The Safety Use Case for Chemical Safety Information

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Keene STATE COLLEGE

Wisdom to make a difference.

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The Pithy Quote

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

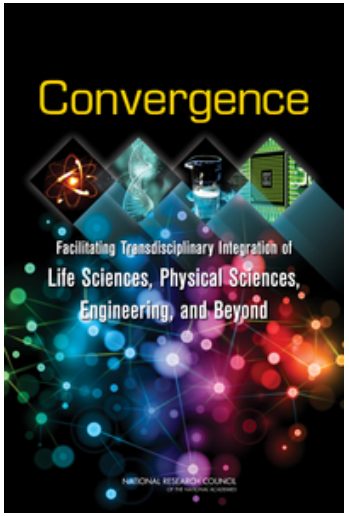
PS: Alas, in these modern times, these young folks just don't know their descriptive chemistry like us old guys do. I predict disaster and catastrophe - as we old guys die off, the world will be left with chemists who don't know descriptive chemistry. Alas and Alak! (or whatever)

- 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.



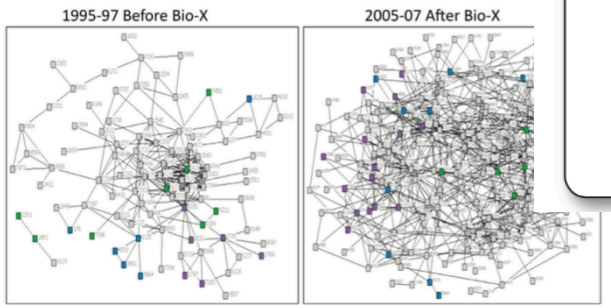


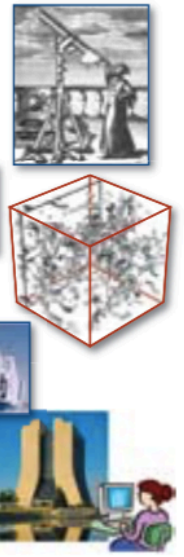
FIGURE 4-2 The web of faculty interactions created by Bio-X. The network of faculty interactions across Stanford has expanded since the establishment of the Bio-X program. The resulting network reportedly appeals to technology com-

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

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



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".
- 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.

Use Cases to Consider

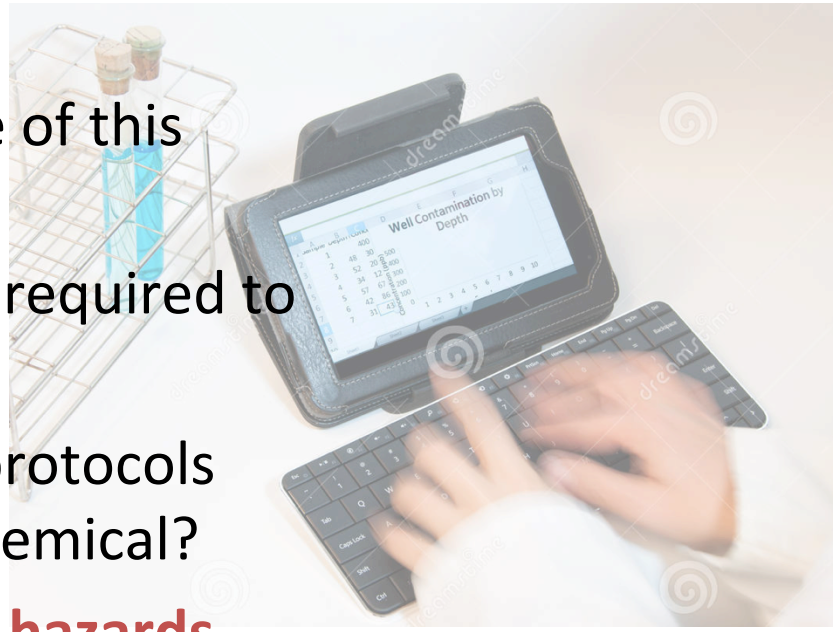
- **Teaching laboratory setting:** short term use of specific chemical concentrations in procedures with expected outcomes; close oversight of inexperienced lab workers by experienced personnel can be assumed.
- **Research laboratory setting:** evolving use of chemicals with uncertain process outcomes 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?



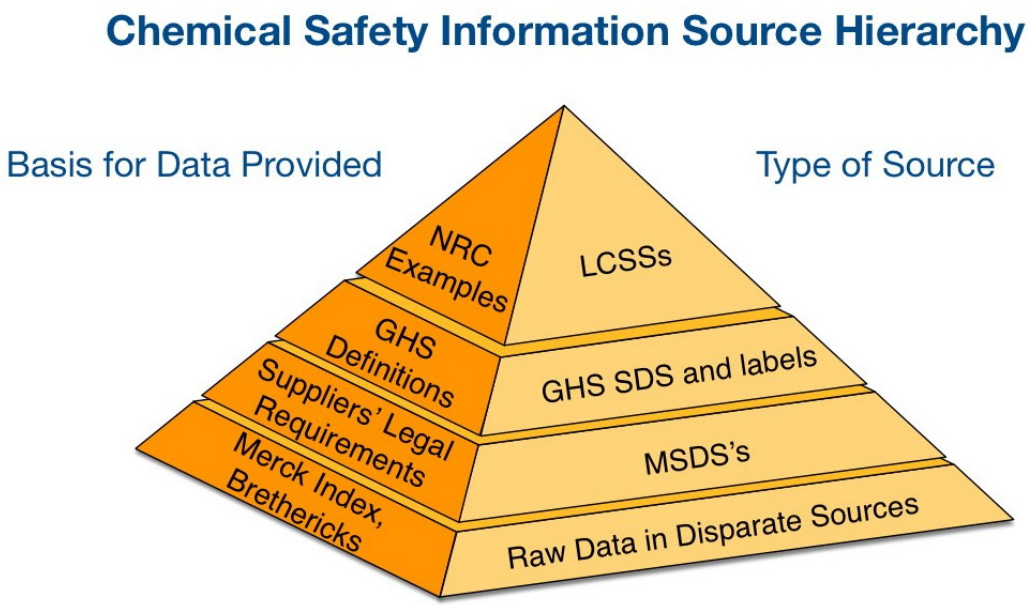
The Structure of Chemical Safety Information

1990's

2000's

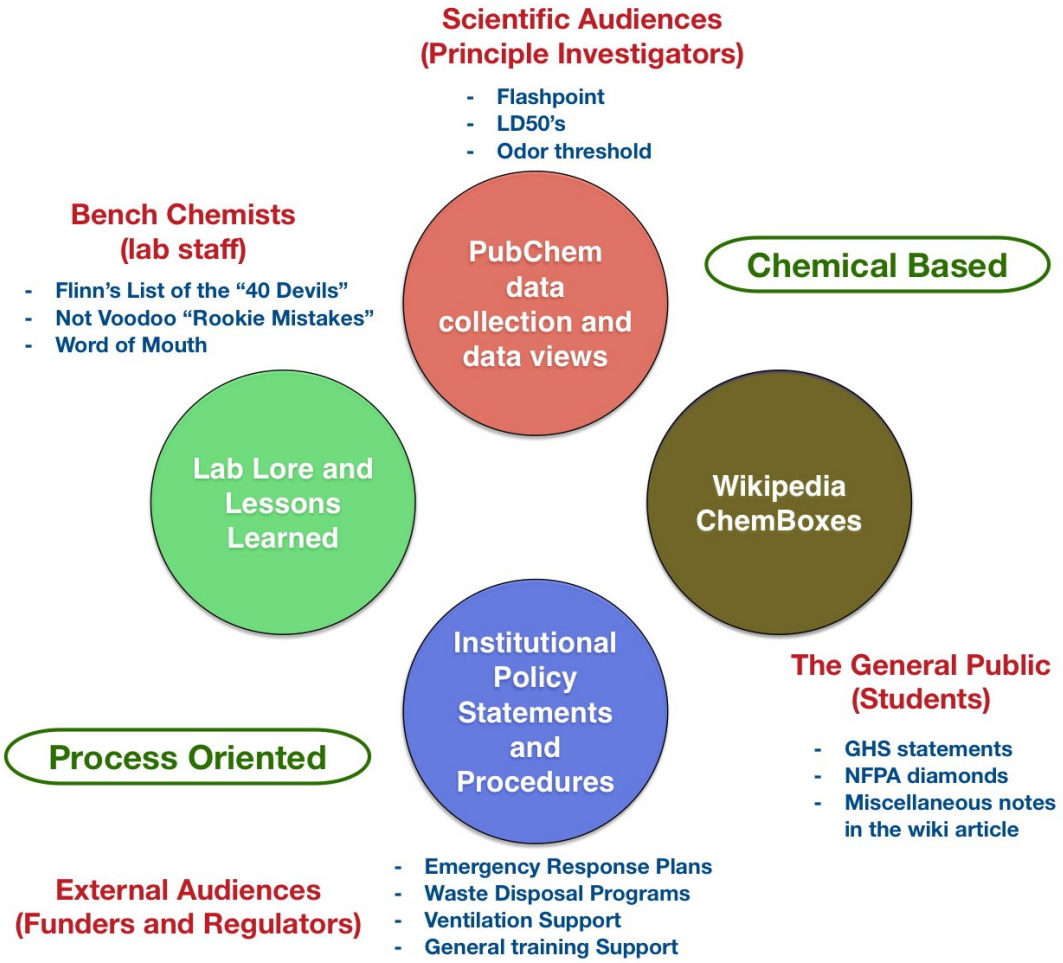
1980's

1970's



Increasingly well-defined; also increasing voluminous

Less Structured Chemical Safety Information

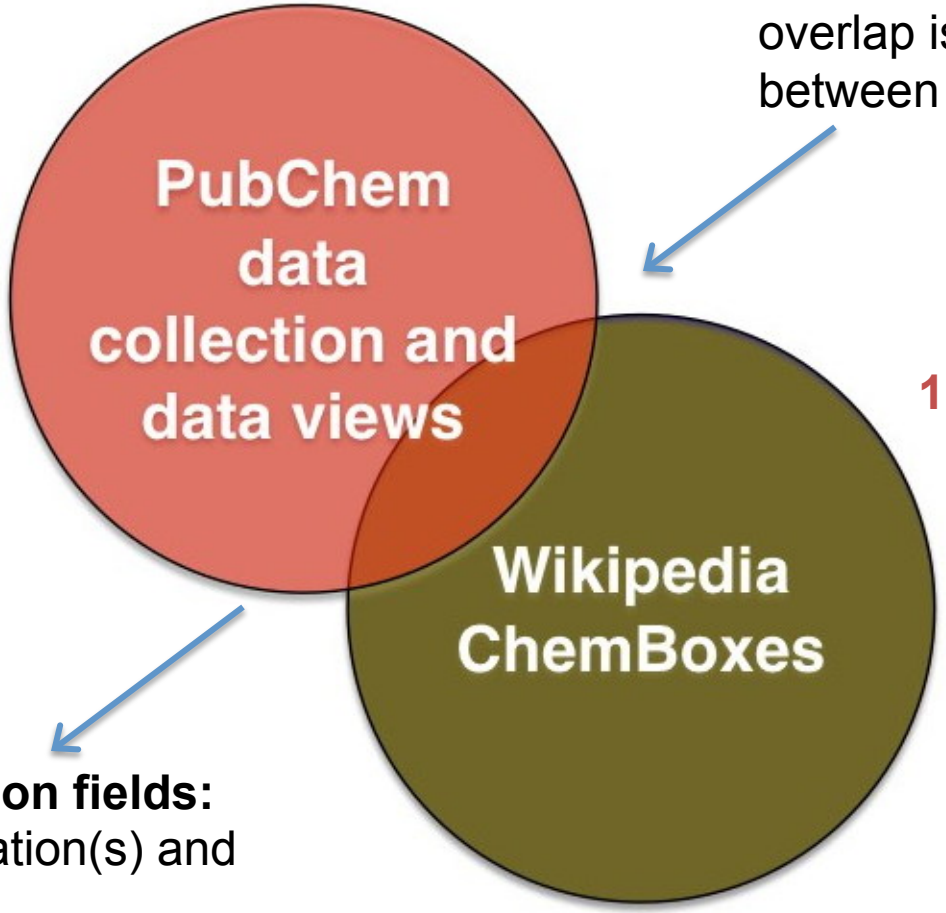


Looking for Structure in the Electronic Data

- 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?



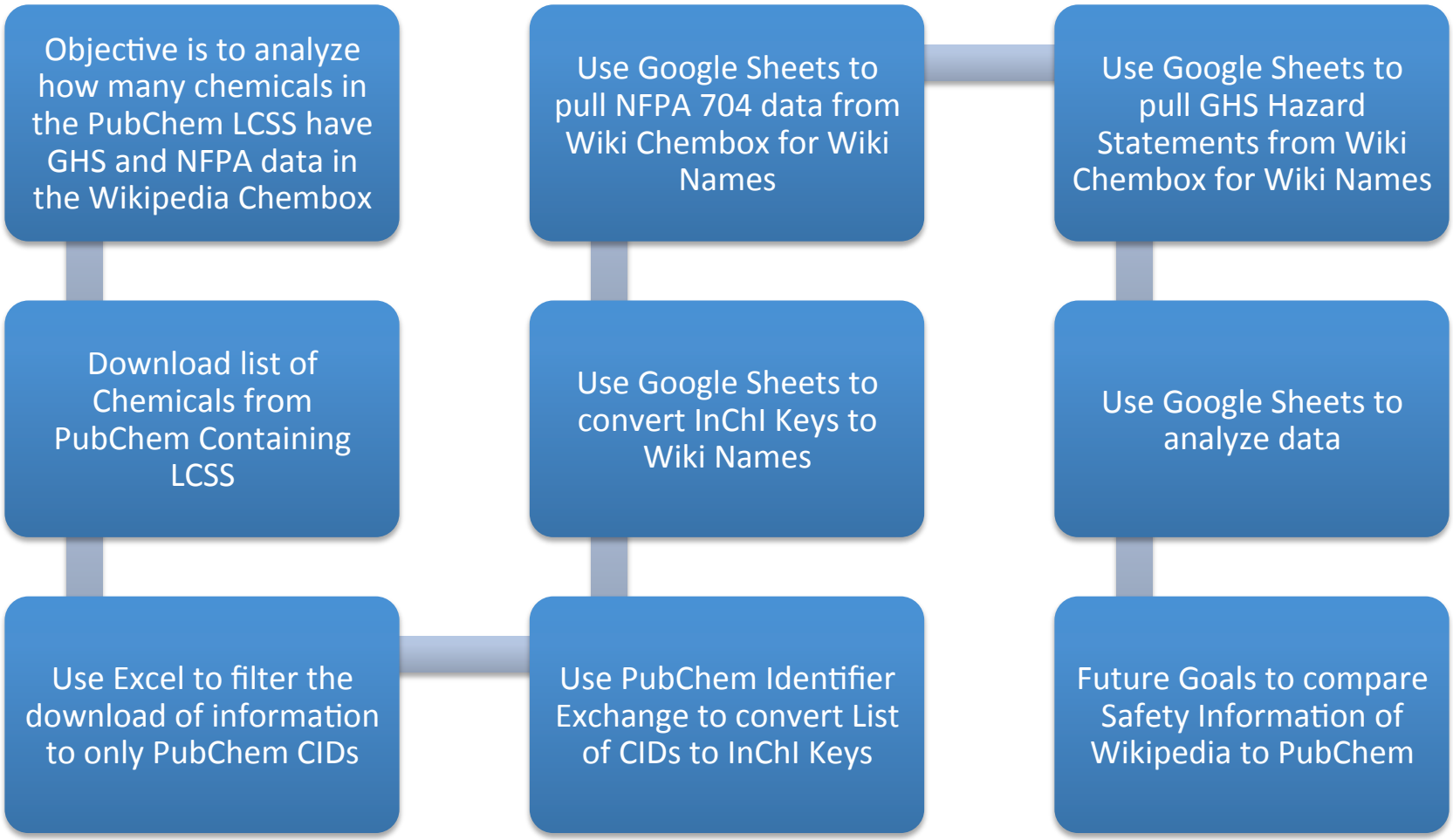
10,000 Chemboxes

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

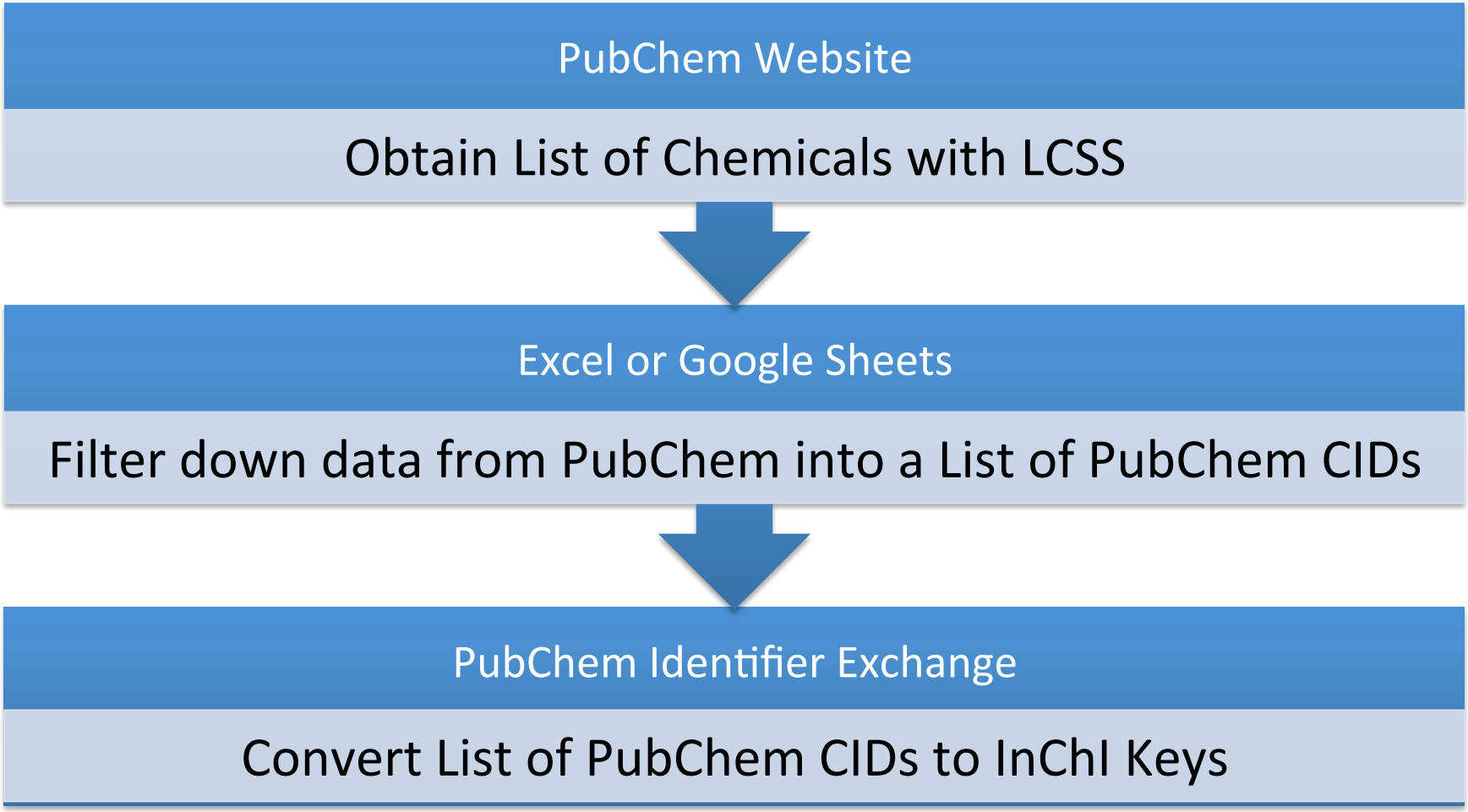
Key safety information fields:

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

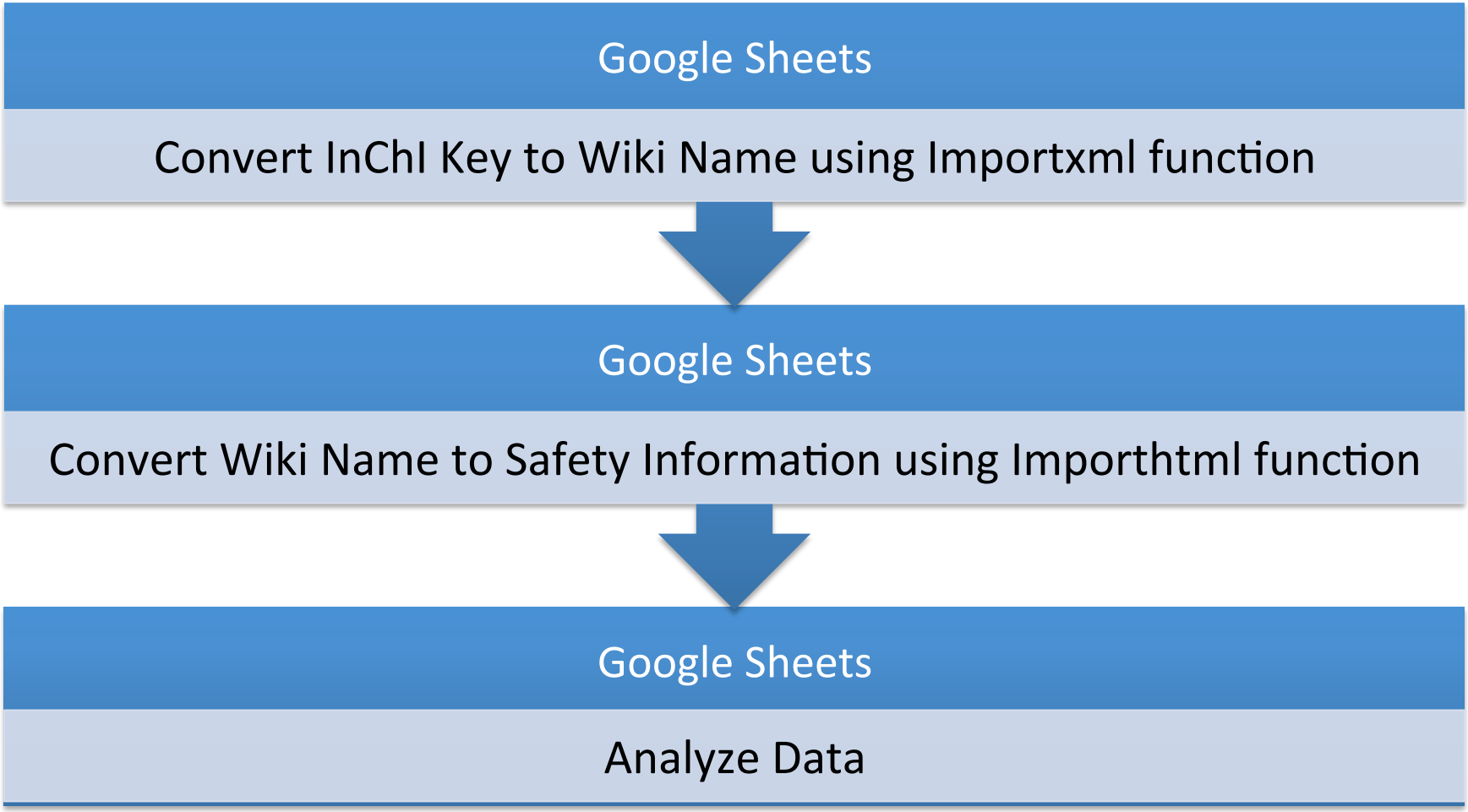
Project Overview



LCSS Data to InChI Key



InChI Key to Safety Information



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

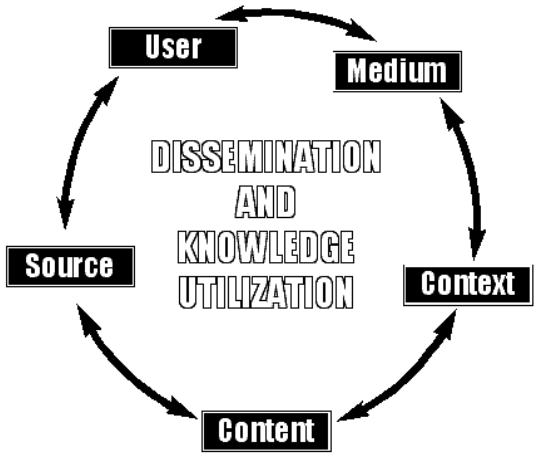
- Understand the Wikipedia Chembox structure to collect information more efficiently
- Develop a Wikipedia – PubChem data link that can provide chemical safety information with provence data to the ChemBox
- Consider what chem safety data makes sense to put in the Wikipedia Chembox and what can be linked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

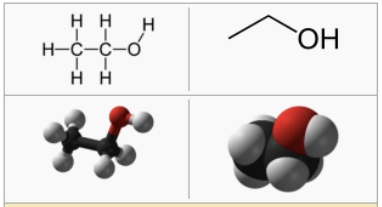
Closing Thoughts

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]