



Organizing chemical information to support lab safety

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Outline

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

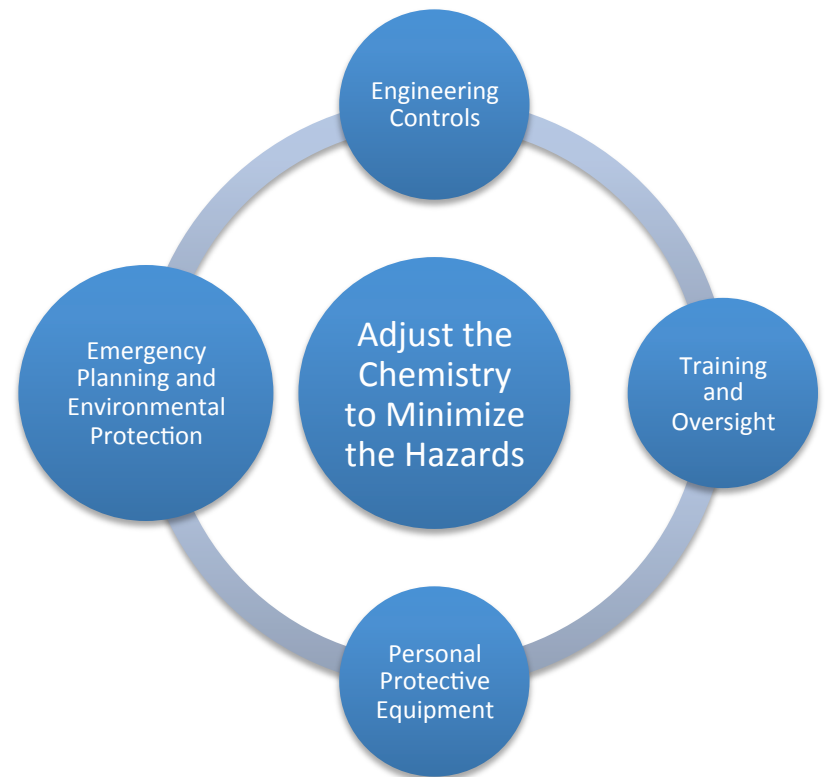
1. Overview of the Lab Safety Use Case
2. The Impact of Information Tools
3. An emerging model for a
Lab Safety-Literate Platform

Safe Chemical Use requires a System, not a Solution

Managing chemical hazards in the lab involves 5 strategies integrated into a **system** (*Stuart*):

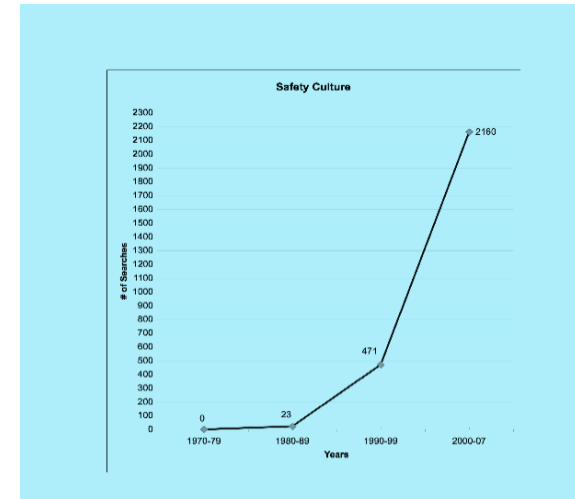
1. Hazard Reduction
2. Engineering Controls
3. Training and Oversight
4. Personal Protective Equipment
5. Emergency Planning and Environmental Protection

This system is appropriate for chemical uses within the scope of the **OSHA lab standard** (*Izzo, Malaby*).

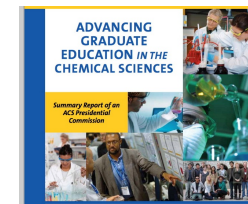


The safety system is held together by an group's Safety Culture

- The idea of **safety culture** emerged in the 1980's, in the aftermath of Bhopal and Chernobyl.
- In the early 1990's, [Arie Rip](#), a Belgian chemist turned sociologist, broadened the idea of "safety culture" to include two types of **Risk Cultures**: Danger Cultures and Safety Cultures
- Lab risk culture is continuing to evolve under social pressure from government, professional and scientific organizations. (*Sangji*)













From Silbey, 2014



Emerging Risk Assessment Tools

- The logic for the system is described in emerging tools developed available since 2010.
 - The Globally Harmonized System (GHS)
 - The RAMP paradigm from **Laboratory Safety for Chemistry Students** (Hill and Finster) (*Hill*)
 - *Identifying and Evaluating Hazards in Research Laboratories* from the ACS







Physical Hazards			Decreasing Hazard	Health Hazards		
Icon	GHS class	Signal Words		Icon	GHS class	Signal Words
	Explosive	Danger or Warning			Corrosive	Danger only (health)
	Oxidizer	Danger or Warning			Toxic	Danger only
	Flammable	Danger or Warning			Health Hazard	Danger or Warning
	Corrosive	Warning only (physical)			Irritant	Warning only
	Compressed Gas	Warning only			Environmental	Warning only
No GHS Hazard Class; No Pictogram						

The RAMP Approach to Laboratory Chemical Safety



Participants in the Lab Risk Assessment Process

- To support safe science while protecting research, safety information must be **scalable, transferable** and **sustainable**.
(Tumidajski)
- 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.

Stakeholders
Bench chemists plan and execute lab scale processes with hazardous chemicals. 
Peer chemists oversee bench chemists in planning projects 
Chemistry librarians help develop chemical information literacy skills and resources. 
Chemical information professionals provide access to chemical information and best practices for maintaining it 
Chemical Health and Safety (CH&S) professionals identify and control chemical hazards for a chemical or process 
Environmental Health and Safety (EHS) professionals guide and promote safe and sustainable chemical practices 

Information Channels Used by the Stakeholders
Raw Information: experimental process information and raw data
Published Literature: peer reviewed articles, methods and data
Curated Chemical Information: chemical literature managed to support assessment of data quality and maintain accessibility
Chemical Health and Safety Assessments: information organized to support chemical risk management
EHS Oversight Process: information designed to support management of chemical hazards

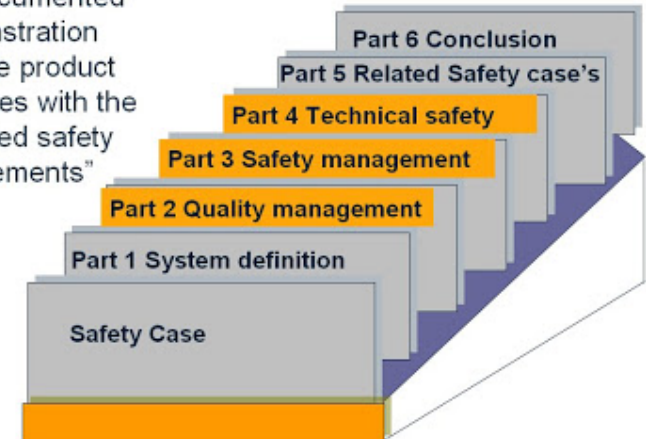
The Goal: A Laboratory Safety Case

- Safety Cases answer the question: *Why do we think this is safe?* for both internal and external audiences
- Established practice for industrial operations, particularly in Europe, but have potential for lab use.

(Mulcahy)

EN 50126 Safety Case =

"The documented demonstration that the product complies with the specified safety requirements"



Information Tools have Cultural Impact

- Culture influences action... by shaping a repertoire or "tool kit" of habits, skills, and styles from which people construct "strategies of action." (Swidler, 1976)
- Current chemistry information tools do not provide robust safety information. (*Kemsley*)



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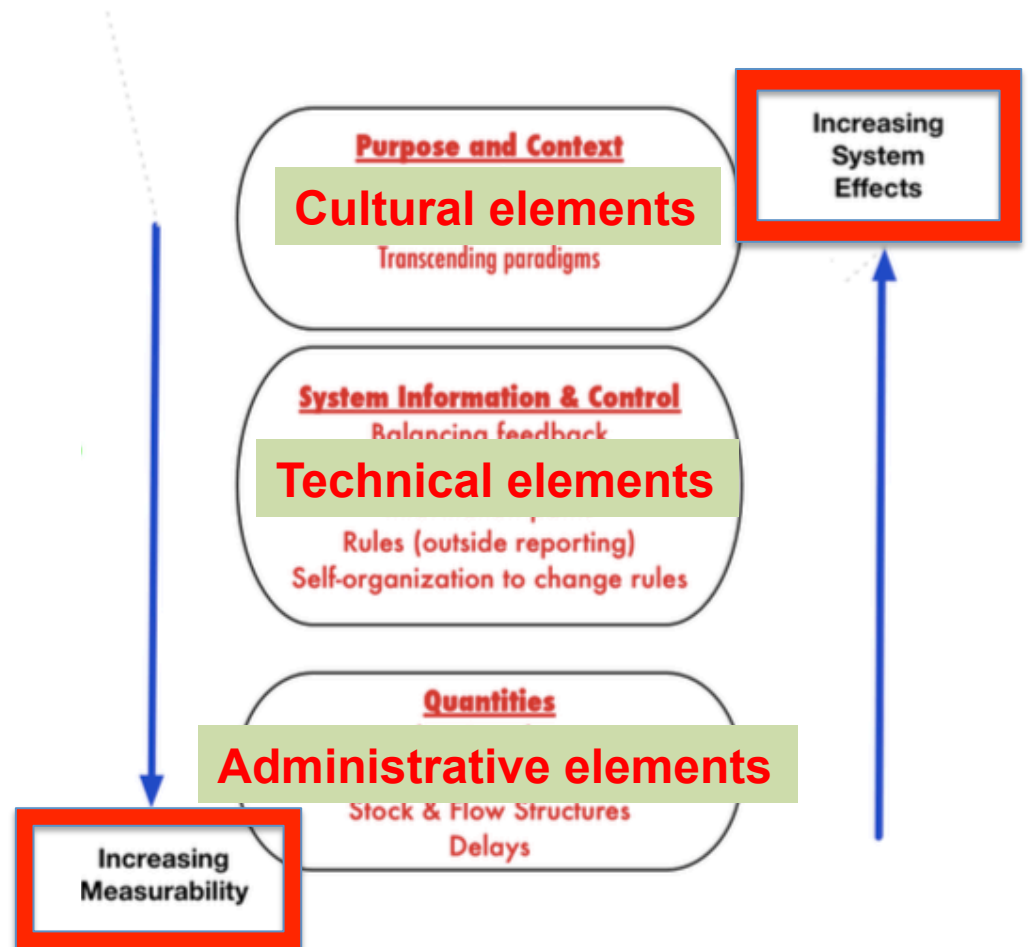
A Cultural History of Networked Technical Information

Identify and Exploit Leverage Points:

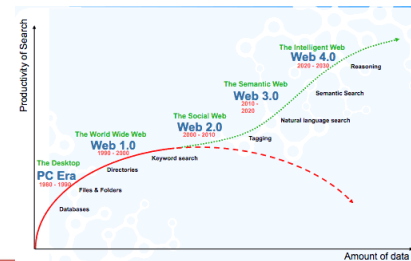
System connections where effective interventions can be applied

Diagram simplified from Donella Meadows

["Leverage Points: Places to Intervene in a System"](#)



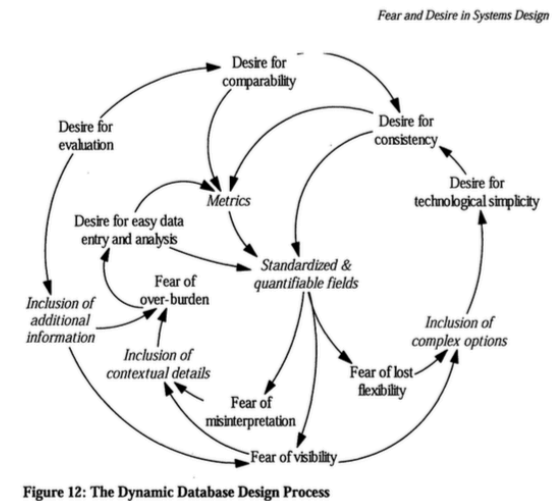
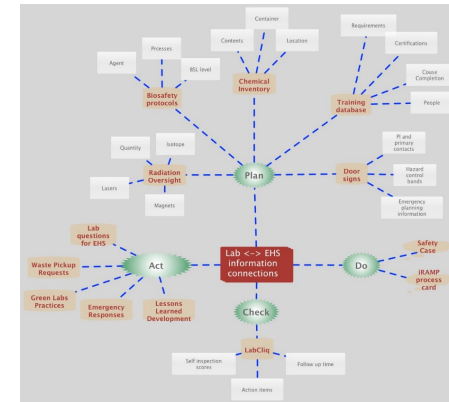
Our Evolving Electronic Tools



- 1990 – 1998: Web 1.0 = **delivery** (e-mail + ftp)
 - Information is managed for delivery from point A to person or group B; **group communication** becomes routine
- 1998 – 2003: Web 1.5 = **discovery** (search engines)
 - Search engines find things that weren't written for you, but are still useful; this development promotes **cross-disciplinary work**
- 2003 – 2010: Web 2.0
 - In Web 2.0, so much information became available that information **brokers** were necessary to support its use.
 - In this setting, brokers developed **siload platforms** (e.g. Electronic Lab Notebooks, Environmental Health and Safety Management Systems) to support specific use cases reasonably well. (*Passante*)

An Example: Lab Safety Information streams

- Institutional data (lab rosters)
- Risk data collections (inventories, SDS's)
- Control banding logic platforms
 - PPE Wizards
 - Lab ventilation wizards
 - ASHRAE lab design criteria
- However, the tension between **organizational fears** and **desires** are also expressed in the EHS system (*Agrawal*)

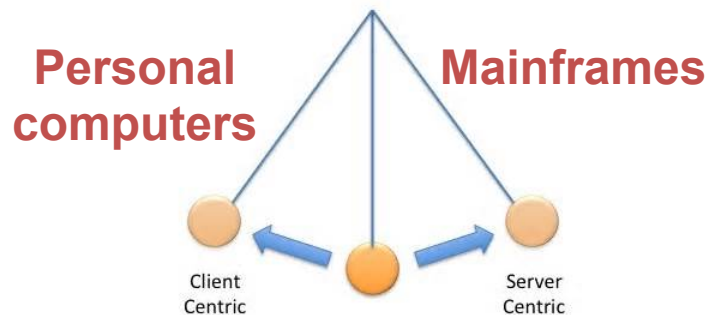


***Fear and Desire in Systems Design:
Negotiating Database Usefulness***

Tanu Agrawal

2010 – 2015: Web 2.5

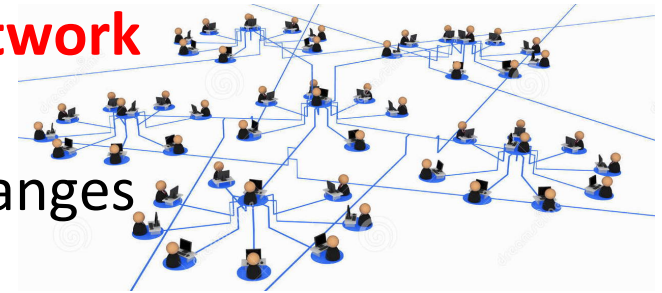
- Changing technologies, external cultural pressure (primarily usability expectations), and the increasing complexity of the lab world broke Web 2.0 efforts.
- Part of the reason for this was **poor information management** practices (competing ontologies; poor provenance) led to **unstructured communication** that competes for attention (i.e. *bedlam*)



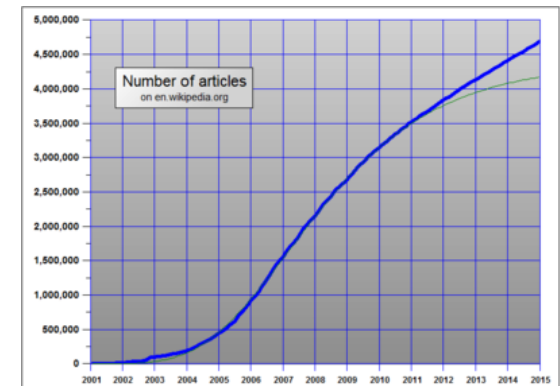
Twitter traffic: 2010-2015

The Vision Beyond 2015

- The emerging web favors:
 - Sites are designed as a **nodes in the network** rather than **drivers** who will become irrelevant as culture and technology changes
 - **Contextual Usability** (i.e. usability considerations beyond the screen)
 - Effective **peer curation**, a la Wikipedia (*Toreki*)



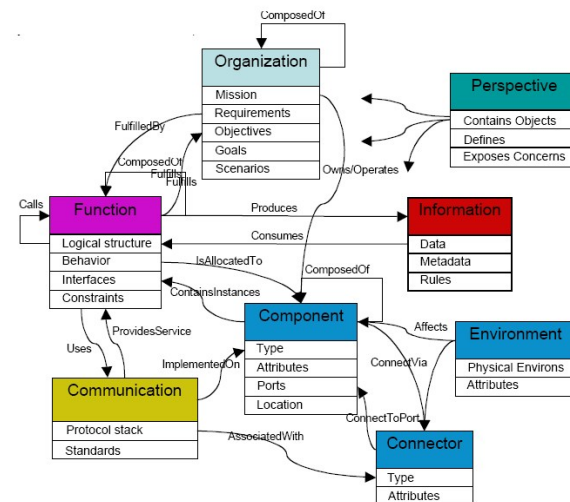
- What is emerging is a flexibly structured **ecosystem** of **data, domain expertise** and **workflow tools** mapped to the **essential commonalities** of the use case and content connected by **good information management practices** (*McEwen*)



Wikipedia articles

Information Practices that Support this Vision

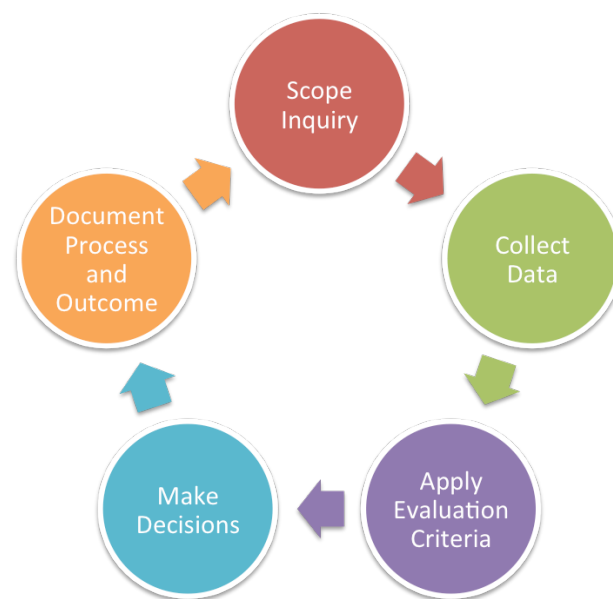
- **Ontology**: the machine readable system of definitions and links between those definitions
- **Annotation**: the human process of prioritizing elements and making decisions based on the available resources and the goal of the project



Chemical Safety Literacy Education

ACRL Literacy Competency Standards for Higher Education

1. Scope the Inquiry
2. Collect Data
3. Evaluate the Information
4. Apply to Decisions
5. Document the Process and Outcome



Lab Safety uses the Information Literacy Skill Set

ACRL Information Literacy Skills	The RAMP model of Chemical Safety
Scope the Inquiry	<i>Safety culture</i>
Collect Data	<i>Recognize hazards</i>
Evaluate the Information	<i>Assess risks</i>
Make Decisions	<i>Manage safety</i>
Document the Process and Outcome	<i>Plan, Protect Share Lessons Learned</i>

iRAMP: Developing a Safety Literate Platform

1 Introduction and Search Screen 2 Recognize 3 Assess 4 Manage 5 Prepare and Protect 6 Safety Case Information 7 Changes and Lessons Learned

[Introduction](#) > [Recognize](#) > [Assess](#) > [Manage](#) > [Prepare and Protect](#) > [Safety Case Information](#) > Changes and Lessons Learned

Welcome to the iRAMP Home Page

This web site provides:

- A search engine to help you identify safety information relevant to planning work laboratory work with specific chemicals or a chemical process
- A process to help you identify relevant hazards and appropriate safety practices relevant to your chemical work in the lab
- A tool to help you document your safety precautions and changes in them as your work proceeds in a convenient way.

IMPORTANT NOTE: The number of hazards provided for in this process is intentionally limited to lab scale process of relatively simple chemistry. The [OSHA lab standard](https://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=standards&p_id=10106) (https://www.osha.gov/pls/oshaweb/owadisp.show_document?p_table=standards&p_id=10106) defines "laboratory scale" as "...work with substances in which the containers used for reactions, transfers, and other handling of substances are designed to be easily and safely manipulated by one person." The risks of more extensive processes should be evaluated using other methods, such as those described in [Identifying and Evaluating Hazards in Research Laboratories](#) from the [American Chemical Society's Committee on Chemical Safety](#).

Use the tabs and breadcrumbs above to explore the process of preparing a [safety case](#) for your work.

Search Here for Lab Safety Information

(enter the name of a chemical or lab process)

(search constrained to curated lab safety information sources)

Web sites with helpful lab technique and lab safety information:

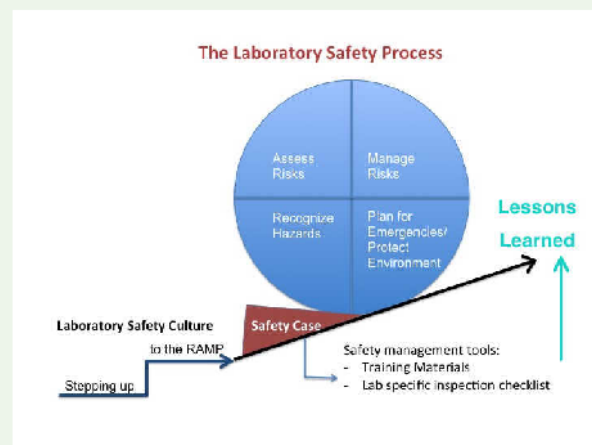
Not Voodoo X:

- For [first-time independent researchers](#)
- For [beginning Ph.D. students](#)
- For [advanced researchers](#)

[Recent Lab Incidents](#)

References

- [Prudent Practices in the Laboratory](#) from the National Research Council (free download)
- The American Chemical Society's [Committee on Chemical Safety](#)
- The [Journal of Chemical Health and Safety](#)



Lab Ramp concept from [Hill and Finster](#)

A Joint Project of:

ACS Division of
Chemical Information

American Chemical Society
Division of Chemical Information




ACS Division of
Chemical Health and Safety




[Feedback appreciated to secretary@dchas.org](mailto:secretary@dchas.org)

An Emerging Risk Assessment Model



iRAMP: A Web-Based Model for Laboratory Chemical Risk Assessment

Leah McEwen, Chemistry Librarian, Cornell University
Ralph Stuart, Chemical Hygiene Officer, Keene State College
Secretaries, ACS Division of Chemical Information and ACS Division of Chemical Health and Safety



Stakeholders

A Conceptual Model

Hazard Management Tools

Bench chemists plan and execute lab scale processes with hazardous chemicals.

Peer chemists oversee bench chemists in planning projects

Chemistry librarians help develop chemical information literacy skills and resources.

Chemical information professionals provide access to chemical information and best practices for maintaining it

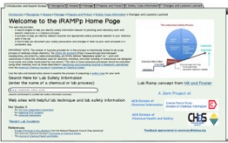
Chemical Health and Safety (CH&S) professionals identify and control chemical hazards for a chemical or process

Environmental Health and Safety (EHS) professionals guide and promote safe and sustainable chemical practices

Goal: A flexibly structured ecosystem of data, domain expertise and workflow tools mapped to the essential connections between the research process and laboratory safety planning in academic labs.



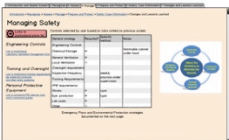
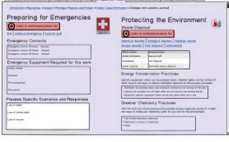
Culture

Stage 1:
The opening section provides an overview of the workflow, access to a search engine of key chemical safety information sources and links to helpful web sites.



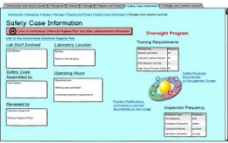
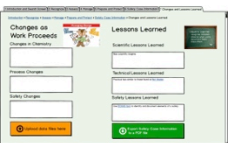
Logic

Stage 2:
The RAMP process is managed through a combination of electronic information and the professional judgement of the user

Learning

Stage 3:
The closing sections enable the user to identify administrative elements of the safety case being developed and to document Lessons Learned as part of the work.

The Globally Harmonized System of Classification and Labelling of Chemicals (GHS)

Physical Hazards		Health Hazards	
GHS Code - Signal Word		GHS Code - Signal Word	
	Explosive		Corrosive
	Oxidizing		Toxic
	Flammable		Health Hazard
	Compressed Gas		Irritant
			Environmental


No GHS Hazard Class, No P-Phrases

Information Resources

Documentation of safety planning is a key element of a laboratory safety culture.


The Hazard Management System

Chemical Specific




Process

Keeping Your Chemical Lab Safe



Standard Operating Procedures


Hazard Analysis Methods



Sources of information:

- Prudent Practices in the Laboratory
- ACS Committee on Chemical Safety publications
- Journal of Chemical Health and Safety
- Not VooDoo X
- recent lab incidents from Google
- DCHAS-L archives

The Hazard Management System



Early Fruits of iRAMP

- We proposed the development of an LCSS format for chemical safety data to PubChem in February; 3200+ LCSS's are being released today (*Bolton*).
- Next steps:
 - Develop descriptors which can data mine the literature to identify process hazards
 - Develop a crowd annotation system for EHS professionals
 - Develop a Chemical Safety Ontology

PubChem OPEN CHEMISTRY DATABASE

LCSS Laboratory Chemical Safety Summary for CID 241

PUBCHEM > COMPOUND > BENZENE > LCSS

Benzene

PubChem CID:	241
Chemical Names:	Benzene; Benzol; Cyclohexatriene; Benzole; Pyrobenzole; Benzine
Molecular Formula:	C ₆ H ₆
Molecular Weight:	78.11184 g/mol

Contents <<

- 1 GHS Classification
- 2 Identifiers
- 3 Physical Properties
- 4 Toxicity Data
- 5 Exposure Limits
- 6 Health and Symptoms
- 7 First Aid
- 8 Flammability and Explosivity
- 9 Stability and Reactivity

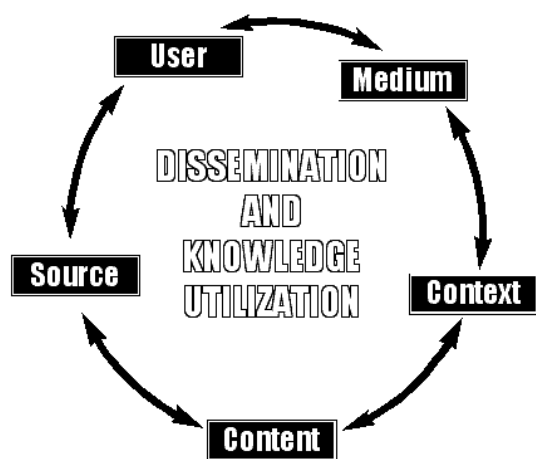
1 GHS Classification

Signal: Dgr

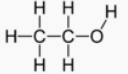
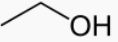
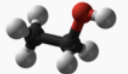

H225 - Highly flammable liquid and vapour
H350 - May cause cancer
H340 - May cause genetic defects
H372 **
H304 - May be fatal if swallowed and enters airways
H319 - Causes serious eye irritation
H315 - Causes skin irritation

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]