



Maximizing Light Yield



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October 13-15, 2026

Physics Opportunity of Large Liquid Scintillator Detectors (II)



Where does LS light yield come from?

From deposited energy to detected photons

- Ionizing particle deposits energy primarily in the **aromatic solvent**.
- Excitation is created in the solvent's energy states.
- Energy migrates among solvent molecules and is transferred to the **primary fluor**, usually PPO.
- PPO converts the excitation into fluorescence at longer wavelength.
- A secondary wavelength shifter such as **bis-MSB** can move the spectrum farther into the detector-sensitive region.
- The observed photoelectron yield depends on every step: excitation production, energy-transfer efficiency, fluor quantum yield, optical transport, and photodetector efficiency.

$$N_{\text{PE}} \sim E_{\text{dep}} \times Y_{\text{exc}} \times \epsilon_{\text{transfer}} \times \Phi_{\text{F}} \times P_{\text{transport}} \times \text{PDE}(\lambda)$$

How energy flows inside a LS system?

Intrinsic fluorescence vs molecular structure

- **Aromatic solvent** Delocalized/Conjugated **π -electron** systems efficiently accept deposited energy and support excitation migration.
- **Primary fluor** High fluorescence quantum yield and strong spectral overlap with solvent emission are desirable.
- **Stokes shift** A larger separation between absorption and emission reduces repeated self-absorption.
- **Non-radiative channels** Internal conversion, intersystem crossing and collisional quenching compete with fluorescence.
- **Purity** Oxygen, metals and absorbing organic impurities can reduce light yield and/or attenuation length.

LAB* $\rightarrow$ PPO* $\rightarrow$ $h\nu$ (and, when used) PPO emission $\rightarrow$ bis-MSB* $\rightarrow$ $h\nu'$

Molecular design should optimize the entire **spectral cascade**, not simply choose the molecule with the highest isolated fluorescence quantum yield.

More fluor does NOT indefinitely mean more light

Optimize energy transfer vs. concentration quenching

- Low fluor concentration is inefficient because an excitation may decay before reaching PPO.
- Increasing PPO therefore initially produces a **large increase in light yield**. But eventually solvent→PPO transfer approaches saturation; and thus PPO self-absorption increases that self-quenching becomes important (potentially negative returns).
- SNO+, DayaBay, PROSPECT (BNL) measurements over **0.1–5 g/L PPO** were described by competing processes: increasing transfer efficiency followed by losses associated with PPO-light absorption/self-quenching.
- JUNO's detector-scale optimization gives a particularly useful demonstration. Initial LY rises rapidly with PPO concentration below about **2 g/L**, after which the increase becomes much weaker. Their optimized large-detector composition was approximately **2.5 g/L PPO + 3 mg/L bis-MSB in purified LAB**.

Optical properties can dominate at large scale

Intrinsic LY $\neq$ detected LY: A small vial may favor one formulation while a 10–30 m detector favors another.

- Absorption length and scattering length determine how far photons can propagate; attenuation combines both processes.
- Self-absorption becomes increasingly costly as detector dimensions grow because photons undergo longer paths and more absorption/re-emission cycles.
- Control of optical contaminants through purification can therefore produce a larger detector-level gain than a small increase in intrinsic photon yield.
- Spectral matching matters: photons should be shifted into a wavelength region with long attenuation length and high PMT/SiPM photon-detection efficiency.
- UNO provides an excellent real-world example: its LS attenuation length requires **>20 m at 430 nm**, and alumina purification demonstrated improvement of LAB from about **20 m to >24 m**.

For large detectors, improving transparency by a few meters can be more valuable than gaining a few percent in intrinsic photon yield.

Wavelength shifting optimizes the spectral window

- **Fluor → WLS → photodetector matching**
- A wavelength shifter does **not create additional excitation energy**. Its purpose is to make existing photons more useful.
- Modern liquid scintillators commonly employ PPO and bis-MSB as a primary fluor and secondary wavelength shifter, respectively, reducing self-absorption by PPO and absorption by LAB, improving effective photon attenuation length, and providing better spectral matching to PMT quantum efficiency.
- JUNO/SNO+ provides a particularly convincing detector-scale result: once the LAB was optically purified, increasing bis-MSB beyond only a few mg/L gave little benefit.
- But every absorption/re-emission cycle has a quantum efficiency loss, so excessive wavelength shifting also loses photons.
- **Can a second WLS with a larger Stokes shift (>450 nm emission) improve long-distance photon survival enough to compensate for the additional fluorescence conversion loss and less PMT QE sensitivity?**

Takeaways

Practical recipe for maximizing detector light yield		
Parameter	Optimize for	Main limitation
Solvent	High excitation/energy-transfer efficiency	intrinsic non-radiative loss
Primary fluor	Efficient solvent→fluor transfer	concentration quenching
WLS	Spectral matching + large Stokes shift	conversion loss/self-absorption
Purity	Long attenuation length	optical impurities/O ₂
Detector optics	High PDE × photon survival	geometry & spectral response

For very large detectors, maximum PE yield is governed not by intrinsic fluorescence alone, **but by the combined optimization of excitation, energy transfer, fluorescence efficiency, quenching, Stokes shift, attenuation length, and photodetector spectral matching.**

