Characterizing Chemicals in Commerce

Development of the High Production Volume Information System (HPVIS)

December 12, 2006
HPV Goals

- Provide public availability of all High Production Volume (HPV) Challenge Program data on the EPA web site
- Provide a data repository for HPV Challenge Program submissions, including test plans, robust summaries, and public comments
HPVIS Goals

- Provide robust search, query, reporting, retrieval and export capabilities balancing the various stakeholder/user-expressed wants and needs
- Ensure transparency in all operations
- Provide compatibility with IUCLID
- Contribute to development of international HPV information systems
HPVIS Development Philosophy

Use a rigorous, systematized approach to software development emphasizing stakeholder identification, participation, and buy-in at all stages of the development process.
Software Development Steps

- Define a management structure
- Gather and prioritize requirements
- Design system to meet short and long-term requirements
- Design and build database
- Develop and test software
- Populate database with legacy data and field the application
Requirements Gathering

- Over 200 initial system requirements were collected from approximately 100 participants
  - 4 workshops with OPPT staff
  - 15 interviews with OPPT managers
  - 4 sessions with outside stakeholders
    - Environmental and chemical organizations
    - EPA Regional staff and State and tribal representatives via FOSTTA
Major HPVIS Design Elements

- Web-based relational database
- Submission-based
- Robust user access and security features
- Submission by single company or consortium of companies for individual chemicals and categories of chemicals
- Flexible data entry and retrieval of chemicals within categories
International Elements

- HPV was built taking into account other international HPV program systems
  - IUCLID 4
  - IUCLID 5 and REACH IT
- Compatibility with OECD efforts to provide global access to HPV data and meet commitments made at the World Summit on Sustainable Development
- eChemPortal implementation 2007
System Implementation

- Database
  - Database structure defined
  - Legacy data population in progress
    - 236 Single Chemical Submissions Complete (92%)
    - 91 Category Chemical Submissions Complete (69%)
    - 848 Sponsored Chemicals Complete (58%)
  - Support for Sponsor direct entry of data (new and revised submissions)
    - Data entry functionality for over 50 defined SIDS and non-SIDS endpoints

236 Single Chemical Submissions Complete (92%)
91 Category Chemical Submissions Complete (69%)
848 Sponsored Chemicals Complete (58%)
System Implementation (continued)

- Data Review and Characterization
  - Sponsor QC (of EPA-entered legacy data) process
  - EPA data adequacy review process
  - Data screening algorithm to identify potential chemicals of interest
• Data Retrieval
  ◆ View Robust Summaries by Chemical (however chemical is entered)
  ◆ View Submission (select by Chemical, Submission Name, Submitter, and/or Sponsor)
  ◆ Ad hoc query (by discipline, endpoint, or across database)
System Implementation (continued)

- Data Retrieval (continued)
  - Matrix of Category Chemicals and Endpoints
    - Single Discipline or All Disciplines
    - User-specified X and Y axis (chemicals by endpoint or endpoints by chemical)
  - Frequency Distribution of Units of Measure (Endpoint Result Report)
    - Select endpoint and result type (e.g., Acute Toxicity and NOAEL)
Category Matrix Report Example

The Category Matrix Report presents results for HPV Challenge Program data that was reported in categories of chemicals. The report is a matrix of the individual chemical members of the category as one axis and the HPVIS endpoints as the other. The intent of the report is to assist users in performing a "read-across" analysis to estimate values for chemicals in the category without a result reported for a specific endpoint.

**Category Selection**
Select a Category Name from the list below.

**Category Name:**
Aliphatic Esters Category

**Endpoint Discipline Selection**
Select an Endpoint Discipline from the list below.

**Endpoint Discipline:**
Physical-Chemical

**Axes selection**
Select category matrix display X and Y axes.

<table>
<thead>
<tr>
<th>Axes</th>
<th>X</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number</td>
<td>Endpoint</td>
<td></td>
</tr>
<tr>
<td>Endpoint</td>
<td>CAS Number</td>
<td></td>
</tr>
</tbody>
</table>

- One CAS Number at a time

Search  <<< Previous  Reset
## Category Matrix Report

**Category Name**: Aliphatic Esters Category  
**Endpoint Discipline**: Physical-Chemical

<table>
<thead>
<tr>
<th>Endpoint Name</th>
<th>Melting Point (12)</th>
<th>Boiling Point (15)</th>
<th>Vapor Pressure (16)</th>
<th>Partition Coefficient (5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>103-24-2 Nonanedioic acid, bis(2-ethylhexyl) ester</td>
<td>Unknown Mels = 79 °C</td>
<td>Unknown Boils = 237 °C @ 5 mm Hg</td>
<td>Unknown 5 mm Hg @ 277 °C</td>
<td>Measured &gt; 2.7 @ 22 °C</td>
</tr>
<tr>
<td>105-52-2 2-Octadecenoic acid (9Z), bis(1,3-dimethylbutyl) ester</td>
<td>Unknown Mels = 30 °C</td>
<td>Unknown Boils = 175 °C @ 20 mm Hg</td>
<td>Measured &lt; 13 Pa @ 25 °C</td>
<td>Measured = 3.74 @ 22 °C</td>
</tr>
<tr>
<td>105-62-4 9-Octadecenoic acid, bis(1,2-ethanediyl) ester</td>
<td>Unknown Mels = 66.5 °C</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Measured &gt; 102 Pa</td>
</tr>
<tr>
<td>106-79-6 Decanedioic acid, dimethyl ester</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 189 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
<tr>
<td>108-63-4 Hexanedioic acid, dimethyl ester</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
<tr>
<td>111-60-4 Octadecanolic acid, 2-hydroxyethyl ester</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
<tr>
<td>11138-60-6 Decanoic acid, 2-(1-oxoctadecyl)oxy[1methyl]-1,3-propanediol octanoate</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
<tr>
<td>115-83-3 Octadecanolic acid, 2,2-bis[(1-oxoctadecyl)oxy][1methyl]-1,3-propanediol octanoate</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
<tr>
<td>122-62-3 Decanedioic acid, bis(2-ethylhexyl) ester</td>
<td>Unknown Mels</td>
<td>Unknown Boils = 191 °C @ 1 mm Hg</td>
<td>Unknown</td>
<td>Unknown Boils = 106 °C @ 5 mm Hg</td>
</tr>
</tbody>
</table>

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**View All Results**
### Melting Point

<table>
<thead>
<tr>
<th>Test Substance - Melting Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>Category Chemical:</td>
</tr>
<tr>
<td>Test Substance:</td>
</tr>
<tr>
<td>Purity/Composition and Other Test Substance Comments:</td>
</tr>
<tr>
<td>Category Chemical Result Type:</td>
</tr>
<tr>
<td>Test Substance Result Type:</td>
</tr>
</tbody>
</table>

#### Results - Melting Point

<table>
<thead>
<tr>
<th>Melting Indicator:</th>
<th>Melts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point Value/Range (Temperature):</td>
<td></td>
</tr>
<tr>
<td>Results: Remarks:</td>
<td></td>
</tr>
</tbody>
</table>

#### Study/Method - Melting Point

<table>
<thead>
<tr>
<th>Key Study Sponsor Indicator:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Year Study Performed:</td>
</tr>
<tr>
<td>Method/Guideline Followed:</td>
</tr>
<tr>
<td>Method/Guideline and Test Condition Remarks:</td>
</tr>
<tr>
<td>GLP:</td>
</tr>
</tbody>
</table>
Ad hoc Query Example

HPVIS Ad Hoc Query

This query allows you to select key data elements from HPVIS to view in tabular form.

There are 3 steps to follow to generate a query:

1. First, select one view of interest from the list below.
2. Select columns (data elements or fields) from the selected view.
3. Enter your search criteria to target specific records from the database.

The HPVIS Ad Hoc Query User’s Guide will provide you with details of how to generate a query. For additional help, select the Online-Tutorial.

To view the below table in tabular form, click Tabular Selection For:

Step 1: Start by selecting one view to be displayed:

- Submission Information
- Discipline Results
- Physical Chemical
- Fate
- EcoToxicity
- Mammalian Health Effects
- Use and Exposure

- Melting Point
- Boiling Point
- Vapor Pressure
- Partition Coefficient
- Water Solubility
- Density/Specific Gravity
- Viscosity
- Surface Tension
- Dissociation Constant
- Non-Saturated pH
- Solubility in Different Media
- Granulometry
- Flash Point
- Flammability
- AutoFlammability
- Explosivity
- Chemical Reactivity
- Oxidation Properties
- Oxidation Reduction Potential
- Physical Chemical Other
Ad hoc Query Example (continued)

**High Production Volume Information System (HPVIS)**

**Selection of Columns**

STEP 2: Select one or more column(s) for your output by clicking on the square box next to the column name. When you are finished selecting columns, click on the "STEP 3: Enter Search Criteria" button at the bottom of this page.

**QUERY NAME:** Melting Point Data, **TABLE NAME:** V_PCHEM_SIDS_1_EZ

- **Category Chemical CAS Number**
  A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical (e.g., 10595-60-5).

- **Category Chemical Name**
  The ninth collective index name of the category chemical.

- **Consortium Name**
  The names of the companies that belong to the consortium or partnership if applicable.

- **Sponsor Name**
  The name of the individual company or consortium (i.e., two or more companies) making a commitment in the HPV Challenge Program to provide data for a chemical or category of chemicals (e.g., Eastman Chemical Company).

- **Sponsored Chemical CAS Number**
  A standardized number assigned by the Chemical Abstracts Service (CAS) to identify a chemical or category (e.g., 10595-60-5).

- **Sponsored Chemical Name**
  The ninth collective index name of the sponsored chemical or category.

- **Submission Name**
  The sponsor provided name associated with the submission.

- **Submitter’s Name**
  The name of the individual company or consortium formally providing test plan related information.
Ad hoc Query Example (continued)

**STEP 3: Enter Search Criteria and Organize the Output**

<table>
<thead>
<tr>
<th>Column Name</th>
<th>Operator Definition</th>
<th>Search Value</th>
<th>Column Display Order</th>
<th>Sort Column</th>
<th>Sort Order</th>
<th>Where Only</th>
</tr>
</thead>
<tbody>
<tr>
<td>Category</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical Number</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sponsored Chemical CAS Number</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Result Type</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substance Result Type</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Melting Indicator</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Value Description</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Test Value</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Test Value Units</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Key Study Sponsor Indicator</td>
<td>Equal to</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Ad hoc Query Example (continued)

#### Query Name: Melting Point Data

<table>
<thead>
<tr>
<th>Category Chemical CAS Number</th>
<th>Sponsored Chemical CAS Number</th>
<th>Sponsored Chemical Result Type</th>
<th>Test Substance Result Type</th>
<th>Melting indicator</th>
<th>Value Description</th>
<th>Test Value</th>
<th>Test Value Units</th>
<th>Key Study Sponsor Indicator</th>
</tr>
</thead>
<tbody>
<tr>
<td>100-02-7</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>114 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-50-5</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>2 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-50-5</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>-100 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-53-8</td>
<td>Measured</td>
<td>Measured</td>
<td>Melts</td>
<td>=</td>
<td>96.1 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-53-8</td>
<td>Measured</td>
<td>Measured</td>
<td>Melts</td>
<td>=</td>
<td>-30 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-53-8</td>
<td>Measured</td>
<td>Measured</td>
<td>Melts</td>
<td>=</td>
<td>-14.9 °C (Key)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-53-8</td>
<td>Measured</td>
<td>Measured</td>
<td>Melts</td>
<td>=</td>
<td>-14.8 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100-69-6</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>15.16 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10081-67-1</td>
<td>Measured</td>
<td>Measured</td>
<td>Melts</td>
<td>=</td>
<td>95 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101-20-2</td>
<td>Estimated by Calculation</td>
<td>Estimated</td>
<td></td>
<td>=</td>
<td>162 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101-20-2</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>260 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101-20-2</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>255.3 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101-80-4</td>
<td>Measured</td>
<td>Measured</td>
<td></td>
<td>=</td>
<td>142 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101-84-8</td>
<td></td>
<td></td>
<td></td>
<td>=</td>
<td>147 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>102-06-7</td>
<td>Unknown</td>
<td></td>
<td></td>
<td>=</td>
<td>161.6 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>102-06-7</td>
<td>Unknown</td>
<td></td>
<td></td>
<td>=</td>
<td>151.6 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>102-06-7</td>
<td>Unknown</td>
<td></td>
<td></td>
<td>=</td>
<td>151.6 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
HPVIS Training/Demonstration

- 4 (identical) sessions of HPVIS training/demonstration available at this conference:
  - Today 1:30 to 3:00 – Session 1C
  - Today 3:30 to 5:00 – Session 2C
  - Tomorrow 10:45 to 12:15 – Session 3B
  - Tomorrow 1:30 to 3:00 – Session 4B
HPVIS Training (continued)

- HPVIS demonstrations will be informal and concentrate on data retrieval
- Data entry functions may also be demonstrated if participants desire
For More Information

- Brion Cook
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