Water-based Liquid Scintillator R&D: a new application for large-scale experiment

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Outlines

- Motivations
- Introduction
- Approaches
- Characterization
- Preliminary Results
- Future Plans
Motivations:

- develop a W-LS to be used as energy spectrometers in large-scale physics experiments
- to replace the hundreds to many tons of unloaded or metal-loaded organic liquid scintillators to
  - simplify the preparation of the sensitive detection medium
  - less compatibility issue
  - cost savings.
- light below Cherenkov region?
~40+ Years of BNL Chemistry and Neutrinos

- **HOMESTAKE** Radiochemical Detector
  - 615 tons of $\text{C}_2\text{Cl}_4$; $^{37}\text{Cl} + \nu_e \rightarrow ^{37}\text{Ar} + e^-$ (~40y)

- **GALLEX** Radiochemical Detector
  - 30 tons of Ga; $^{71}\text{Ga} + \nu_e \rightarrow ^{71}\text{Ge} + e^-$ (1986 - 1998)

- **SNO** Water Čerenkov Detector (SNOLab)
  - 1-k tons of ultra-pure $\text{D}_2\text{O}$ (1996 - 2006)

- **SNO+ Neutrinoless Double Beta Decay** Real-time Detector
  - 1-k tons of 0.1% Nd in Liquid Scintillator (b. 2005~)

- **LENS** Real-time LS Detector (R&D)
  - 100 tons of ~8% $^{115}\text{In}$ in Liquid Scintillator (b. 2000~)

- **Very Long-Baseline Neutrino Oscillations (R&D)**
  - $\nu_\mu$ beam from accelerator to DUSEL (b. ~2002)

- **High-Precision Reactor $\theta_{13}$ Real-time Detector**
  - 200 tons of 0.1% Gd in Liquid Scintillator (b. 2003~)

- **Neutrino Application**
  - Geo-neutrino, Nonproliferation
  - Li/Ca-loaded Liquid Scintillator

- **Water-based Liquid Scintillator (b. 2009)**
Components of LS

- **Aromatic solvent** that contains a high density of $\pi$-electrons for energy transfer
- **Fluor** that transfers the energy ($<400 \text{ nm}$) to light ($>400 \text{ nm}$) within the optimal detection range of PMT
Common Features of LS Detector

1. high light yield at 30 – 50% anthracene
2. adequate attenuation length of ~15m after purification
3. long stability of 3+ years

Cons

- careful chemical treatment
- high cost
- less compatible with materials
- extensive liquid handling
- chemical safety in the confined space of underground laboratories
Is water-based LS compatible?

- photon yield is less than that of pure liquid scintillator
- superior attenuation length of water (80 – 100m) compensates p.e./MeV?
Open Issues

- **LS loading technology**
- **Purification**
  - *LS* – distillation, dry column, solvent wash
  - *Water* – UV lamp, exchange resin, RO, filtration
  
  > What can we do for LS-water system?

- **Light-yield**
  - Quenching effect
    - non-radioactive transfer
    - re-absorption

- **Attenuation length**

- **Chemical stability**
Basic Principal: Polarity, solubility, and miscibility

- polar (hydrophilic) and non-polar (lipophilic) determines what types of solvents or liquid compounds are miscible with.
- a rule of thumb: "like dissolves like".
- Similarly, water and organic solvent are not miscible with each other and will quickly separate into two layers even after being shaken well.
- Need a surfactant to reduce the tension between polar and non-polar surface
Approaches

Fundamental:

- **sufficient concentration** of liquid scintillator in a water medium is essential to the success of water-based liquid scintillator.

- **Engineering** a complexing medium (surfactant) to stabilize the lipophilic and hydrophilic molecules with
  - Long attenuation length
  - Chemical stability for 3+ years

- Two approaches are proposed
A1: Investigation of Surfactant
systematic studies of commercial LS (PC, PXE, DIN, PCH, LAB), which can be produced in large quantity
to research (or develop) a suitable amphiphilic surfactant containing both lipophilic (non-polar) and hydrophilic (polar)
• The degree of tension reduction is a function of surfactant concentration, which could also affect the optical and stability properties of W-LS.
anionic surfactants (carboxylates, phosphates or sulphates) are most interested
Selection of Liquid Scintillator

- high density, flash point, low toxicity, and low cost
- chemical compatibility
- high light yield and long attenuation
- Any of them be loaded in the water?

linear alkyl chains of 10-13 C atoms with a benzene ring; used primarily for the production of biodegradable synthetic detergent

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiling Point (°C)</td>
<td>275 - 307</td>
</tr>
<tr>
<td>Melting Point (°C)</td>
<td>&lt; -50</td>
</tr>
<tr>
<td>Flash Point (°C)</td>
<td>130</td>
</tr>
<tr>
<td>Vapor Pressure (mmHg)</td>
<td>&lt; 0.1 mmHg @ 20°C</td>
</tr>
<tr>
<td>Vapor Density (Air = 1)</td>
<td>8.1</td>
</tr>
<tr>
<td>Solubility in Water</td>
<td>Insoluble</td>
</tr>
<tr>
<td>Molecule Weight</td>
<td>233 – 237 g/mol</td>
</tr>
<tr>
<td>pH</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Viscosity</td>
<td>5 – 10 cps @ 20°C</td>
</tr>
<tr>
<td>Evaporation Rate (water = 1)</td>
<td>Not applicable</td>
</tr>
</tbody>
</table>

high light yield, high flash point, low toxicity, cheap → an ideal scintillator for neutrino experiment
# Parameters of Liquid Scintillator

<table>
<thead>
<tr>
<th></th>
<th>Metal Loading</th>
<th>$d$ (g/cm$^3$)</th>
<th>UV Abs$^{430}$ before/after</th>
<th>Abs$_{260}$</th>
<th>$n^{20}$</th>
<th>Light Yield</th>
<th>$H$ atoms$^\dagger$ per c.c</th>
<th>Flash Point</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PC</strong></td>
<td>Yes</td>
<td>0.889</td>
<td>0.008 / 0.002</td>
<td>2</td>
<td>1.504</td>
<td>1</td>
<td>$5.35 \times 10^{22}$</td>
<td>48 C</td>
</tr>
<tr>
<td><strong>PCH</strong></td>
<td>Yes</td>
<td>0.95</td>
<td>0.072 / 0.001</td>
<td>1.7</td>
<td>1.526</td>
<td>0.46</td>
<td>$5.71 \times 10^{22}$</td>
<td>99 C</td>
</tr>
<tr>
<td><strong>DIN</strong></td>
<td>Yes</td>
<td>0.96</td>
<td>0.040 / 0.023</td>
<td>&gt;10</td>
<td>-</td>
<td>0.87</td>
<td>$5.45 \times 10^{22}$</td>
<td>&gt;140 C</td>
</tr>
<tr>
<td><strong>PXE</strong></td>
<td>Yes, but not stable</td>
<td>0.985</td>
<td>0.044 / 0.022</td>
<td>2.1</td>
<td>-</td>
<td>0.87</td>
<td>$5.08 \times 10^{22}$</td>
<td>167 C</td>
</tr>
<tr>
<td><strong>LAB</strong></td>
<td>Yes</td>
<td>0.86</td>
<td>0.001 / 0.000</td>
<td>1</td>
<td>1.482</td>
<td>0.98</td>
<td>$6.31 \times 10^{22}$</td>
<td>130 C</td>
</tr>
<tr>
<td><strong>Mineral Oil $C_{24-28}$</strong></td>
<td>No</td>
<td>0.85</td>
<td>0.002 / 0.001</td>
<td>1</td>
<td>~1.46</td>
<td>~</td>
<td>$6.73 - 8.00 \times 10^{22}$</td>
<td>215 C</td>
</tr>
<tr>
<td><strong>Dodecane</strong></td>
<td>No (&lt;20%)</td>
<td>0.75</td>
<td>0.001 / 0.000</td>
<td>1</td>
<td>1.422</td>
<td>~</td>
<td>$6.89 \times 10^{22}$</td>
<td>71 C</td>
</tr>
</tbody>
</table>
A2: Linear Alkyl Benzene Derivatives

- Linear Alkyl Benzene was first identified by SNO+ as the choice of detection medium (Daya Bay, SNO+ and LENS).
- LAB has a long alkyl chain (10-13 C) and a benzene ring (unsaturated π-electrons) for scintillation light.
- Several advantages as LS: (1) optically transparent of 15m at 430nm; (2) relatively high photon yield (30% anthracene); and high flash point at 140°C.
- The worldwide industrial uses of LAB is millions of tons per year. The manufacture quantity and cost are adequate for large-scale neutrino experiments.
A2: LAB Derivatives (continued)

- **chemical basis of LAB-S is a possible candidate**
  - LAB acting as a solvent to extract oils and grease (lipophilic)
  - attached sulfonate group (hydrophilic) can dissolve in water.

- **A surfactant and liquid scintillator simultaneously, very promising candidate for water-based liquid scintillator (or organo-scintillator loaded water detector).**
Characterizations

- Solubility of LS in H2O
  - HPLC
  - Fluorescence emission
  - UV
  - Dielectric constant or dipole moment
- Photon production
- Fluor investigation
- Attenuation length
- Stability as a function of time
M-LS Characterization (I)

- $L_{1/e}$ (att. length) by 10-cm UV-Vis and 2-m dual-beam, vertical LED system.

- Light Yield (S%)

\[ L = \frac{\log(e) L}{A(L)} \]

Extinction of LED502SE Light in 1000 cm H$_2$O

18.9 ± 1.2 m for 18MΩ H$_2$O at 525 nm, J. Goett

Brookhaven Science Associates
**LS Characterization (II)**

- Impurities by XRF and colorimetric

\[ \delta < 3\% \]

\[ y = 0.4634x - 0.0008 \]

\[ R^2 = 0.9966 \]
Characterization of LS (III)

- surfactant by IR
  - $[\text{H}_2\text{O}]$ by Karl-Fischer titrator
  - $[\text{NH}_4^+]$ and $[\text{Cl}^-]$ by electrochemistry
  - $[\text{RCOOH}]$ by acid-base titration
Characterization of LS (IV)

- **Radioactive Background**

  - Sensitivity at 50 ppb U/Th for 100-hr counting
  - Plan to upgrade another Compton-suppression well counter
Preliminary Results

- We started the R&D in 2009
- Primary interest in LS’s that are commercially available for mass production
- Samples stable for 4+ months since preparation
- in contact with the vendors capable of providing large quantity
LS- solubility test in H2O (preliminary)
LS – H2O light yield (preliminary)

~18% of $S_{\text{LAB}}^\text{LAB}$
LS-M solubility in H2O (preliminary)
[LS] in H2O characterization (Preliminary)

\[ y = 59.374x + 0.0744 \]
\[ R^2 = 0.9924 \]
What can we do to improve?

- *Purification, purification, Purification!*
  - Remove the impurities to (1) improve optical length and (2) increase stability
  - Remove the color to avoid re-absorption of solvent

*We have extensive experiences in both organic and water*
Organic Purification

A – E: 5 drums of Petresa LAB came from 2007
BNL unpurified/purified: 1 drum of Petresa LAB from 2006
Water Purification
SNO water purification
Near-term Goals

- **feasibility check for water-based LS synthesis**
  - systematic study of chemical form and physical property of surfactant
  - investigation of commercial scintillation cocktails (from Bicron & National Diagnostic) in water
  - Geant4 simulation using Daya Bay package
  - suitability of commercial liquid scintillator (PC, PCH, PXE, LAB) in water
  - surfactant (mainly carboxylate, phosphate, and sulphate) emulsion or solubilisation check
  - general chemical form of LAB-S as surfactant and scintillator
  - solubility (w%) of LAB-S in water

- **stability, photon yield and optical purification of water-based LS**
  - photon yield comparison with plastic scintillator or anthracene
  - water-quenching effect on light yield
  - stability test of water-based liquid scintillator
  - optical transmission and purification development for all components of the composition of water-based liquid scintillator
  - feasibility check of large-scale production
Long-term Goals

- Long-term stability check and aging test of water-based liquid scintillator
- Addition of fluor and wavelength-shifter to Water-based Liquid Scintillator
- Metal-loaded water-based liquid scintillator
- Material compatibility assessment with water-based liquid scintillator
- Water-based liquid scintillator prototype
Material Compatibility Program

- Impacts of material to liquid: UV, light Yield
- Impacts of liquid to material; XRF, ICP-MS, Microscope
- Over 400 samples (polymers, SS, coatings, liners, etc) were tested in Water and LS
- For LS, the blue scintillation light (at 430nm)
- For water, the Cerenkov light (>300 nm)
A Water-based LS Demonstrator

Scale-up from many tens to ton of liters
Inter-departmental collaborations

- Daya Bay
- DUSEL – LBNE
- Compatibility program
- 2-m dual-beam vertical attenuation system
- Periodical neutrino group discussion
- Water-based liquid Scintillator
- ...etc
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