Liquid Argon optical properties to be used in Geant4 and Opticks Simulations

Hans Wenzel¹

¹ Fermilab PO Box 500, Batavia, IL 60510, USA

E-mail: wenzel@fnal.gov

Abstract. In Geant4 and Opticks optical properties like e.g. the materials refractive index are inputs that have to be provided. In this paper we collect the optical properties relevant for liquid Argon TPC's.

1. Introduction

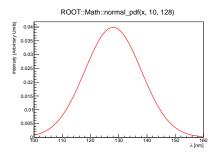
In Geant4 and Opticks optical properties like e.g. the materials refractive index are inputs that have to be provided when the detector is constructed. High-precision modeling of light production, transport and detection in liquid Argon experiments requires the use of the best available values to describe the properties of liquid Argon. In this article we briefly describe the physical processes relevant to the production, transport and detection of optical photons in liquid Argon. We collect the values and parameterizations of optical properties relevant for liquid Argon TPC's. We provide scripts that plot this quantities and that convert this values into a gdml description that can be directly used in the Geant4 Detector description. All values are summarized in the file material.xml which can be found in the github repository [6]. Usually quantities are given as a function of photon wavelength but Geant4 requires the photon energy. The motion of the charged particles liberates charge from the surrounding argon (ionization) and produces light (scintillation)

$$E_{\gamma}(eV) = \frac{hc}{\lambda_{\gamma} 10^{-9}} \tag{1}$$

with:

speed of light: c = 299792458m/sec

Planck constant: $h = 4.13566743 \times 10^{-15} eV/sec$



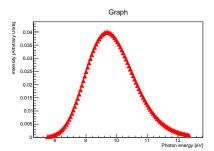


Figure 1. Scintillation emmission spectrum.

2. Light production

There are two relevant sources of light production when a charged particle passes through a medium. The two sources have very different characteristics and yield. One is Scintillation light produced when a charged particle ionizes the material. The light is emitted isotropically from the point where it is produced.

Cherenkov radiation is electromagnetic radiation emitted when a charged particle (such as an electron) passes through a dielectric medium at a speed greater than the phase velocity (speed of propagation of a wavefront in a medium) of light in that medium. herenkov radiation as conical wave front

2.1. Scintillation Properties of liquid Argon

Efficient scintilator with typical Light yields in the order of a few 10,000's of photons per MeV deposited (depends on E field, particle type and purity) (SCINTILLATIONYIELD: 50000/MeV when no electric field present) Scintillation yield is E-field and particle dependent. For a proton: 24,000 photons / MeV, E = 500 V / cm 40,000 photons / MeV, E = 0 V / cm

Liquid argon produces scintillation light via two distinct scintillation mechanisms, each of which has a different characteristic time constant. The emmssion spectra are passed to Geant4 as a 2 column matrix where the first column is the photon energy and the second is the value.

Property/Geant4 keyword	value
light yield/SCINTILLATIONYIELD	$50000\gamma's/MeV$ (no electric field)
Wavelength of emission/SCINTILLATIONCOMPONENT1	128nm (FWHM = 10nm)
Wavelength of emission/SCINTILLATIONCOMPONENT2	128nm (FWHM = 10nm)
fast component/SCINTILLATIONTIMECONSTANT1	6ns
fast fraction/SCINTILLATIONYIELD1	0.75
slow component/SCINTILLATIONTIMECONSTANT2	1500ns
slow fraction/SCINTILLATIONYIELD2	0.25
?????/RESOLUTIONSCALE	1

Table 1. Scintillation Properties of liquid Argon.

Scintillation Quenching, Birks

2.2. Cerenkov spectrum and Yield

A charged particle radiates if its speed is greater than the local phase speed of light v_p In Geant4 the process is not contributing to energy loss.

the charged particle travels in a medium with speed v_p such that $\frac{c}{n} < v_p < c$. from [12]

$$\cos(\theta_C) = \frac{1}{n\beta} \tag{2}$$

$$\frac{d^2N}{dEdx} = \frac{2\pi\alpha z^2}{\lambda^2} \left(1 - \frac{1}{(\beta^2 n^2(\lambda))} \right)$$
 (3)

Cerenkov photons

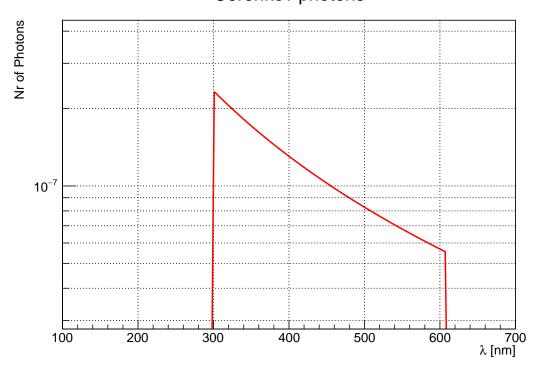


Figure 2. Cerenkov spectrum

3. Light propagation

In this section we discuss the material properties related to light propagation in a medium. The values are passed to Geant4 as a 2 column matrix where the first column is the photon energy and the second is the value.

optical material property	Geant4 Keyword
Refraction index as function of photon energy	RINDEX
Absorption length as function of photon energy	ABSLENGTH
Rayleigh scattering length as function of photon energy	RAYLEIGH

Table 2. Material properties related to light propagation in a medium

3.1. Refraction Index and group velocity

In [9] the refraction index and group velocity at 128nm are measured at $n=1.358\pm0.003$ and $\frac{1}{vg}=7.46\pm0.08ns/m$. (compared to $n=1.45\pm0.07$ [8])

The Sellmeier equation 4 below is an empirical relationship between refractive index and wavelength for a particular transparent medium.

$$n^2 = a_0 + \frac{a_{UV}\lambda^2}{\lambda^2 - \lambda_{UV}^2} + \frac{a_{IR}\lambda^2}{\lambda^2 - \lambda_{IR}^2}.$$
 (4)

Scintilation λ	UV Resonance λ	IR Resonance λ
(nm)	(nm)	(nm)
128	106.6	908.3

Table 3. blabla bla.

T(K)	a_0	a_{UV}	a_{IR}
83.81	1.24 ± 0.09	0.27 ± 0.09	0.00047 ± 0.007
90	1.26 ± 0.09	0.23 ± 0.09	0.0023 ± 0.007

Table 4. Sellmeier coefficents

where the parameters a_0 , a_{UV} and a_{IR} known as Sellmeier coefficients have to be determined experimentally.

The relation between group velocity and the refraction index is given by:

$$v_g(\lambda) = \frac{c}{n - \lambda \frac{\partial n}{\partial \lambda}} \tag{5}$$

3.2. Absorption length

Argon is highly transparent to its own scintillation light. (ABSLENGTH) > 1.1m (ArXiv:1511.07725)

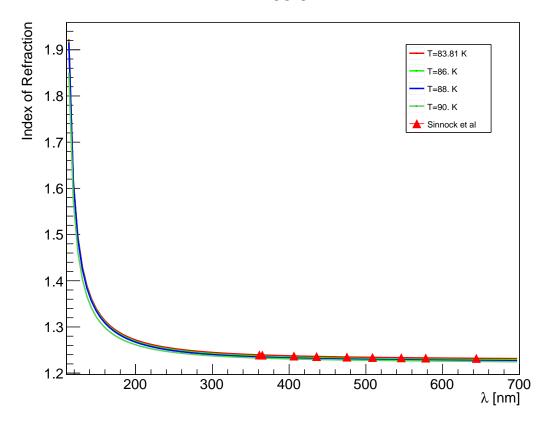


Figure 3. refraction index

3.3. Rayleigh Scattering length

Rayleigh scattering length (RAYLEIGH). In the literature one can find the following calculated values at 128nm: 90 cm [9] and $55 \pm 5cm$ [8]. The range of values for the Rayleigh scattering length is due to the refraction index at 128nm n input to the 6 below:

$$l^{-1} = \frac{16\pi^3}{6\lambda^4} \left[kT \rho^2 k_T \left(\frac{(n^2 - 1)(n^2 + 2)}{3} \right)^2 \right]$$
 (6)

with:

4. Boundary processes

4.1. Refraction and total internal reflection

In physics, refraction is the change in direction of a wave passing from one medium to another or from a gradual change in the medium. Total internal reflection is the optical phenomenon in which waves arriving at the interface (boundary) from one medium to another (e.g., from water to air) are not refracted into the second ("external") medium, but completely reflected back into the first ("internal") medium. It occurs when the second medium has a higher wave speed (lower refractive index) than the first, and the waves are incident at a sufficiently oblique angle on the interface. For light, refraction follows Snell's law, which states that, for a given pair of

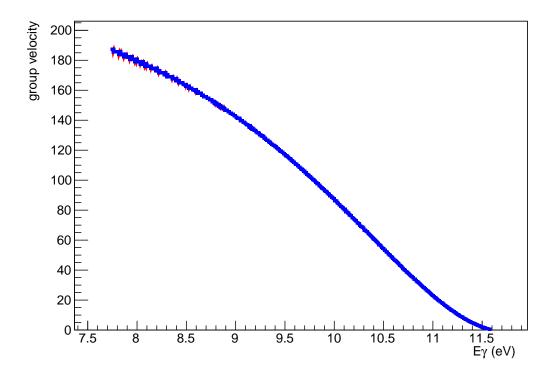


Figure 4. group velocity

media, the ratio of the sines of the angle of incidence θ_1 and angle of refraction θ_2 is equal to the ratio of phase velocities (v1 / v2) in the two media, or equivalently, to the indices of refraction (n2 / n1) of the two media.

$$\frac{\sin \theta_1}{\sin \theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1} \tag{7}$$

n which waves arriving at the interface (boundary) from one medium to another The Fresnel equations (or Fresnel coefficients) describe the reflection and transmission of light (or electromagnetic radiation in general) when incident on an interface between different optical media. (boundary between liquid Ar and wls, wls and photodetector.)

4.2. reflection

Specular reflection, or regular reflection, is the mirror-like reflection of waves, such as light, from a surface. The law of reflection states that a reflected ray of light emerges from the reflecting surface at the same angle to the surface normal as the incident ray, but on the opposing side of the surface normal in the plane formed by the incident and reflected rays. (boundary between liquid Argon and metal walls of cryogenic vessel)



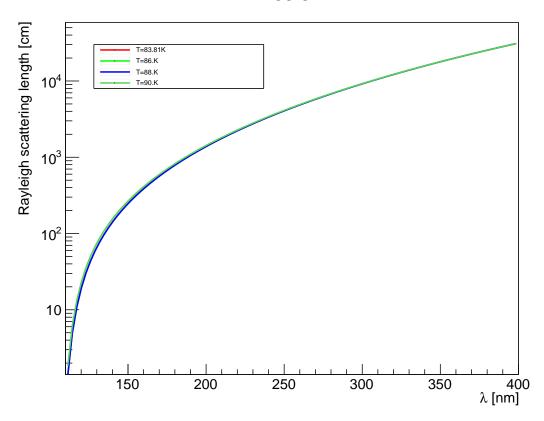


Figure 5. rayleigh scattering length.

5. Photon Detection

5.1. Quantum efficiency and absorption length of the tetraphenyl butadiene (TPB) wave length shifter
[7]

optical material property	Geant4 Keyword	value
Emission spectrum as function of photon energy	WLSCOMPONENT	see Figure ?? (from [7])
Absorption length as function of photon energy	WLSABSLENGTH	400 nm at 128 nm
emmission time const	WLSTIMECONSTANT	0.5 ns

Table 5. Properties of the TPB wavelength shifter (values from [7])

FitReemissionSpect.csv

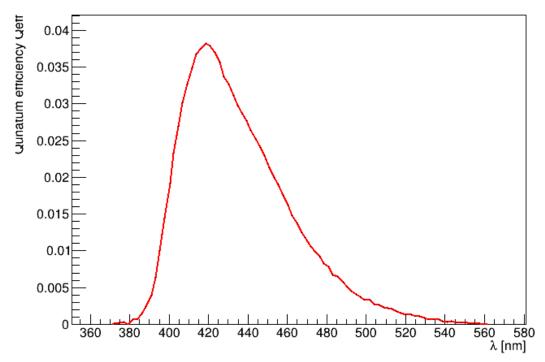


Figure 6. TPB wave length spectrum extracted form [7].

6. Conclusions and Outlook

References

- [1] https://github.com/hanswenzel/LArProperties.
- [2] https://github.com/hanswenzel/CaTS.
- [3] Allison J et al. 2016, Nuclear Instruments and Methods in Physics Research A 835 (186–225).
- [4] http://geant.cern.ch/.
- [5] High-Energy Physics Literature Database, http://inspirehep.net/.
- $[6] \ \mathtt{https://github.com/hanswenzel/CaTS/tree/master/scripts/LAr.C.}$
 - https://github.com/hanswenzel/CaTS/tree/master/scripts/wls.C.
- [7] Christopher Benson, Gabriel D. Orebi Gann, Victor Gehman,

 Measurements of the intrinsic quantum efficiency and absorption length of tetraphenyl butadiene thin films
 in the vacuum ultraviolet regime.
 - Eur. Phys. J. C (2018) 78:329
- [8] Emily Grace, Alistair Butcher, Jocelyn Monroe, James A. Nikkel,
 - $Index\ of\ refraction,\ Rayleigh\ scattering\ length,\ and\ Sellmeier\ coefficients\ in\ solid\ and\ liquid\ argon\ and\ xenon.$
 - ArXiv:1502.04213
- [9] A measurement of the group velocity of scintillation light in liquid argon, M. Babicz et al, 2020 JINST 15 P09009
- [10] Ben Jones, Introduction to Scintillation Light in Liquid Argon http://microboone-exp.fnal.gov"/
- [11] E. Morikawa, R. Reininger, P. Gürtler, V. Saile, and P. Laporte,
 Argon, krypton, and xenon excimer luminescence: From the dilute gas to the condensed phase.
 J. Chem. Phys. 91, 1469 (1989); https://doi.org/10.1063/1.457108
- [12] P.A. Zyla et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2020, 083C01 (2020) and 2021 update. https://pdg.lbl.gov/.