The State of Data in Explosives and Ignitable Liquids

Michael Sigman and Mary Williams
National Center for Forensic Science
University of Central Florida
Acknowledgements

The NCFS Databases have been partially supported by:

1. The National Center for Forensic Science, A State of Florida Type II Research Center.

2. Award Numbers 2005-MU-MU-K044, 2008-IJ-CX-K401, 2011-DN-BX-K539, 2015-DN-BX-K051 awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this presentation are those of the authors and do not necessarily reflect those of the Department of Justice.

3. The Prevention of and Fight against Crime Programme of the European Union. This project has been funded with support from the European Commission. This publication reflects the views only of the author, and the European Commission cannot be held responsible for any use which may be made of the information contained therein.
Presentation Outline

• Overview of NCFS databases and partnerships
• Detailed Descriptions
  – Ignitable Liquids Reference Collection Database
  – International Database of Ignitable Liquids
  – Substrates Database
  – Smokeless Powders Database
• Future needs and directions
• Summary
NCFS Database Time Line

2000
IGNITABLE LIQUIDS REFERENCE COLLECTION

2010
Substrate Database

2011
Smokeless Powders Database

2016
International Database of Ignitable Liquids

T/SWGFX Partnership

ENFSI (+) Partnership
NCFS Database Development

Database projects are driven by needs of the forensic science community and conducted as partnerships with the community.

Databases are designed to meet the daily needs of analysts performing casework. Database growth to answer new questions and meet new casework needs is anticipated.

Combining Community Partnerships and Casework Focus with literature and community driven research support is a strong basis for obtaining competitive funding.
Ignitable Liquids Reference Collection Database

Evaporated and Bio Degraded IL Records

DB

1085 Records

Freely Available on Web – Data Download

Consensus ASTM E1618 Classifications
## ILRC Database: Search Results

**Ignitable Liquids Reference Collection**

<table>
<thead>
<tr>
<th>SRN</th>
<th>Brand Name</th>
<th>HC Range</th>
<th>Predominant ion profile</th>
<th>Classification</th>
<th>Major Peaks</th>
</tr>
</thead>
<tbody>
<tr>
<td>0096</td>
<td>BP Regular Unleaded Gasoline</td>
<td>C 6-C 14</td>
<td>Aromatics</td>
<td>Gasoline</td>
<td>1,2,4-trimethylbenzene, o-p-ethyltoluene, m-p-xylene, toluene</td>
</tr>
<tr>
<td>0097</td>
<td>BP Regular Unleaded Gasoline</td>
<td>C 6-C 14</td>
<td>Aromatics</td>
<td>Gasoline</td>
<td>1,2,4-trimethylbenzene, o-p-ethyltoluene, m-p-xylene, toluene</td>
</tr>
</tbody>
</table>

**Sample detail & download section**
ILRC Database: Sample Detail & Download
ILRC Database: Related Samples
Modeling Fire Debris: Classification Models
Fire Debris 0 – 100% SUB, Validation Data

Tippett Plot
Fire Debris 0 – 100% SUB, Validation Data

H_p: The sample is positive for ILR
H_D: The sample is not positive for ILR
International Database of Ignitable Liquids

National Center for Forensic Science
University of Central Florida

Co-funded by the Prevention of and Fight against Crime Programme of the European Union

http://ncfs.ucf.edu/internationaldb/
International Database of IL

DB

240 Records

Unevaporated Ignitable Liquid GC-MS Data

Freely Available on Web – Data Download

Regional Committee Data Review & Entry for QA
International Database of Ignitable Liquids

Search Database

Ignitable Liquid Information
- **SRN**
- **Brand Name**
- **Country Purchased**
- **Product Use**
- **Date Purchased**
- **Data Source**
- **Data Source SRN**
- **Country of Data Source**
- **Region**
- **Keyword**
- **Advanced Keyword**

Classification Information
- **HC Range**
- **Low >=**
- **High <=**
- **Predominant Ion profile**
- **Classification**
- **Major Peaks**
- **CAS #**
- **TIC Image width**

Show All Liquids
Clear
Search
### Released Samples

<table>
<thead>
<tr>
<th>SRN</th>
<th>Brand Name</th>
<th>HC Range</th>
<th>Predominant Ion profile</th>
<th>Classification</th>
<th>Major Peaks</th>
</tr>
</thead>
</table>
| 0032 | Netherlands | C 6-C 23 | Alkanes                 | Heavy petroleum distillate (HPD) | 1. methylcyclohexane  
2. toluene  
3. n-heptadecane  
4. n-octadecane  
5. n-nonadecane |
| 0037 | Gasoline, DP Ultimate | C 6-C 12 | Aromatics               |                | 1. 2-ethoxy-2-methylpropane (ETBE)  
2. 2,2,4-trimethylpentane  
3. toluene  
4. m/p xylene  
5. 1,2,4-trimethylbenzene |

---

**Sample detail & download section**
International Database of Ignitable Liquids

Sample Reference Number: 0032

1. methylcyclohexane
2. toluene
3. n-heptadecane
4. n-octadecane
5. n-nonadecane
http://ilrc.ucf.edu/substrate/
Substrate Database

Burned and Unburned Headspace Data

DB

210 Records

Freely Available on Web – Data Download

ILRC Committee Review for IL Class Characteristics
Substrate Database: Search Page

Search Database

<table>
<thead>
<tr>
<th>Field</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MRN</td>
<td></td>
</tr>
<tr>
<td>Material use class</td>
<td>Search</td>
</tr>
<tr>
<td>Material use sub-class</td>
<td>Search</td>
</tr>
<tr>
<td>Condition</td>
<td>Search</td>
</tr>
<tr>
<td>Ignitable Liquid Residue Present</td>
<td>Search</td>
</tr>
<tr>
<td>Product Name/Description</td>
<td></td>
</tr>
<tr>
<td>HC Range</td>
<td></td>
</tr>
<tr>
<td>Low &gt;=</td>
<td>Search</td>
</tr>
<tr>
<td>High &lt;=</td>
<td>Search</td>
</tr>
<tr>
<td>Major Peaks</td>
<td>Search</td>
</tr>
<tr>
<td>Predominant ion profile</td>
<td>Search</td>
</tr>
<tr>
<td>Material Composition</td>
<td>Search</td>
</tr>
<tr>
<td>Keyword</td>
<td>Advanced Keyword</td>
</tr>
<tr>
<td>Show All Records</td>
<td></td>
</tr>
</tbody>
</table>

View complete List

Clear  Search
### Substrate Database: Search Results

<table>
<thead>
<tr>
<th>MRN</th>
<th>Product Name/Description</th>
<th>HC Range</th>
<th>Condition</th>
<th>Material use class</th>
<th>Major Peaks</th>
</tr>
</thead>
<tbody>
<tr>
<td>0007</td>
<td></td>
<td>C 7-C 19</td>
<td></td>
<td>Flooring</td>
<td>benzylidene styrene</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Carpet</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>None</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Burned</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>major Peaks</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Cycloalkanes/alkanes</td>
<td>Sample detail &amp; download section</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>polypropylene</td>
<td></td>
</tr>
</tbody>
</table>

### Sample detail & download section

<table>
<thead>
<tr>
<th>MRN</th>
<th>HC Range</th>
<th>Material use class</th>
<th>Material use sub-class</th>
<th>Product Name/Description</th>
<th>Ignitable Liquid Residue Present</th>
<th>Condition</th>
<th>Major Peaks</th>
<th>Predominat Profile</th>
<th>Material Composition</th>
<th>Sample detail &amp; download section</th>
</tr>
</thead>
<tbody>
<tr>
<td>0008</td>
<td>C 10-C 18</td>
<td>Flooring</td>
<td>Carpet</td>
<td>Olefin Carpet</td>
<td>None</td>
<td>Unburned</td>
<td>Peaks not identified</td>
<td>Cycloalkanes/alkanes</td>
<td>polypropylene</td>
<td>Sample detail &amp; download section</td>
</tr>
</tbody>
</table>
Substrate Database: Sample Detail & Download

Material Reference Number 0007

Abundance

1. styrene
2. benzaldehyde

Time (s)

Data of Run: 04/02/2007
Ignitible Liquid Residue Present: None
Material use class: Flooring
Material use sub-class: Carpet
HC Range: C 7 - C 10
Product Name/Description: Olefin Carpet
Sample Information: 100% Olefin
Manufacturer: Shaw
Color: Viking-Stingray
Condition: Burned
Predominant Ion Profile: Cycloalkanes/alkenes
Material Composition: polypropylene

To download the datasets, spreadsheet or additional sample information of scalable TICs, click on the icons below.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Spreadsheet</th>
<th>Additional Sample Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dataset M0000007.exe</td>
<td>Spreadsheet M0000007.xls</td>
<td>Sample Information M007.pdf</td>
</tr>
</tbody>
</table>
Substrate Database: Current Expansion Work

• Addition of 1350 new records
• Multiple burn methods
• Tabulation of frequency of occurrence of 255 major compounds in each ILRC and Substrates Database record
• Investigation of improved modeling of fire debris using new substrate pyrolysis data

2015-DN-BX-K051 awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice
http://www.ilrc.ucf.edu/powders/
Smokeless Powders Database

Physical and Chemical Characteristics Data

829 Records

Freely Available on Web – Data Download

Explosives Committee Consensus Methods & Properties
## Smokeless Powders Database: Search Page

### Search Database

<table>
<thead>
<tr>
<th>Powder Information</th>
<th>Physical Description</th>
<th>Chemistry</th>
<th>Result Layout</th>
</tr>
</thead>
<tbody>
<tr>
<td>SRN</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Data Source</td>
<td>Select Value</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Data Source SRN</td>
<td>Select Value</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Product use</td>
<td>Federal Bureau of Investigation</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td></td>
<td>National Center for Forensic Science</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Distributor Name</td>
<td>Netherlands Forensic Institute</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Product Name</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Date Obtained</td>
<td></td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Lot Number</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Date of Analysis</td>
<td></td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Manufacturer</td>
<td>Select Value</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Date Manufactured</td>
<td></td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Comments</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
</tbody>
</table>

[Search Button]
### Smokeless Powders Database: Search Page

#### Search Database

<table>
<thead>
<tr>
<th>Powder Information</th>
<th>Physical Description</th>
<th>Chemistry</th>
<th>Result Layout</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape</td>
<td>Select Value</td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Perforation</td>
<td>Yes</td>
<td>No</td>
<td>Help</td>
</tr>
<tr>
<td>Distinguishing Features</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ teardrops</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ dumb bells</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ agglomerates</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ bias cut</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ striation</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>□ Oblongs</td>
<td></td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Color</td>
<td>Select Value</td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Luster</td>
<td>Select Value</td>
<td></td>
<td>Help</td>
</tr>
<tr>
<td>Marker Color</td>
<td>Green □ Red □ Blue □ Yellow □ Purple □ Orange □ White</td>
<td>Help</td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>min. mm</td>
<td>max. mm</td>
<td>Help</td>
</tr>
<tr>
<td>Average</td>
<td>mm</td>
<td>mm + / - mm</td>
<td>Help</td>
</tr>
<tr>
<td>Length/thickness</td>
<td>min. mm</td>
<td>max. mm</td>
<td>Help</td>
</tr>
<tr>
<td>Average</td>
<td>mm</td>
<td>mm + / - mm</td>
<td>Help</td>
</tr>
</tbody>
</table>

Clear Parameters

Search
### Search Database

The Smokeless Powders Database Search Page includes options for searching by Powder Information, Physical Description, and Chemistry. The active area is highlighted in blue.

#### Main Components
- Nitroglycerin
- 2,4-Dinitrotoluene
- Diethyl phthalate
- Diphenylamine
- Methyl centralite
- Ethyl centralite
- Dibutyl phthalate
- 2-nitrodiphenylamine
- 4-nitrosodiphenylamine
- Amyl phthalate
- 4-nitrodiphenylamine
- Dicyclophthalate
- 2-nitrosodiphenylamine

#### Other Components
- Camphor

**Clear Parameters**

**Search**
### Search Database

<table>
<thead>
<tr>
<th>Powder Information</th>
<th>Physical Description</th>
<th>Chemistry</th>
<th>Result Layout</th>
</tr>
</thead>
</table>

#### Display Image
- GC-MS TIC
- Powder
- Canister
- FTIR Spectrum
- None

#### Image Size
- 400 pixel
- 600 pixel
- 800 pixel
- 1000 pixel

**Clear Parameters**

[Search]
Smokeless Powders Database: Search Results

0101  Winchester 296

SRN  0101
Distributor  Winchester
Product Name  296
Shape  flattened ball
avg. Diameter  0.50 mm
avg. Length/thickness
List of components
Nitroglycerin
Dioctyl phthalate
Diphenylamine
Ethyl celtraite
Dibutyl phthalate
2-nitrodiphenylamine
4-nitrodiphenylamine
Sample detail & download section

0139  Hodgdon HS-6

SRN  0130
Distributor  Hodgdon
Product Name  HS-6
Shape  flattened ball
avg. Diameter  0.90 mm
avg. Length/thickness
List of components
Nitroglycerin
Diphenylamine
Ethyl celtraite
Dibutyl phthalate
2-nitrodiphenylamine
4-nitrodiphenylamine
Sample detail & download section
Smokeless Powders Database: Sample Detail & Download

1. Nitroglycerine
2. Diphenylamine
3. Ethyl cresylic
4. Glyceryl phthalate
5. 2-nitrodiphenylamine
6. 4-nitrodiphenylamine
Evidentiary/Investigative Value of DB Match

Forensic Databases: Future Needs and Directions

- Big Data Partnerships with Private Sector
- International Standards to Promote Sharing of Information
- Global DB to Address Criminals Without Boarders
- Larger DB to Reflect or Allow Modeling of Relevant Populations
Trace Problems: Comparison & Classification

- **Comparison Problem**: Association between two or more items


- **Classification Problem**: Assign an object into one of several classes

  - Rarity, Variance, Feature correlation

  \[
  \frac{P(H_P|E)}{P(H_D|E)} = \frac{P(E|H_P)}{P(E|H_D)} \cdot \frac{P(H_P)}{P(H_D)}
  \]

  - Likelihood Ratio (LR)

    \[
    LR = \frac{f(E|H_P)}{f(E|H_D)} \text{ (Continuous Data)}
    \]

### Database vs Relevant Population

#### FL 1992-2013 (n=70,521)
- AR: 331 (0.47%)
- GAS: 23,243 (32.96%)
- ISO: 219 (0.31%)
- MISC: 4,104 (5.82%)
- NA: 127 (0.18%)
- NP: 233 (0.33%)
- OXY: 860 (1.22%)
- PD: 4,386 (6.22%)
- SUB: 37,016 (52.49%)

#### ILRC + Substrate (n=1,305)
- AR: 74 (5.67%)
- GAS: 111 (8.51%)
- ISO: 88 (6.74%)
- MISC: 203 (15.56%)
- NA: 58 (4.44%)
- NP: 55 (4.21%)
- OXY: 169 (12.95%)
- PD: 337 (25.82%)
- SUB: 210 (16.09%)

---

Carl E. Chasteen, B.S., CPM, F-ABC, Chief of Forensic Services, Bureau of Forensic Fire and Explosives Analysis, Division of State Fire Marshal, Department of Financial Services, State of Florida
Summary

• Databases:
  – 2 Ignitable Liquid, 1 Substrate, 1 Smokeless Powders
  – Designed for casework and training as partnerships with forensic community
  – Research applications have been secondary to casework

• Expansion and Future Databases
  – Should consider representation of relevant population
  – Should account for: rarity, variance, feature correlation
  – International databases
  – ANSI/ISO data standards to promote sharing of data
    • i.e., netCDF data files
  – Additional funding/Private sector partnerships
Thank you.

NCFS Ignitable Liquids and Explosives Research Group 2016.