Chemical Management Applications for the University of California

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Outline

• Overview of the UC Chemical Management Solution
  - Stakeholders
• Data Challenges
  - Unique Identifiers
• Lessons Learned
Example Researcher Workflow

- To quickly add a chemical container to an inventory
Stakeholder: Researchers

- Who: Undergraduate, Graduate Researchers at 10 University of California Campuses, Medical Centers
- Use: Locations, Quantities, Physical Properties and Hazards, Chemical Reagent Sharing
- Interface: Edit and Maintain (Inventory) Data
Stakeholder: Chemicals User

• Who: Facilities, Fleet Services, Theater shop, etc.
• Use: Hazard information (Safety Data Sheets)
• Interface: Edit and Maintain (Inventory) Data
Stakeholder: First Responders

- Who: Emergency Service Providers
- Use: Aggregate of Acute Hazards in a Room
- Interface: View Only
Fire Marshal

- **Who:** Campus Fire Marshals, Fire Prevention
- **Use:** Compliance Reports: Maximum Allowable Quantity (MAQ)
  - Aggregate by Control Area (Building, Floor, Room)
- **Interface:** View Only (Inventory)
Safety Professional

- **Who:** Campus Health and Safety
- **Use:** Compliance reports, Business Intelligence, Carcinogens
- **Interface:** View and Edit Inventory (Campus Dependent)
Data Challenges: Unique Identifiers
Ex) Butyl Lithium nomenclature across the University of California Inventory

- 443 “Unique” Names
- Removing capitalization: 151

= ~60 Total Materials

https://www.knime.org/
Unique Identifier: CAS

Ex) Diisobutyl aluminum hydride solution

<table>
<thead>
<tr>
<th>CAS Number</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>214981</td>
<td>1.0 M in THF</td>
</tr>
<tr>
<td>214949</td>
<td>1.0 M in cyclohexane</td>
</tr>
<tr>
<td>214973</td>
<td>1.0 M in methylene chloride</td>
</tr>
<tr>
<td>214965</td>
<td>1.0 M in heptane</td>
</tr>
<tr>
<td>256846</td>
<td>1.0 M in heptane</td>
</tr>
<tr>
<td>190306</td>
<td>1.0 M in hexanes</td>
</tr>
<tr>
<td>256870</td>
<td>1.0 M in toluene</td>
</tr>
</tbody>
</table>

Peroxide former

OSHA specifically regulated carcinogen
## Unique Identifier: Group by Hazard Assessment?

<table>
<thead>
<tr>
<th>Color</th>
<th>% H₂O₂</th>
<th>External structures:</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="false" alt="Yellow" /></td>
<td>3-30%</td>
<td>Chemical Facilities Anti Terrorist Standards (CFATS): 2 divisions (&lt;35%)</td>
</tr>
<tr>
<td><img src="true" alt="Purple" /></td>
<td>30%</td>
<td>Occupational Safety and Health Administration (OSHA): 3 divisions (&lt;20%; 21-60%; &gt;61%)</td>
</tr>
<tr>
<td><img src="false" alt="Blue" /></td>
<td>30-35%&lt;</td>
<td></td>
</tr>
<tr>
<td><img src="true" alt="Red" /></td>
<td>50%</td>
<td>International Fire Code (IFC) Appendix E: 4 divisions (8-27.5%; 27.5-52%; 59-91%, &gt;91%)</td>
</tr>
</tbody>
</table>

### Individual Entries:

- **216763**: contains inhibitor, 30 wt. % in H₂O, AC5 reagent
- **316389**: contains potassium stannate as inhibitor, 30-32 wt. % in water, semiconductor grade, 99.999% trace metals basis
- **HS410**: contains inhibitor, 30 wt. % in H₂O, meets USP testing specifications
- **18511**: for ultratrace analysis
- **95321**: ≥30%, for trace analysis
- **51642**: ≥30%, for trace analysis
- **68597**: 3%, for microbiology
- **31642**: 30% (w/w)
- **95294**: tested according to Ph.Eur.
- **40230**: ≥30% (w/w)
- **40309**: ≥30% (w/w)
- **95290**: purum p.a., ≥95% (RI)
- **15304**: meets analytical specification of Ph. Nord., 34.5-36.5%
- **88597**: 3%, for microbiology
- **51642**: 30% (w/w)
Unique Identifier: Why InChI for Mixtures

- Most (all) substances are mixtures *in practice*
- Many use cases for documenting mixtures of substances
  - Inventories
  - Catalogs
  - Tracking (including during experiments, across literature)
  - Other reporting
- Lack of existing systematic notation
- Machine readable chemical composition useful in these large systems

http://www.inchi-trust.org/
http://iupac.org/
Lessons Learned
Lesson Learned: (Step 2) Find the Chemical

- Expectation: You know what my container is.
- Reality: 1000s of vendors, numerous products
- User Question: How do I find the right entry?
- Unique Identifiers Displayed to User vs Space
- Purchasing?

https://www.knime.org/
Lessons Learned: Ease of Utility

• Free Entry vs Picklist

Free Entry

Comments

Picklist

Type

Choose a Type
Choose a Type
Above Ground Tank
Ampule
Bag
Box
Can
Carboy
Cryogenic Dewar
Cylinder
Fiber Drum
Glass Bottle
Other
Plastic Bottle
Plastic/Non-metallic Drum
Steel Drum
Tank Inside Room
Underground Tank
Lessons Learned: Ontologies

• Mapping of External Database Unique Identifiers to Internal Structures
  ex.) BoilingPoint – Boiling point, BP, Boiling Point, Boilpoint, etc.

• How/What Should be Grouped

Can of Paint → Color → Vendor?
Practicality

• Ease of Access
• High turnover items
• Lab supplies
External Collaborators

- American Chemical Society
  - Division of Chemical Health and Safety
  - Division of Chemical Information
- Cornell University
- International Union of Pure and Applied Chemistry/ International Chemical Identifier (IUPAC-InChI)
- Keene State
- Millipore-Sigma
- National Institute of Health (PubChem)
- SciQuest
- ThermoFisher Scientific
- U.S. Environmental Protection Agency (CompTox)
Questions?
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http://risksafety.universityofcalifornia.edu/
Stakeholders
Lessons Learned

• Find and Add to my Inventory
• Ease of Utility vs Accuracy
• Ontologies?
• Practicality
• Multiple/One record? (searching is a struggle) (aggregation/disaggregation and affects on search results)

Search add
multiple

• High turnover containers (barcoding an area)
• Information displayed to help identify container (Helping users filter search results down to what they have)