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Through-Container Measurement of Acoustic Signatures for Classification/Discrimination of Liquid Explosives (LEs) and Precursor Threat Liquids

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Topics of Discussion

- Need for Effective Container Screening
- Objective of the Study
- Description of the Technology
  - Capabilities and Functionality
  - Principles of Operation
- Description of Measurement Protocol
- Results
- Analysis of Results
- Conclusions and Future Work

The Need for Effective Container Screening

- **Driven by DHS and Law Enforcement**
  - **Border and Transportation Security**
  - **Security at High Profile Venues and Events**
  - **Emergency Preparedness and Response**
  - **Vulnerabilities to Liquid-Based Homemade Explosives (HMEs)**

- **This work addresses container screening for liquid threats (chemical weapons agents, liquid explosives, precursors, etc.)**
- **An effective acoustics-based approach offers a non-invasive, nondestructive method for screening liquid filled containers rapidly and reliably.**

Objective of the Study

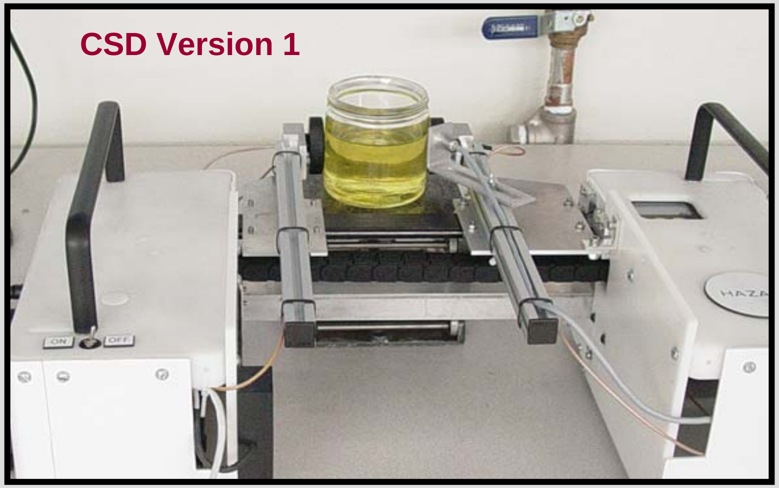
<u>Objective:</u> To address critical measurement discrimination and sensitivity issues required for analyzing and quantifying the effectiveness of PNNL's Container Screening Device (CSD) prototype for classifying and discriminating threat-liquids from non-threat liquids.

US Pat #7,246,522 issued in July, 2007

Description of the Technology

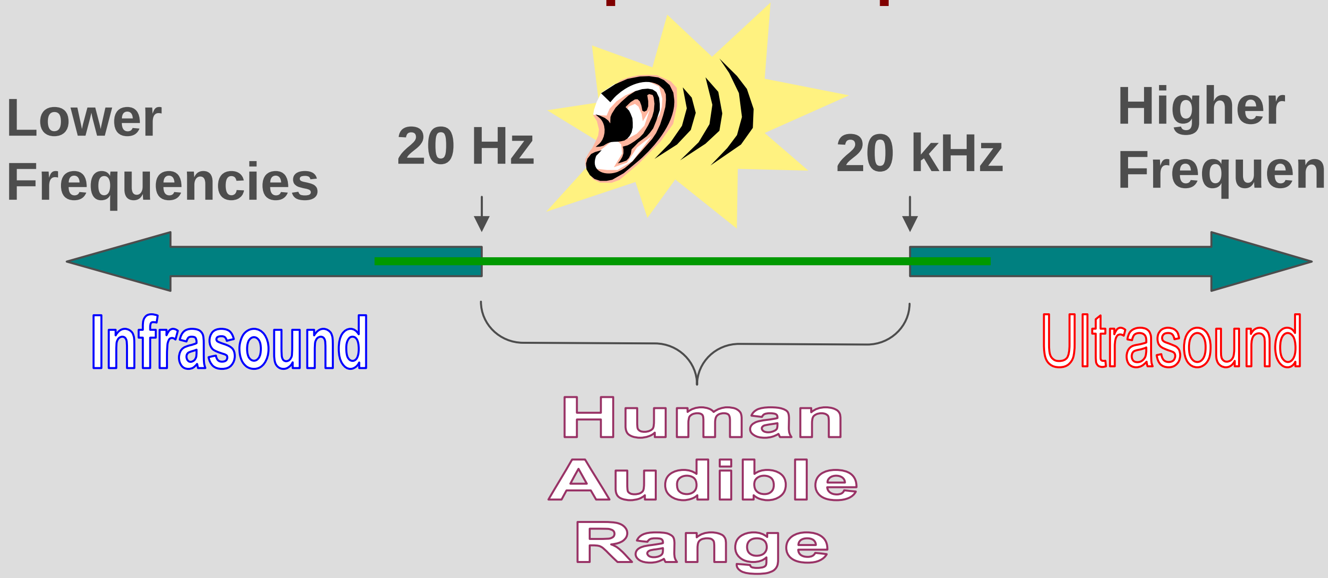
Capabilities and Functionality of the CSD Platform:

- Detect Contraband (or Hidden Compartments) in Liquid-filled Containers and Bulk Solid Commodities
- Rapidly Sort Liquid Types (and many Solids) into Groups of Like and Unlike
- Classify/Discriminate Liquids in Sealed Containers and some Bulk Solids
- Determine Liquid Fill Level in a Sealed Container



Description of the Technology

Principles of Operation:



Measured Characteristics

- Path Length (Distance)
- Echo Detection
- Time of Flight/Temperature
- Signal Amplitude/Phase
- Frequency Content

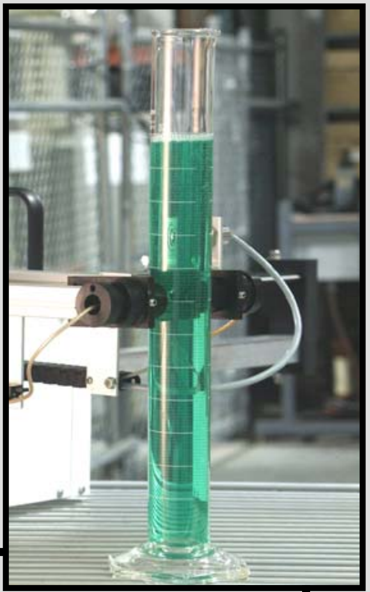
Resultant Properties

- Acoustic Velocity
- Relative Attenuation
- Absorption Spectra
- Liquid Density
- Viscosity

Description of the Technology

Principles of Operation:

- Two Transducers (Pitch-Catch modality)
- Opposite Orientation, Alignment is Critical
- Transducers use a dry-couplant (liquid filled membrane)
- Low V, Long Duration, FM Chirp from 2-8 MHz (Transmit)
- Ultrasonic energy travels through the container wall-liquid-wall configuration and is received by the opposite transducer
- Sound field is modified by the container walls and the liquid where density, viscosity, elasticity, compressibility, and temperature play key roles in influencing the velocity and relative attenuation



c=velocity

E=Young's Modulus

K=bulk modulus

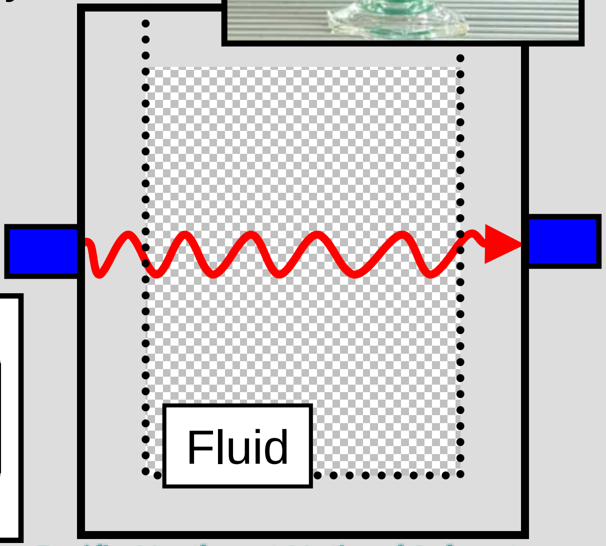
ρ=density

$$E_j = \sum_{i=1}^{n} f^2 \, FFT_i \, \Delta f$$

$$c_{solids} = \sqrt{\frac{E}{\rho}}$$

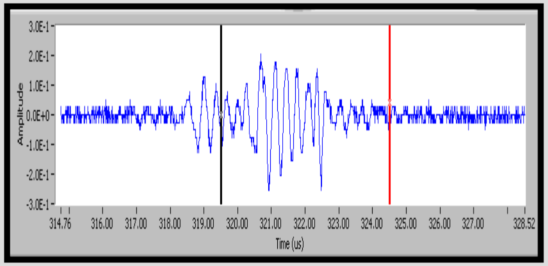
$$c_{fluid} = \sqrt{\frac{K}{\rho}}$$

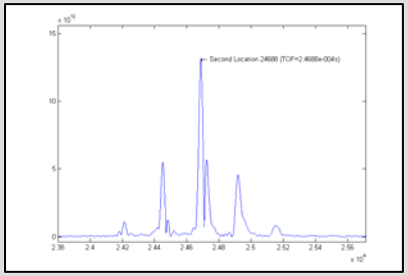
$$\alpha_{coeff} = \left(\frac{E_2}{E_1}\right)$$

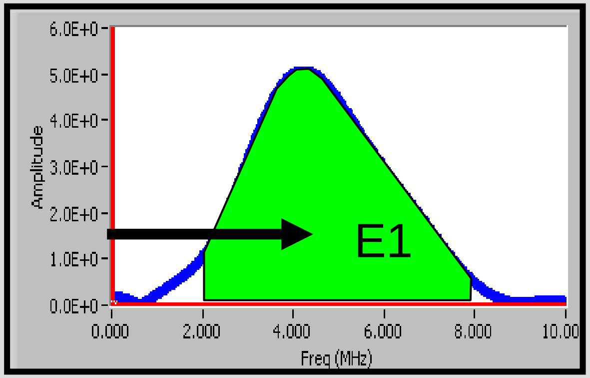


Description of the Technology

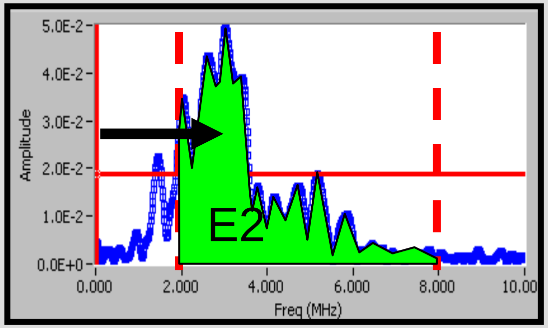
Principles of Operation:







- Received ultrasonic echoes undergo signal conditioning, amplification and 16-bit digital sampling
- Algorithms perform deconvolution process (cross-correlation of input chirp with received chirp)
- Automated container temperature and distance values are measured and ported to the algorithms for computation of sound speed and relative attenuation
- Raw ultrasonic data is automatically compensated for wall thickness, and processed values are compared to a database listing for a sequential “closest-match”



V and α →

Alcohol
Mineral Oil
Castor Oil
Motor Oil
Water
Shampoo
Antifreeze
Aluminum

Description of Measurement Protocol

- All measurements acquired at near room temperature
- Containers used were Polyethylene Terephthalate – (PETE) 120 ml containers
- 21 total liquids evaluated in Phase 1
- Key measured parameters include container diameter, acoustic velocity, relative attenuation and surface temperature of the container
- Multiple measurements taken for each liquid and for each testing scenario
  - Over 20 identical PETE containers used in Phase 1 evaluation
  - De-ionized, de-gassed water used for baseline testing
- Three primary datasets were obtained to evaluate:
  - Effects of container variability on the measurement
  - Inherent CSD measurement variability
  - Discrimination/Classification capability (21 liquid set)

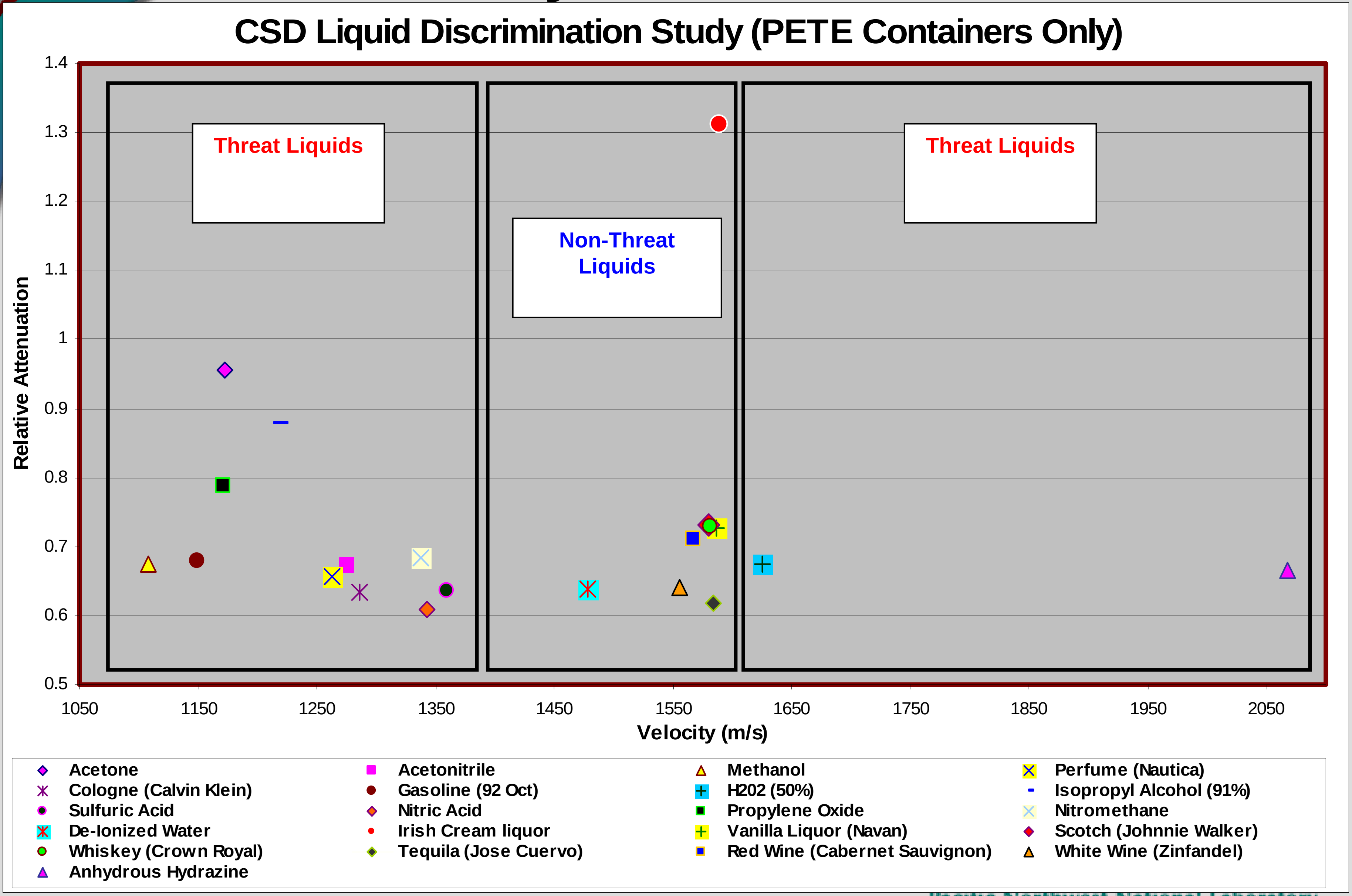
Liquids Evaluated in Phase 1

Liquid Name:	Concentration:	Category Descriptor:
Acetone	99%	Solvent/Fuel Additive
Acetonitrile	99.5+% A.C.S. Reagent	Solvent
Anhydrous Hydrazine	98%	Ignition Source/Propellant
Cologne (Calvin Klein® CKBe)	Not Provided	Benign Commercial Product
De-ionized De-gassed Water (H_2O)	Not Applicable	Benign Commercial Product
Gasoline	92 octane	Ignition Source/Fuel
Hydrogen Peroxide (H_2O_2)	50% in solution	Oxidizer/Propellant/LE Component
Irish Cream Liquor (Carolyn's®)	17% alcohol (34 proof)	Benign Commercial Product
Isopropyl Alcohol	91% concentration	Solvent
Methanol	99.9%	Solvent/Fuel
Nitric Acid	≥ 90% A.C.S. Reagent	Oxidizer/Acid/LE Component
Nitromethane	95+% A.C.S. Reagent	Solvent/Fuel/LE Component
Perfume (Nautica®)	Not Provided	Benign Commercial Product
Propylene Oxide	99% ReagentPlus®	Thermobaric Explosive
Red Wine (Woodbridge® Cabernet Sauvignon)	17.5% alcohol (35 proof)	Benign Commercial Product
Scotch (Johnnie Walker's®)	40% alcohol (80 proof)	Benign Commercial Product
Sulfuric Acid	98% A.C.S. Reagent	Acid/LE Component
Tequila (Jose Cuervo®)	40% alcohol (80 proof)	Benign Commercial Product
Vanilla Liquor (Navan®)	40% alcohol (80 proof)	Benign Commercial Product
Whiskey (Crown Royal®)	40% alcohol (80 proof)	Benign Commercial Product
White Wine (Sutter Home® White Zinfandel)	9.5% alcohol (19 proof)	Benign Commercial Product

Summary of Phase 1 Results

Liquid	Ave. Velocity (m/s)	Velocity Std Dev (m/s)	Ave. Atten. (unitless)	Atten. Std. Dev	Total Trials
Acetone	1172.781	5.136	0.9565	0.0792	20
Acetonitrile	1275.916	0.682	0.6712	0.0438	20
Methanol	1108.681	7.691	0.6745	0.0648	20
Perfume (Nautica®)	1263.172	7.101	0.6554	0.0786	20
Cologne (Calvin Klein® CKBe)	1286.350	7.138	0.6348	0.0548	20
Gasoline (92 Octane)	1149.085	0.487	0.6783	0.0399	20
Hydrogen Peroxide (50% in solution)	1625.768	2.762	0.6747	0.0447	20
Isopropyl Alcohol (91%)	1214.029	1.119	0.8789	0.0943	20
Sulfuric Acid	1359.412	1.043	0.6357	0.0730	20
Nitric Acid	1342.502	6.610	0.6079	0.0927	20
Propylene Oxide	1170.968	0.525	0.7875	0.0832	20
Anhydrous Hydrazine	2067.550	1.379	0.6656	0.0621	20
Nitromethane	1337.749	0.400	0.6847	0.0221	20
De-ionized, de-gassed water (200 total measurements)	1478.322	6.841	0.6389	0.0542	200
Irish Cream Liquor (Carolyn's® 17% alcohol)	1588.879	3.635	1.3120	0.1709	20
Vanilla Liquor (Navan® 40% alcohol)	1586.823	4.098	0.7272	0.0701	20
Scotch (Johnnie Walker's® 40% alcohol)	1580.185	4.575	0.7319	0.052	20
Whiskey (Crown Royal® 40% alcohol)	1580.916	1.13	0.7281	0.0529	20
Tequila (Jose Cuervo® 40% alcohol)	1583.601	0.592	0.618	0.0242	20
Red Wine (Woodbridge®, Cabernet Sauvignon 17.5% alcohol)	1566.915	2.71	0.7119	0.0778	20
White Wine (Sutter Home®, White Zinfandel 9.5% alcohol)	1555.280	6.382	0.6408	0.0366	20
De-ionized, de-gassed water (no-decoupling between individual measurements)	1482.413	0.3675	0.6197	0.0059	40

Summary of Phase 1 Results



Analysis of Phase 1 Results

- Two basic classification algorithms were used to investigate the ability to distinguish between the different liquids evaluated in this study.
- These methods were the Classification and Regression Tree Algorithm (CART), and the Linear Discrimination Algorithm (LDA).
- Results from these two methods presented here represent preliminary runs using commercially available versions of these statistical evaluation methods.
- No adjustments (standardization, averaging, etc.) were made to the independent variables for these initial runs.
- As expected, some liquids are easily classified using these two statistical methods while others are more difficult to classify/discriminate correctly.

Analysis of Phase 1 Results

CART ANALYSIS

Acetone	0.0000000
Acetonitrile	0.0000000
Anhydrous Hydrazine	0.0000000
CKBe® Cologne	0.0000000
De-ionized water	0.0000000
Gasoline	0.0000000
H2O2 50%	0.0000000
Irish Cream	0.0000000
Isopropyl Alc (91%)	0.0000000
Methanol	0.0000000
Nautica®	0.0000000
Nitric Acid	0.0000000
Nitro Methane	0.0000000
Propylene Oxide	0.0000000
Red Wine	0.0000000
Scotch	0.7272727
Sulfuric Acid	0.0000000
Tequila	0.0000000
Vanilla Liquor	0.1818182
Whiskey	0.0909091
White Wine	0.0000000

- A classification "tree" resulting from using the CART algorithm on all of the available data was generated, and nearly all of the branching that occurs on this tree is based upon velocity with only a few branches based upon attenuation.
- The CART model incorporates a "smearing" affect where probabilities of association are assigned to each liquid category as each "new" observation (measurement) is tested.
- For example, given a certain combination of measured velocity, attenuation, and temperature values obtained for a certain liquid, the CART model assigns probabilities of association to the different liquids.
- For this example, the liquid would be classified as scotch because it has the highest associated probability.

Analysis of Phase 1 Results

CART ANALYSIS

A Confusion Matrix was generated using a "leave-one-out" re-sampling approach. The process involves repeatedly selecting a random observation (velocity, attenuation, and temperature measurements) from among the observations (measurement data) available for a given liquid, and applying the CART model fit using the remaining observations (the remaining observations over all liquids) to the selected observation. The probabilities of association are summed over the repeated tests for a given liquid, and the results are divided by the number of tests for that liquid. Over 10,000 trials were executed for this matrix.

Analysis of Phase 1 Results

CART ANALYSIS

	DeI H2O	Acetone	IsopAlc	CKBe	Acetonitrile	Methanol	Nautica	Gasoline	Nitro Meth	Anhyd Hyd	Propyl Ox	H2O2 50%	Sulf.Acid	Red Wine	White Wine	Irish Cream	Scotch	Whiskey	Vanilla Liq	Tequila	Nitric Acid
DeI H2O	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Acetone	0	0.95	0.05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
IsopAlc	0	0.01	0.83	0	0	0	0.16	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CKBe®	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Acetonitrile	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nautica®	0	0.01	0.04	0	0	0	0.95	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gasoline	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Nitro Meth	0	0	0	0	0	0	0	0	0.87	0	0	0	0	0	0	0	0	0	0	0	0.13
Anhyd Hyd	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Propyl Ox	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
H2O2 50%	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
Sulf.Acid	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Red Wine	0	0	0	0	0	0	0	0	0	0	0	0	0	0.95	0	0	0.00	0.00	0	0.04	0
White Wine	0	0	0	0	0	0	0	0	0	0	0	0	0	0.09	0.91	0	0	0	0	0	0
Irish Cream	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Scotch	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00	0	0	0.80	0.05	0.08	0.07	0
Whiskey	0	0	0	0	0	0	0	0	0	0	0	0	0	0.01	0	0	0.02	0.88	0.00	0.09	0
Vanilla Liq	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00	0	0	0.10	0.05	0.73	0.12	0
Tequila	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.08	0.01	0.11	0.80	0
Nitric Acid	0	0	0	0	0	0	0	0	0.06	0	0	0	0	0	0	0	0	0	0	0	0.94

Analysis of Phase 1 Results

LDA ANALYSIS

As with the CART analysis, LDA assigns probabilities of association to each liquid category for each "new" observation tested. The same "leave-one-out" re-sampling approach used for CART was used to generate a confusion matrix based on the LDA classification method.

Analysis of Phase 1 Results

LDA ANALYSIS

	De-I H2O	Acetone	Isopropyl Alc	CKBe®	Acetonitrile	Methanol	Nautica®	Gasoline	Nitro Meth	Anhyd Hyd	Propyl Ox	H2O2 50%	Sulf. Acid	Red Wine	White Wine	Irish Cream	Scotch	Whiskey	Vanilla Liq	Tequila	Nitric Acid
De-I H2O	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Acetone	0	0.99	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0	0
Iso. Alc.	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CKBe®	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Acetonitrile	0	0	0	0	0.96	0	0.04	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nautica®	0	0	0	0	0.24	0	0.76	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Gasoline	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Nitro Meth	0	0	0	0	0	0	0	0	0.9	0	0	0	0	0	0	0	0	0	0	0	0.1
Anhyd Hyd	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Propyl Ox	0	0.04	0	0	0	0	0	0	0	0	0.96	0	0	0	0	0	0	0	0	0	0
H2O2 50%	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
Sulf.Acid	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
Red Wine	0	0	0	0	0	0	0	0	0	0	0	0	0	0.85	0.08	0	0.03	0.02	0	0.03	0
White Wine	0	0	0	0	0	0	0	0	0	0	0	0	0	0.2	0.79	0	0	0	0	0	0
Irish Cream	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
Scotch	0	0	0	0	0	0	0	0	0	0	0	0	0	0.08	0	0	0.39	0.29	0.11	0.12	0
Whiskey	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.29	0.38	0.19	0.14	0
Vanilla Liq	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.12	0.25	0.51	0.13	0
Tequila	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.11	0.15	0.1	0.65	0
Nitric Acid	0	0	0	0	0	0	0	0	0.22	0	0	0	0	0	0	0	0	0	0	0	0.78

Conclusions and Future Work

- Results indicate that ultrasonic physical property measurements can be effective metrics for liquid classification and discrimination
- Measurement variability is manageable but will require further improvement through engineering design and enhancements to signal-detection and processing algorithms
- Attenuation measurements require additional work to compensate for beam divergence, coupling variations and wall-material to liquid-boundary acoustic impedance corrections/compensation
- More measurements are planned on threat liquids (to be studied in Phase 2 – April/May 2008) and include

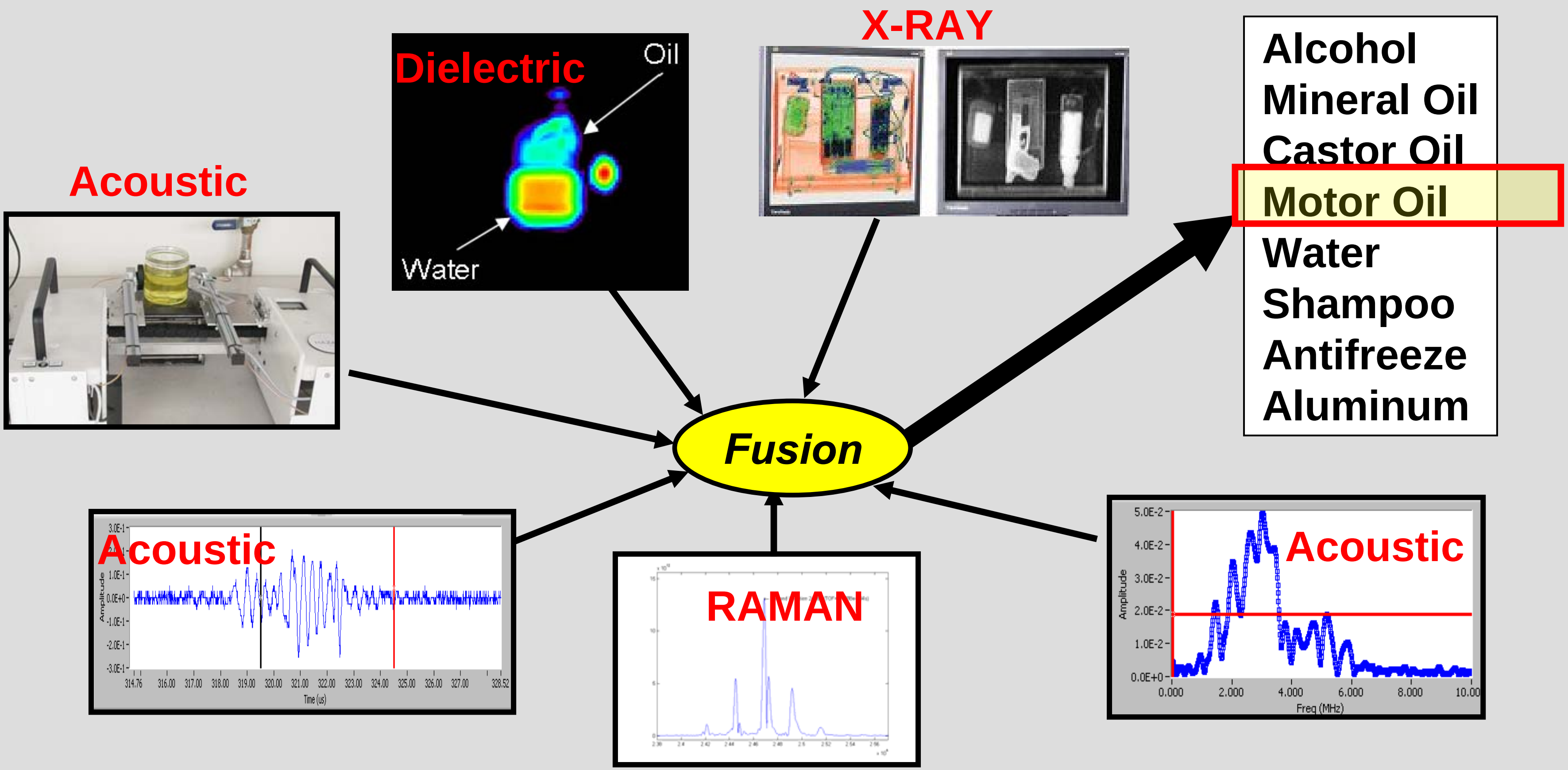
TNT RDX HMX PETN Nitroglycerin

Conclusions and Future Work

- Orthogonal modalities and additional acoustic signatures will be studied in the future
- The effects of container variation (both geometrical and wall material) need to be addressed after the algorithms are enhanced
- Addressing a COTS approach to container material identification for integration with the CSD platform
- Enable the pulse-echo modality onboard the CSD
- Incorporate advanced statistically-based decision algorithms:
  - Chemometric analysis
  - Feature analysis
  - Clustering algorithm

Conclusions and Future Work

- Incorporate multi-modal, multi-physical property measurement approach with an effective **data-fusion** technique to strengthen effectiveness of classification, discrimination and confidence levels



Questions & Discussion

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