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

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Abstract

In Geant4 and Opticks optical properties like e.g. the refractive index, absorption length, rayleigh scattering length etc. as well as surface properties are inputs that have to be provided. In this paper we collect the optical properties relevant for liquid Argon TPC's.

Contents

1 Introduction

In Geant4 [1] and Opticks [4] optical properties like e.g. the materials refractive index or rayleigh scattering length 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 [8]. Usually quantities are given as a function of photon wavelength but Geant4 requires the photon energy.

A nice overview about the properties of Scintillation Light in Liquid Argon can befound in [12]. The motion of the charged particles liberates charge from the surrounding argon (ionization) and produces light (scintillation)

The Geant4 keywords used in this article refer to Geant4 version > 11.0 released in December 2021. The latest version introduced changes to the Geant4 API with regards to optical material properties.

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

with:
speed of light: $c = 299792458 m/sec$
Planck constant: $h = 4.13566743 \times 10^{-15} eV/sec$

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 isotropic from the point where it is produced.

Cerenkov radiation ([14],[15]) is electromagnetic radiation emitted when a charged particle 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. Cerenkov radiation as conical wave front with the emission angle given by

$$\cos\theta = \frac{1}{n\beta} \tag{2}$$

with:
ratio between the speed of the particle v_p and the speed of light as $\beta = \frac{v_p}{c}$.

2.1 Scintillation Properties of liquid Argon

Efficient scintillator 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 emission 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	$128nm$ $(FWHM = 10nm)$ see 1
Wavelength of emission	SCINTILLATIONCOMPONENT2	$128nm$ $(FWHM = 10nm)$ see 1
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 law below:

$$\frac{dL}{dx} = S\frac{\frac{dE}{dx}}{1 + kB\frac{dE}{dx}}. \tag{3}$$

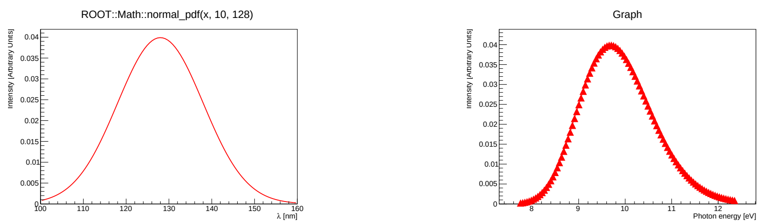

Figure 1: Scintillation emission spectrum.

where L is the light yield, S is the scintillation efficiency, dE/dx is the specific energy loss of the particle per path length, kB is the Birks coefficient. Its value depends on the scintillating material and particle type.

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 [14]

$$\cos(\theta_C) = \frac{1}{n\beta} \tag{4}$$

$$\frac{d^2N}{dEdx} = \frac{2\pi\alpha z^2}{\lambda^2}\left(1 - \frac{1}{(\beta^2 n^2(\lambda))}\right) \tag{5}$$

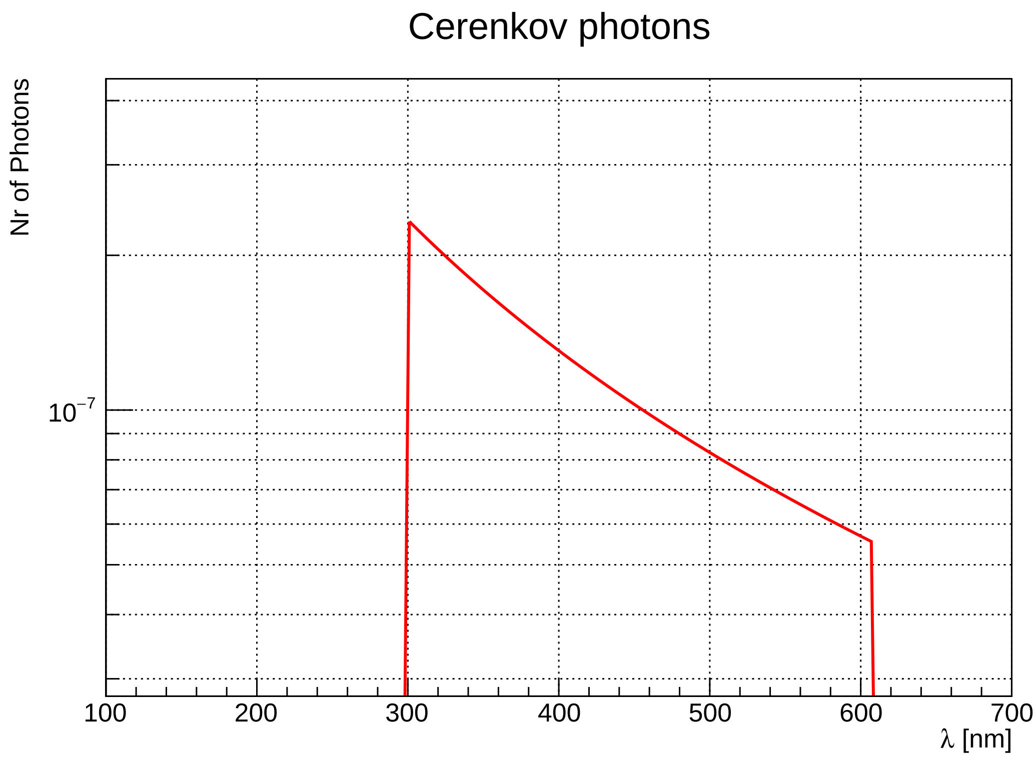

Figure 2: Cerenkov spectrum

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 [11] the refraction index and group velocity at $128nm$ are measured at $n = 1.358 \pm 0.003$ and $\frac{1}{vg} = 7.46 \pm 0.08ns/m$. (compared to $n = 1.45 \pm 0.07$ [10])

$\frac{1}{vg} = 7.46 \pm 0.08ns/m$ corresponds to $0.134m/nsec$ which is approximately $c_0/2240$ where c_0 is the speed of light in vacuum. (reading it from the gdml dump calculated by Geant4 one gets $c_0/2600$)

The Sellmeier equation 6 below is an empirical relationship between refractive index and wavelength for a particular transparent medium.

$$n^2 = a_0 + \frac{a_{UV}\lambda^2}{\lambda^2 - \lambda_{UV}^2} + \frac{a_{IR}\lambda^2}{\lambda^2 - \lambda_{IR}^2}. \tag{6}$$

Scintillation λ (nm)	**UV Resonance** λ_{UV} (nm)	**IR Resonance** λ_{IR} (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 coefficients

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:

$$v_g(\lambda) = \frac{c}{n - \lambda\frac{\partial n}{\partial \lambda}} \tag{7}$$

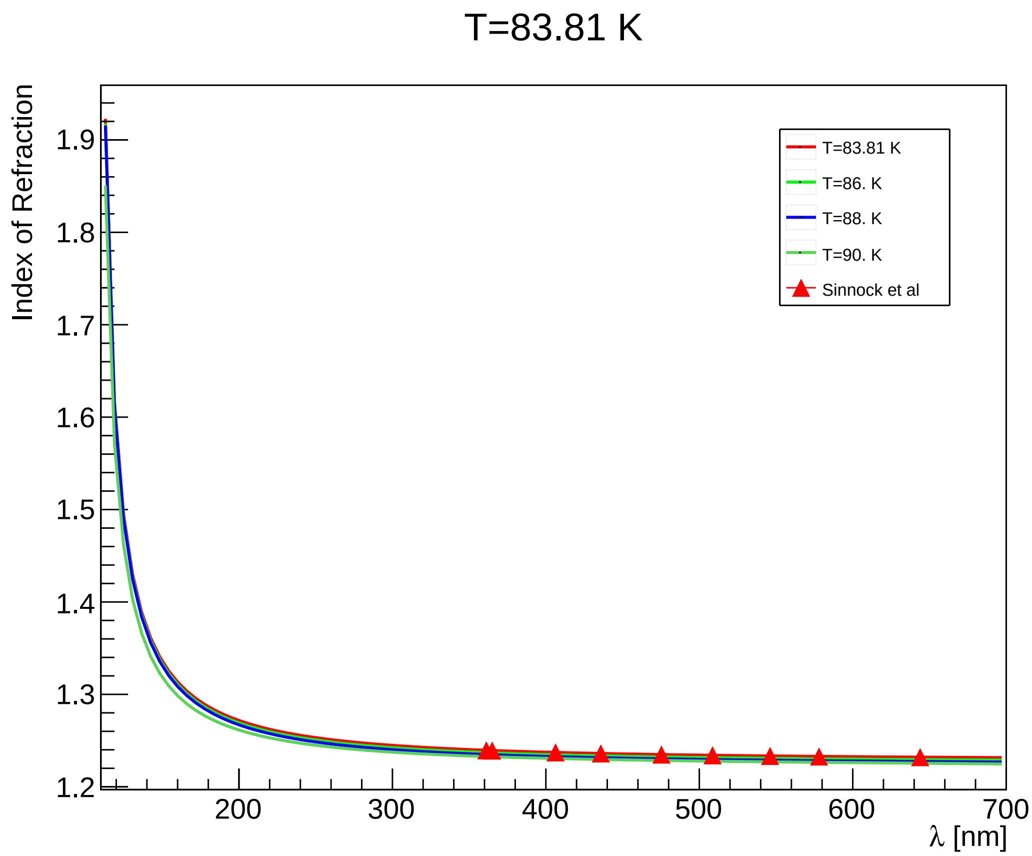

Figure 3: Refraction index. The experimental data is from [5].

3.2 Absorption length

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

3.3 Rayleigh Scattering length

Rayleigh scattering length (RAYLEIGH). In the literature one can find the following calculated values at $128nm$: 90 cm [11] and $55 \pm 5cm$ [10]. The range

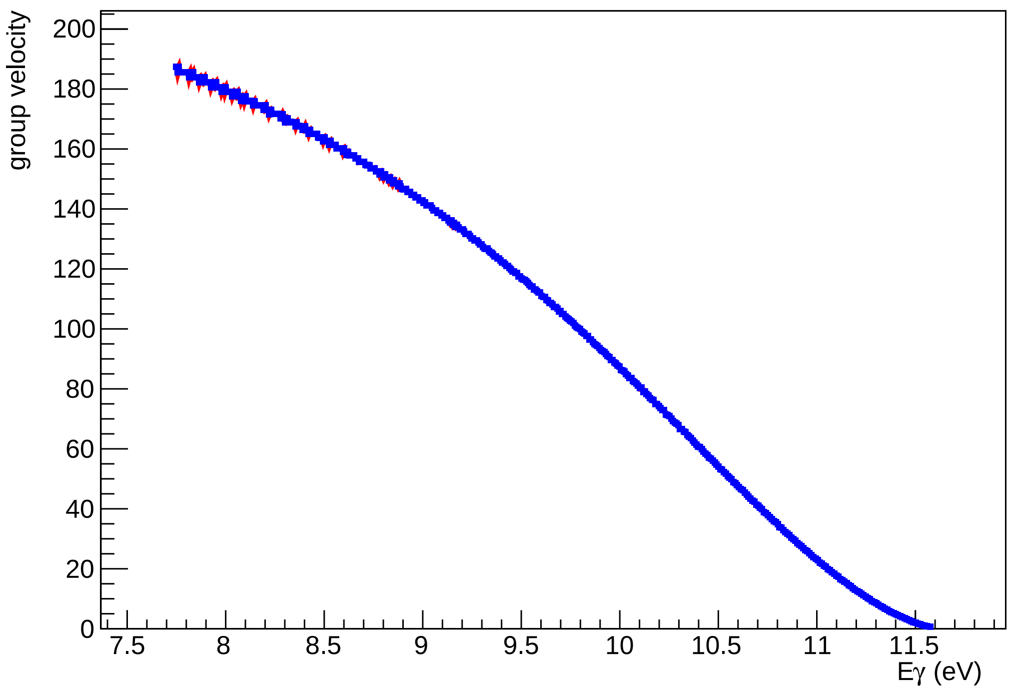

Figure 4: group velocity

of values for the Rayleigh scattering length $l$is due to the different refraction indices n at $128nm$ input to equation 8 below:

$$l^{-1} = \frac{16\pi^3}{6\lambda^4}\left[kT\rho^2 k_T \left(\frac{(n^2-1)(n^2+2)}{3}\right)^2\right] \tag{8}$$

with
l: the scattering length
λ: the wavelength of light
n: the index of refraction corresponding the wavelength of light
T: the temperature
ρ: the density
k_T: the isothermal compressibility
k: the Boltzman constant

Figure 5 shows the rayleigh scattering length as a function of λ calculated using formula 8.

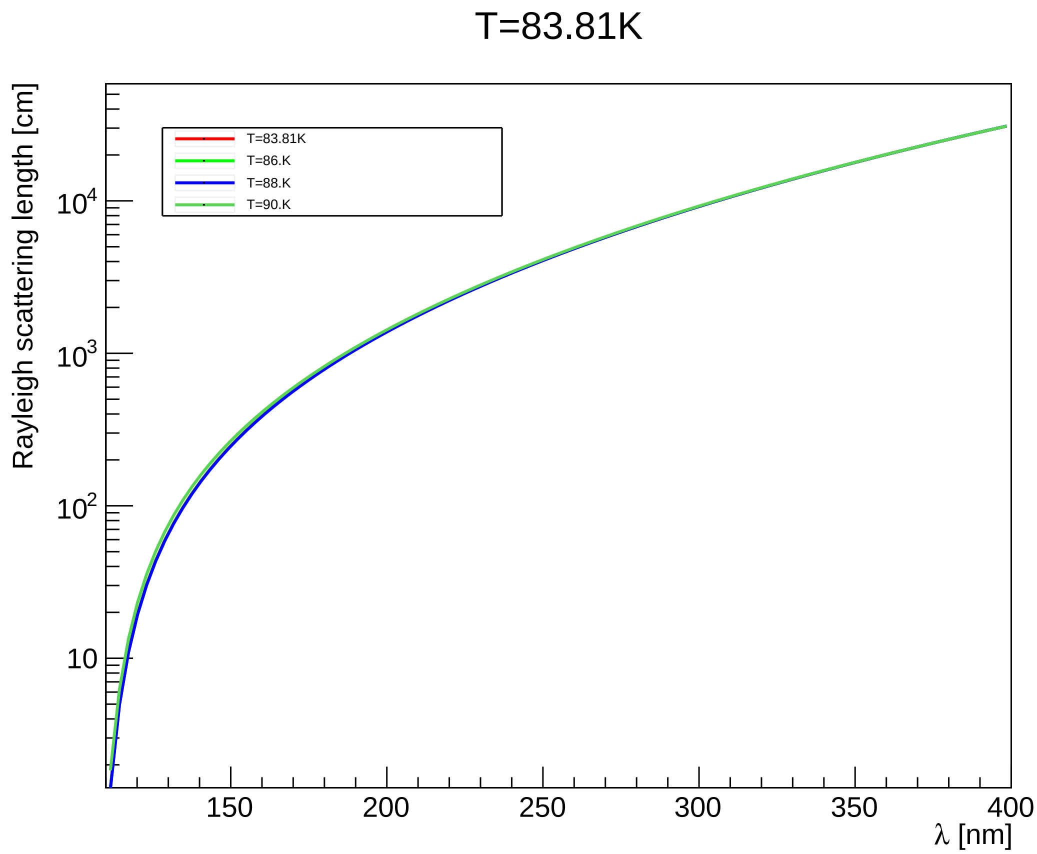

Figure 5: rayleigh scattering length as a function of λ.

4 Boundary processes

4.1 Refraction and total internal Reflection

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 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.

$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{v_1}{v_2} = \frac{n_2}{n_1} \tag{9}$$

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 photo-detector.)

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)

5 Photon Detection

5.1 Quantum efficiency and absorption length of the tetraphenyl butadiene (TPB) wave length shifter

optical material property	**Geant4 Keyword**	**value**
Emission spectrum as function of photon energy	WLSCOMPONENT	see Figure 6 (from [9])
Absorption length as function of photon energy	WLSABSLENGTH	$400nm$ at $128nm$
emission time const	WLSTIMECONSTANT	$0.5ns$

Table 5: Properties of the TPB wavelength shifter (values from [9]).

6 Conclusions and Outlook

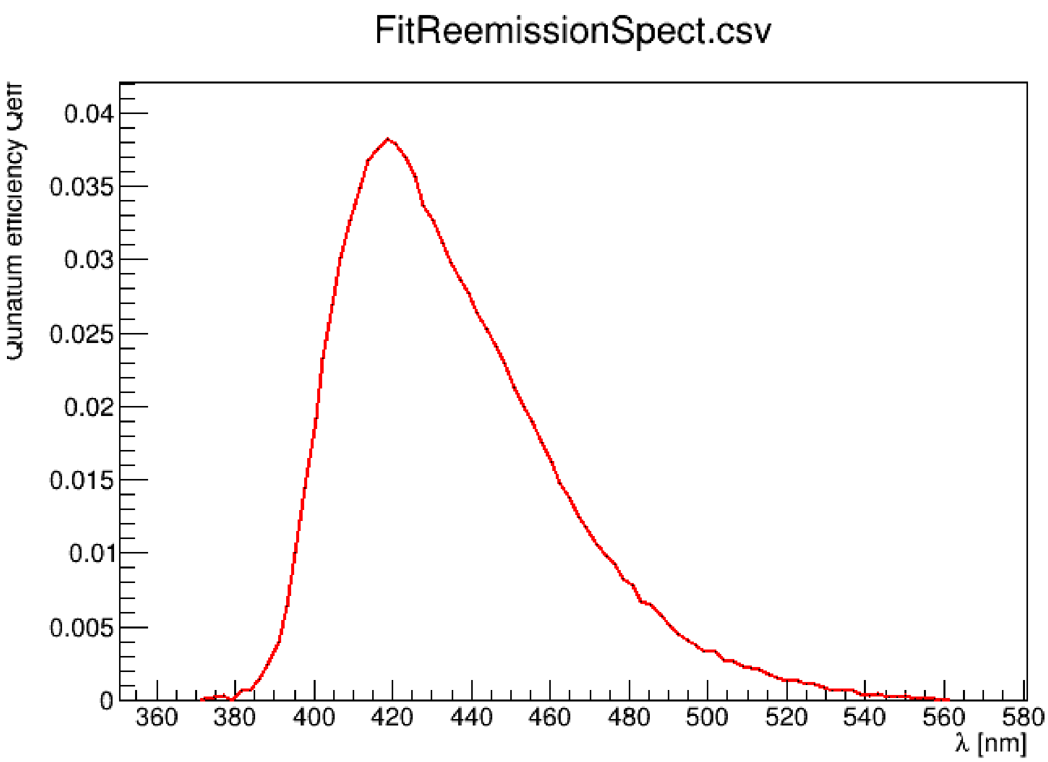

Figure 6: TPB wave length spectrum extracted from [9].

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