSB Safety Bulletin
U.S. Chemical Safety and Hazard Investigation Board

October 2014

Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations
Eliminating Flash Fire Hazards by Substituting or Minimizing the use of Flammable Chemicals and Performing an Effective Hazard Review Will Prevent Injuries

Key Lessons Summaries:

- Due to flash fire hazards and the potential for serious injuries, do not use bulk quantities of flammable chemicals in educational demonstrations when small quantities are sufficient.
- Employers should implement strict safety practices when demonstrating hazardous handling hazardous chemicals — including written procedures, effective training, and the highest level of appropriate personal protective equipment for all participants.
- Conduct a comprehensive hazard review prior to performing any educational demonstration.
- Provide a safety barrier between the demonstration and the audience.

le safety
u seek the Material
om a reliable source

nfpfa
+ A new proposal for campus fire safety
October 2013

HEY KIDS, WATCH THIS
NFPA 45 and the problem of school science lab demos gone wrong

CSB - Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations

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.

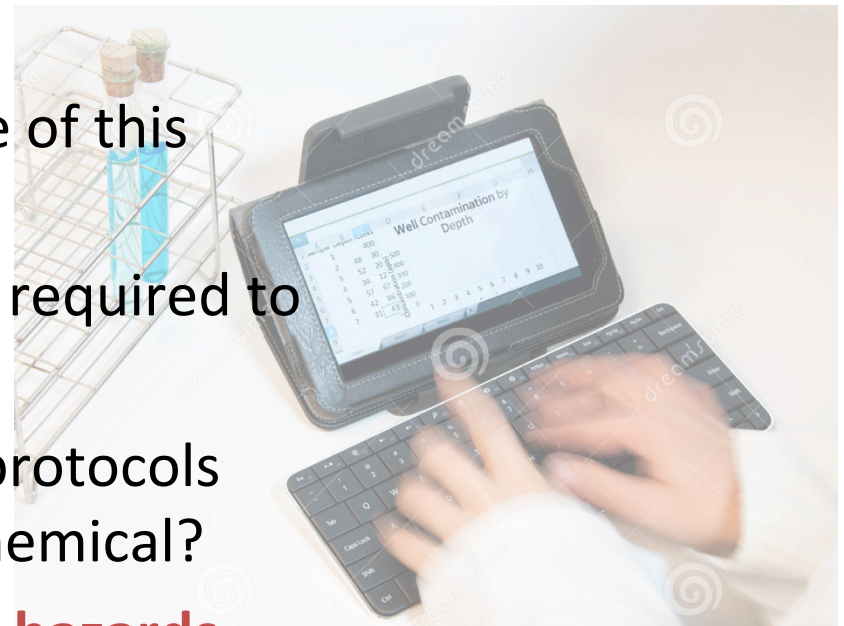


Non Lab Use Cases Identified by *Prudent Practices*

- Non Lab Use Cases
 - Household use of commercial chemical products
 - Large scale manufacturing use of chemicals
 - Medical aspects of long term exposures (drug use, etc.)
 - Environmental impacts
 - HAZMAT response
 - Transportation considerations

The Lab Use Case 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 Structure of Chemical Safety Information

Chemical Safety Information Source Hierarchy

1990's

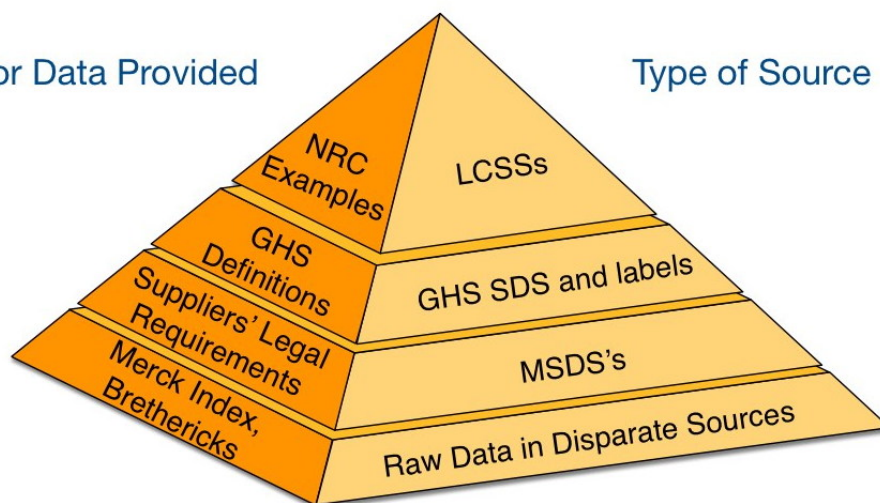
Basis for Data Provided

Type of Source

2000's

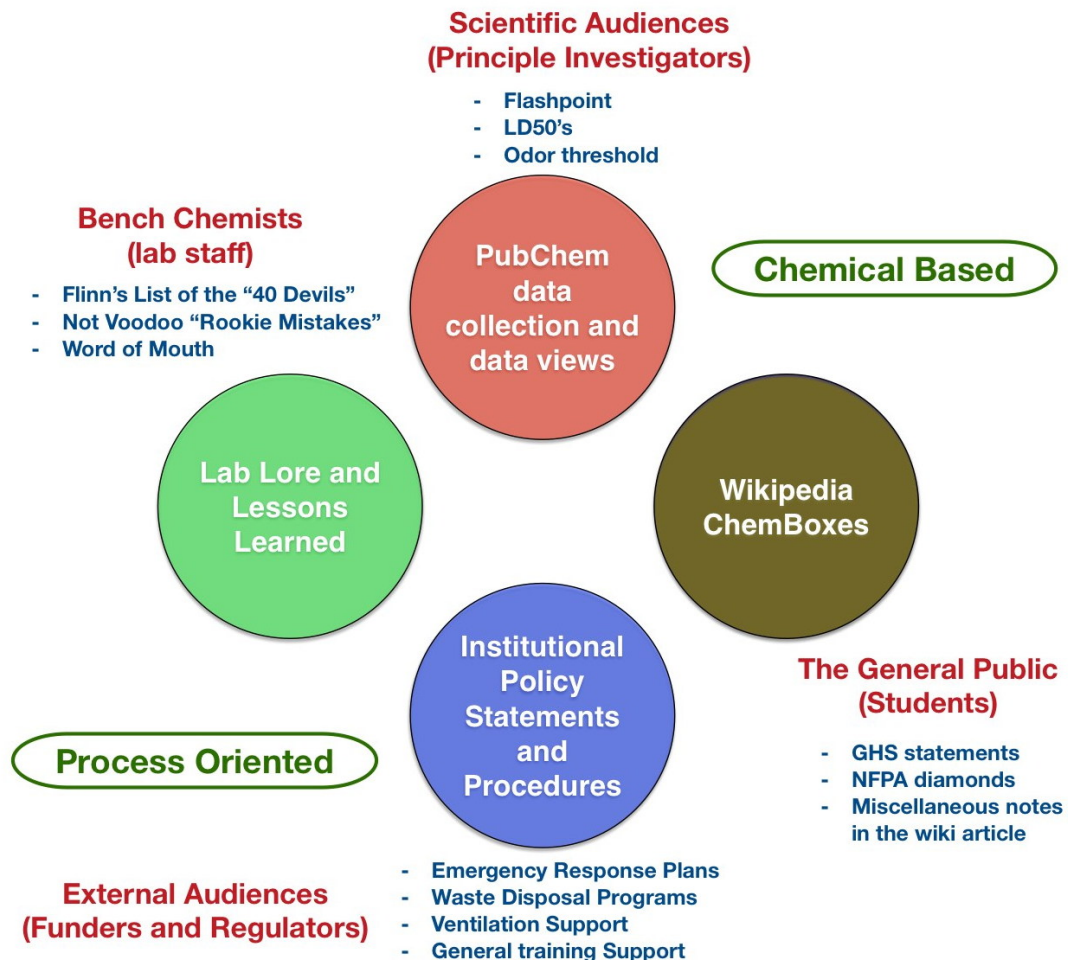
1980's

1970's



Increasingly
well-
defined;
also
increasing
voluminous

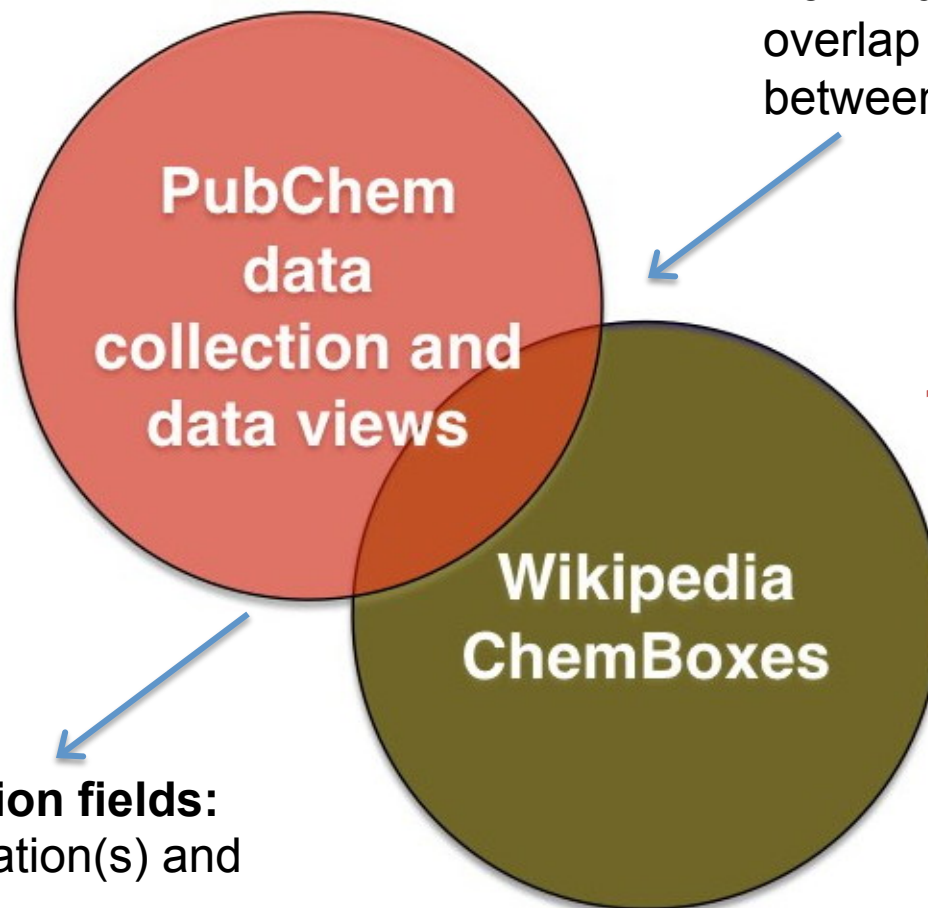
Less Structured Chemical Safety Information



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)?

Millions of chemicals;
3500 with GHS info



How much overlap is there between the two?

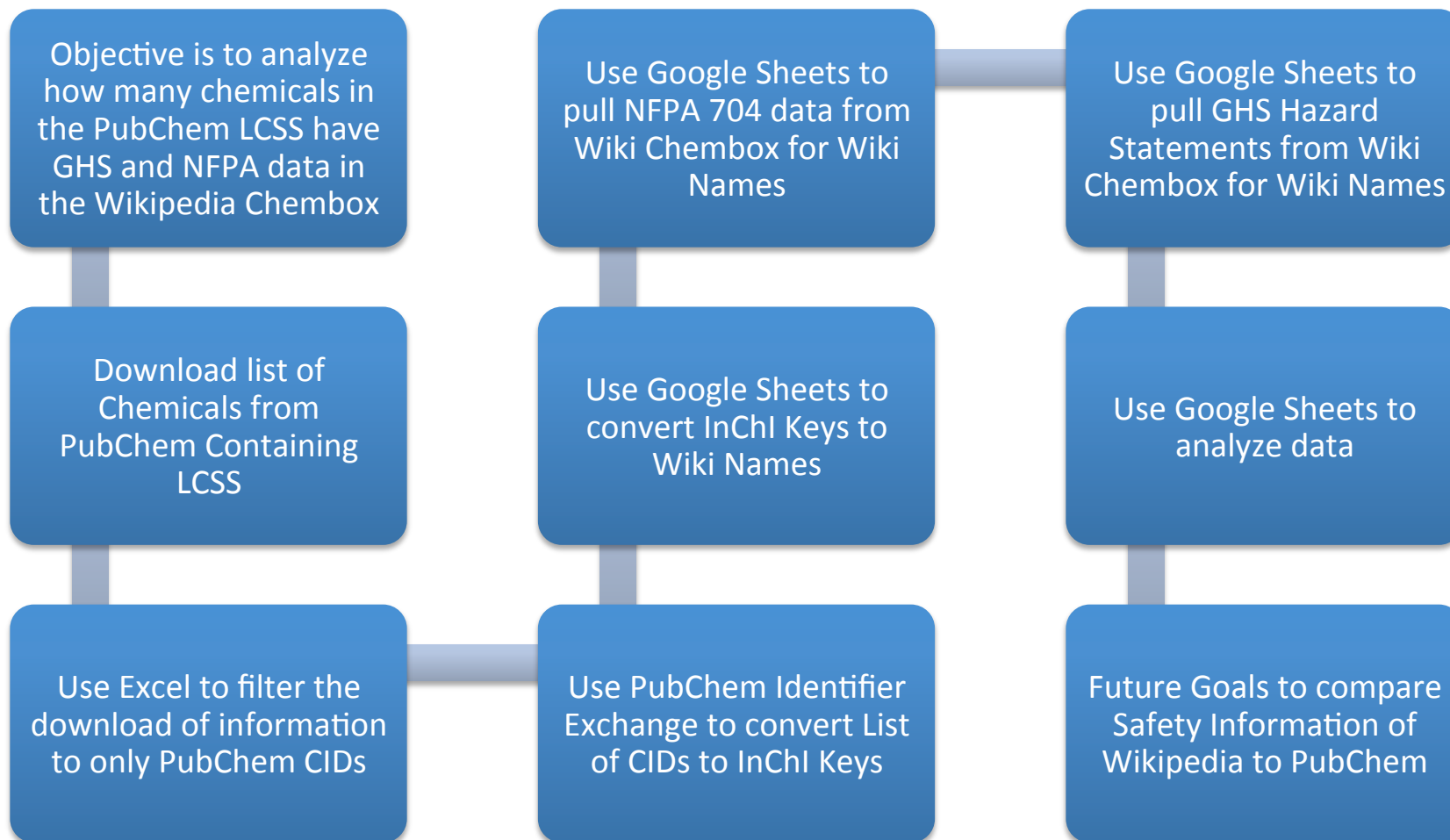
10,000 Chemboxes

Key safety information fields:

- GHS class designation(s) and signal word
- NFPA diamond information

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

Project Overview



LCSS Data to InChI Key

PubChem Website

Obtain List of Chemicals with LCSS



Excel or Google Sheets

Filter down data from PubChem into a List of PubChem CIDs



PubChem Identifier Exchange

Convert List of PubChem CIDs to InChI Keys

InChI Key to Safety Information

Google Sheets

Convert InChI Key to Wiki Name using Importxml function



Google Sheets

Convert Wiki Name to Safety Information using Importhtml function



Google Sheets

Analyze Data

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

	Not in Wikipedia	In Wikipedia	GHS Hazard Statement	NFPA 704	Total
n	2441	1038	157	431	3486
%	70.02%	29.78%	4.50%	12.36%	

Future Directions

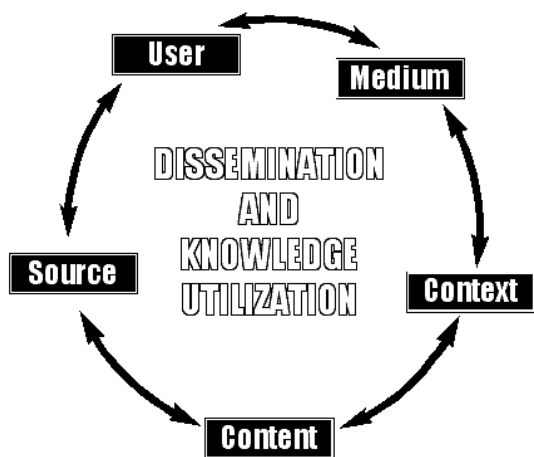
- Understand the Wikipedia Chembox structure to collect information more efficiently
- Develop a Wikipedia – PubChem data link that can provide chemical safety information with provenance data to the ChemBox
- Consider what chem safety data makes sense to put in the Wikipedia Chembox and what can be linked to there

The hazard portion of the **acetone** chembox

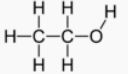
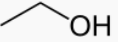
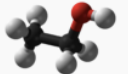

Hazards	
Safety data sheet	See: data page
GHS pictograms	
GHS signal word	DANGER
GHS hazard statements	H225 , H319 , H336
GHS precautionary statements	P210 , P261 , P305+351+338
EU classification (DSD)	
R-phrases	R11 , R36 , R66 , R67
S-phrases	(S2) , S9 , S16 , S26
NFPA 704	
Flash point	-20 °C (-4 °F; 253 K)
Autoignition temperature	465 °C (869 °F; 738 K)
Explosive limits	2.6–12.8% ^[10]
Threshold Limit Value	1185 mg/m ³ (TWA), 2375 mg/m ³ (STEL)
Lethal dose or concentration (LD, LC):	
LD ₅₀ (Median dose)	5800 mg/kg (rat, oral) 3000 mg/kg (mouse, oral) 5340 mg/kg (rabbit, oral) ^[11]
LC ₅₀ (Median concentration)	20,702 ppm (rat, 8 hr) ^[11]

Closing Thoughts

*The Medium is the Message:
the form of a medium embeds
itself in the message, creating a
symbiotic relationship by which
the medium influences how the
message is perceived.
(Wikipedia)*



*"Wikipedia is the last
refuge of the Internet
optimist"
Christopher Lydon*

Ethanol	
	
	
Names	
Systematic IUPAC name	ethanol ^[1]
Other names	Absolute alcohol, alcohol, cologne spirit, drinking alcohol, ethane monoxide, ethylic alcohol, EtOH, ethyl alcohol, ethyl hydrate, ethyl hydroxide, ethylol, grain alcohol, hydroxyethane, methylcarbinol
Identifiers	
CAS Registry Number	64-17-5 ✓
ChemSpider	682 ✓
InChI	[show]
IUPHAR/BPS	2299
Jmol-3D images	Image ↗
PubChem	702
SMILES	[show]