Ions Transport equations and El.Field Distortion from Space Charge in LAr Ionization Chambers

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Charge Transport equation: General Concepts

Transport equation: the case of a LAr Ionization Chamber

Transport equation in LAr Ionization Chamber: the protoDUNE TPC case

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Charge Transport equations: General Concepts

- The transport equation is a general conservation equation for the motion of a scalar quantity (Charge) in some medium (Gas, Liquid, Solid) through a domain (1D , 2D, 3D interval).
- Definitions: "Charge" q, density ρ $[m^{-3}]$, current density $\vec{J}\,[m^{-2}s^{-1}]$ with $\vec{J} = q\rho\vec{v}$ where $\vec{v}$ $[m\ s^{-1}]$ is the bulk velocity.
- The net "transport" of q is the balance of:
    - the **Influx** of q across the boundaries into the domain
    - the **Outflux** of q across the boundaries from the domain
    - the **Generation** of q within the boundaries of the domain
    - the **Loss** of q within the boundaries of the domain.
    - the **Accumulation** of q in the domain
- A general Conservation Law of the Charge q is assumed to hold:

$$q_{Accumul} = q_{In} - q_{Out} + q_{Gen} - q_{Loss} \tag{1}$$

Charge Transport equation: General Concepts

- where:
  - **Accumulation**: $q_{Accumul}$ is the Charge accumulation **in Time** in the interval dt inside the Volume dV:

$$q_{Accumul} = \frac{\partial(q\rho)}{\partial t} dtdV$$

  - **Influx** and **Outflux**: the net difference of Influx and Outflux through the Volume dV:

$$(q_{In} - q_{Out}) = -\nabla \cdot \vec{J}\, dtdV$$

  - **Generation** and **Loss**: sources and sinks of charge $S_k[m^{-3}s^{-1}]$ may be present in the Volume dV. The net difference between charge-generation and charge-loss in the interval dt and in the Volume dV is:

$$(q_{Gen} - q_{Loss}) = S_{Gen} dtdV - S_{Loss} dtdV = \Delta S\ dtdV$$

- The Conservation Law of the Charge in the Volume (Eq.1) can thus assume the (more familiar) form of continuity equation in its differential form:

$$\frac{\partial(q\rho)}{\partial t} + \nabla \cdot \vec{J} = \Delta S \qquad (2)$$

  - l.h.s.- first term (time variation): Accumulation term
  - l.h.s.- second term (space variation): Influx and Outflux through the Volume dV
  - r.h.s. : balance of the Generation and Loss due to Sources and Sinks of Charge in the Volume.

Charge Transport equation: The Stationary case

- Systems where no charge accumulation occurs, i.e. where $(q_{Out} - q_{In}) = (q_{Gen} - q_{Loss})$,
  are "Stationary" systems and $\partial(q\rho)/\partial t = 0$.
- Example: systems where (1) no charge is emitted into the Control Volume from the surface delimiting the Volume and (2) all the charge reaching the surface is absorbed.
- In these cases the Charge Conservation Law of Eq.2 reduces to:

$$\nabla \cdot \vec{J} = \Delta S \tag{3}$$

Charge Transport equation: the case of the Ionization Chamber - [Charge $= e^-, I^+$]

- Parallel plate Ionization Chamber: Anode plane ($x_A = 0$), Cathode plane ($x_C = d$), $\vec{E} = (E_0, 0, 0)$ [with $E_0 = V_0/d$ established by V_0 voltage at the Cathode].
- The parallel plate IC geometry represents a 1-D domain where free charged particles of opposite sign (e^-, I^+) generated by Ionization move in opposite direction along x with different drift velocities $\rightarrow$
- Transport Equations:
  - **Medium**: any dielectric material (relative permittivity ϵ_r)
  - **Domain**: 1D interval $[0, d]$ - Anode to Cathode Drift distance (along x) -
  - **Scalar quantities**:
    Electron Charge ($q = -1$):
    $\vec{v}_d^{\,e} = (-v_d^e, 0, 0)$, $\vec{J}_e = (J_e, 0, 0)$ with $J_e = -v_d^e\; n_e$; $\mathbf{n_e(x)}$ **el-density**
    Ion Charge ($q = +1$): $\vec{v}_d^{\,+} = (v_d^+, 0, 0)$, $\vec{J}_+ = (J_+, 0, 0)$ with $J_+ = v_d^+\; n_+$; $\mathbf{n_+(x)}$ I^+**-density**
- Drift velocities dependance on Electric Field:
  - drift velocities (and Current density) depend on the E-Field strength in the domain
  - ${v_d}^e = \mu_e E$, ${v_d}^+ = \mu_+ E$ with μ_e, μ_+ $[m^2 s^{-1} V^{-1}]$ electron and Ion *mobility* (independent from E in first approximation)

Charge Transport equation: the case of the Ionization Chamber - [Charge $= e^-, I^+$]

- Assuming Stationary systems in 1-D domain, the Charge Conservation Law of Eq.3 provide the Transport Equations System:

$$\begin{cases} \frac{\partial J_e}{\partial x} = S_{Gen}(e^-) - S_{Loss}(e^-) \\ \frac{\partial J_+}{\partial x} = S_{Gen}(I^+) - S_{Loss}(I^+) \end{cases} \tag{4}$$

- In case the density of the slow Ion charge is large enough to modify the uniform electric field established in the parallel plate IC, the divergence of the actual electric field $E(x)$ depending on the charge density enclosed in the IC volume (Gauss Law) should be added to the System:

$$\begin{cases} \frac{\partial(-\mu_e \ E \ n_e)}{\partial x} = S_{Gen}(e^-) - S_{Loss}(e^-) \\ \frac{\partial(\mu_+ \ E \ n_+)}{\partial x} = S_{Gen}(I^+) - S_{Loss}(I^+) \\ \frac{\partial E}{\partial x} = \frac{1}{\epsilon}(n_+ - n_e) \end{cases} \tag{5}$$

Ionization in LAr and the Initial Microscopic Fast Processes

- Ionization from radiation penetrating/crossing the LAr volume is the production mechanism for (e^{-}, Ar^{+}) pair generation:

$$Ar + W_{ion} \rightarrow e^{-} + Ar^{+} \; ; \; W_{ion} = 23.6 \; eV/\text{pair in LAr}$$

- Ar^{+} ions rapidly associate in multi-body collisions with ground-state atoms to form Ar_2^{+} molecular ions:

$$Ar^{+} + Ar \rightarrow Ar_2^{+}$$

- e^{-} and Ar_2^{+} undergo fast (Columnar) Recombination whose fraction R depends upon the actual El. Field in the LAr Volume

Initial Microscopic Fast Processes

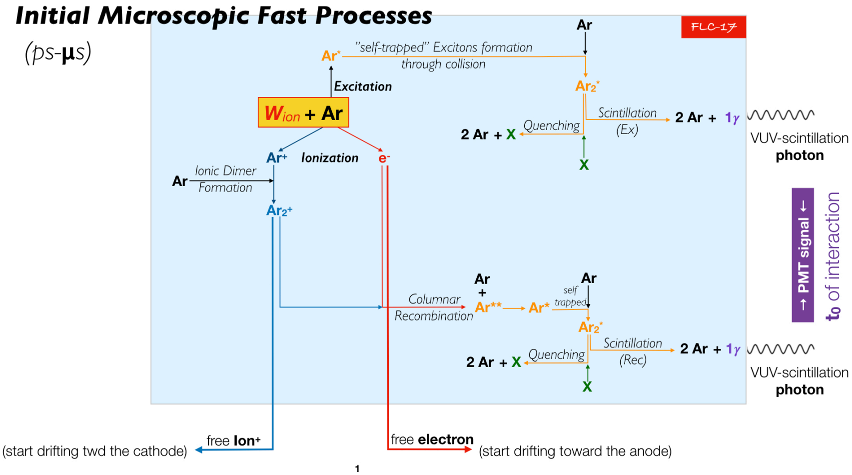


Figure: Initial Microscopic Fast Processes from energy deposit by Ionization

protoDUNE LArTPC in Parallele Plate IC approximation, and Ionization process from Cosmic Muons

- ProtoDUNE TPC - 2 Drift Volumes, each with Dimensions: $\Delta x = 3.6\ m,\ \Delta y = 6\ m,\ \Delta z = 7\ m \ \rightarrow\ V = 150\ m^3$
- ProtoDUNE TPC - Anode-Cathode ΔV: $V_0 = 180 kV \ \rightarrow$ (Nominal) E Field in Drift Volume: $\vec{E} = (E_0, 0, 0),\ \ E_0 = 500\ V/cm$
- Recombination Factor $R(E_0)\ =\ 0.7$ (fraction of charge surviving initial Recombination at nominal Field)
- Cosmic Muon Rate in Drift Volume: $r_\mu = 13\ kHz$ $[\leftarrow R^{\mu @ surf}_{Tot} = 200 \mu/m^2 s]$
- Average muon track length in Drift Volume: $\langle \ell_\mu \rangle\ =\ 3.4\ m$
- Total muon track length per unit of time in Drift Volume: $L^\mu_{Tot}\ =\ 44,200\ m\ s^{-1}$
- Ionization Rate of (e^-, I^+) pairs freed: $N^i_{Pairs}\ =\ L^\mu_{Tot}\ \frac{dE}{dx}\ \frac{1}{W_{ion}}\ R(E_0)\ =\ 2.8 \times 10^{11}\ \left[s^{-1}\right]$
- Ionization Rate per Unit of Volume of (e^-, I^+) pairs freed: $n^i_{Pairs}\ =\ \frac{N^i_{Pairs}}{V}\ =\ 1.9 \times 10^9\ \left[m^{-3}\ s^{-1}\right]$ uniformly distributed in the drift volume and constant in time

Charge Generation in LAr from Initial Processes

- e^- Charge generation rate per unit Volume:
  $S^i_{Gen}(e^-) \ = \ n^i_{Pairs} \quad \left[m^{-3} \ s^{-1}\right]$

- Positive Ion Charge generation rate per unit Volume:
  $S^i_{Gen}(Ar_2^+) \ = \ n^i_{Pairs} \quad \left[m^{-3} \ s^{-1}\right]$

Subsequent Processes during drift time

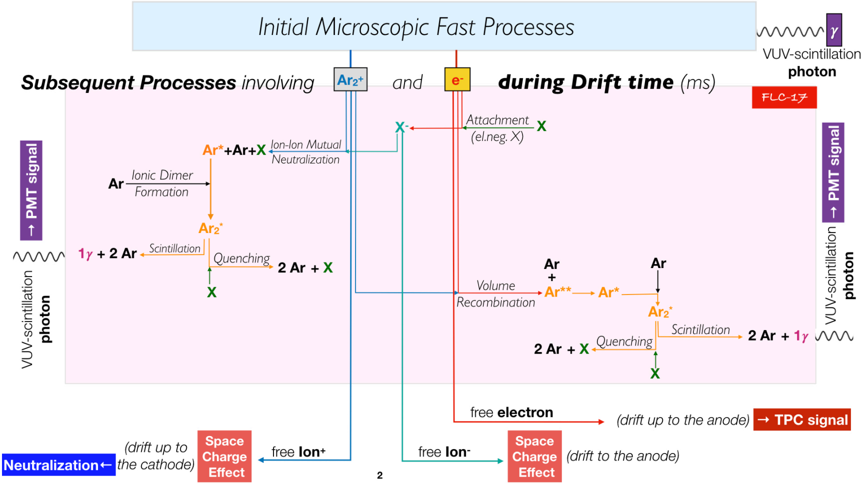


Figure: Susequent Processes during drift time

Charge Loss and Charge Generation in LAr from Microscopic Processes during Drift time

- Volume Recombination: $e^- + Ar_2^+ \;\rightarrow Ar^{**} + Ar$
  $S^R_{Loss}(e^-) \;=\; S^R_{Loss}(Ar_2^+) \;=\; -\; k_R \; n_e \; n_+ \quad \left[m^{-3}\; s^{-1}\right]$

- Electron Attachment to el.negative Impurity X: $e^- + X \;\rightarrow X^-$
  $S^A_{Loss}(e^-) \;=\; -\; k_A \; n_e \; n^0_X \quad \left[m^{-3}\; s^{-1}\right]$
  - X concentration in LAr: n^0_X $[m^{-3}]$ from e-lifetime measurement, assumed constant in time and uniformly distributed in the Volume

- the loss of electrons by attachment corresponds to the generation of negative Ions (X^-):
  $S^A_{Gen}(X-) = \; -\, S^A_{Loss}(e^-) \;=\; +\; k_A \; n_X \; n_e \quad \left[m^{-3}\; s^{-1}\right]$

- Ion-Ion Mutual Neutralization: $Ar_2^+ + X^- \;\rightarrow Ar^{**} + Ar + X$
  $S^{MN}_{Loss}(Ar_2^+) \;=\; S^{MN}_{Loss}(X^-) \;=\; -\; k_{MN} \; n_- \; n_+ \quad \left[m^{-3}\; s^{-1}\right]$

Rate Constants of Processes during drift time

Table: Rate Constants

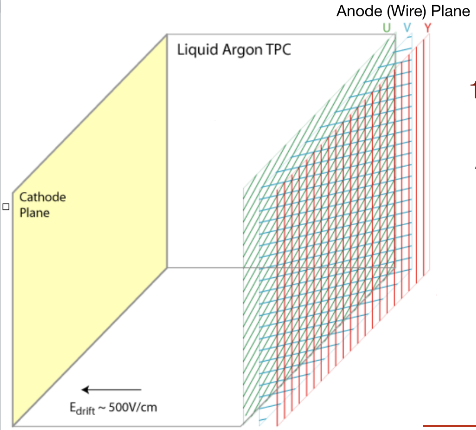
Process	El. Field	Rate Constant	Ref.
(e^-, X) Attachment to Impurity $X = H_2O$ $X = O_2$	100 V/cm 500 V/cm	$k_A = 1.4 \times 10^{-15}\ m^3\ s^{-1}$ $k_A = 1.4 \times 10^{-16}\ m^3\ s^{-1}$	Pordes (MTS + PrM data) Bakale
(e^-, Ar_2^+) Recombination	500 V/cm	$k_R = 1.1 \times 10^{-10}\ m^3\ s^{-1}$	Shinsaka
(X^-, Ar_2^+) Mutual Neutralization $X^- = H_2O^-$ $X^- = O_2^-$	no dependence reported	$k_{MN} = 2.8 \times 10^{-13}\ m^3\ s^{-1}$ $k_{MN} = 1.8 \times 10^{-13}\ m^3\ s^{-1}$	Miller Miller

Drift velocity and mobility

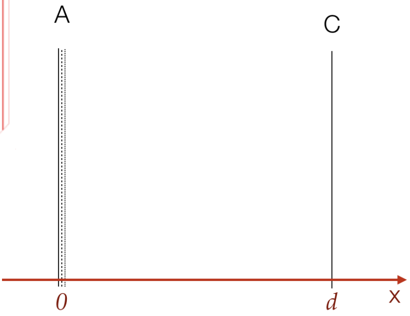
Table: Drift velocity (and mobility) for e^-, Ion$^+$, Ion$^-$

	Mobility	El. Field	Drift Velocity	Ref.
e^-	$\mu_e = 3.2 \times 10^{-2} \frac{m^2}{V\ s}$	500 V/cm	$v_d^e = 1.61 \times 10^{+3} \frac{m}{s}$	[Walkowiak]
Ar_2^+	$\mu_+ = 8.0 \times 10^{-8} \frac{m^2}{V\ s}$	500 V/cm	$v_d^+ = 4 \times 10^{-3} \frac{m}{s}$	[Rutherfoord-ATLAS] [Dey et al.] [Henson] [Davis et al.]+[Rice (Theory)]
$X^- = H_2O^-$ $X^- = O_2^-$	$\mu_- = 9.2 \times 10^{-8} \frac{m^2}{V\ s}$ $\mu_- = 7.8 \times 10^{-8} \frac{m^2}{V\ s}$	500 V/cm 500 V/cm	$v_d^- = 4.6 \times 10^{-3} \frac{m}{s}$ $v_d^- = 3.9 \times 10^{-3} \frac{m}{s}$	FLC guesstimate... [Dey]: ref. to [Davis et al.] +[Rice (Theory)]

Reference System and 1D Domain



1D Domain $x = [0,d]; \quad d = 3.6\ m$



Conservation Laws and Transport through the LAr Volume for 3 Charge Species and Electric Field distortion

- Expanding from Eq.5 → System of differential equations for the Conservation and Transport of all particles generated in the LArTPC volume and the Electric Field distortion by Space Charge effect

$$
\begin{cases}
-\mu_e \; n_e \; \dfrac{\partial E}{\partial x} - v_d^e \; \dfrac{\partial n_e}{\partial x} = + \; n_{pair}^i - k_R \; n_+ \; n_e - k_A \; n_X \; n_e \\
-\mu_+ \; n_+ \; \dfrac{\partial E}{\partial x} + v_d^+ \; \dfrac{\partial n_+}{\partial x} = + \; n_{pair}^i - k_R \; n_+ \; n_e - k_{MN} \; n_- \; n_+ \\
-\mu_- \; n_- \; \dfrac{\partial E}{\partial x} - v_d^- \; \dfrac{\partial n_-}{\partial x} = + \; k_A \; n_X^0 \; n_e - k_{MN} \; n_- \; n_+ \\
\dfrac{\partial E}{\partial x} = \dfrac{1}{\epsilon_0 \epsilon_r}(n_+ - n_- - n_e)
\end{cases}
\tag{6}
$$

with (liquid) Ar relative permittivity $\epsilon_r = 1.51$

- Solution (numerical integration):
  Charge Densities $n_+(x)$, $n_-(x)$, $n_e(x)$ and E Field $E(x)$
  in the 1-D domain $x = [0, \; d]$

Boundary Conditions

- The following set of boundary conditions holds:

$$\begin{cases} n_e(x=d) & = 0 \\ n_+(x=0) & = 0 \\ n_-(x=d) & = 0 \\ E(x=0) & = \beta\ E_0 \end{cases} \tag{7}$$

- $n_X^0(\text{const.}) = 3 \cdot 4.6 \times 10^{16} m^{-3}$ density corresponds to 3 ppt(w) impurity X=H_2O concentration (ref. lifetime $\tau_e = 6$ms)
- the parameter β is determined iteratively:
  Start value: $\beta = 0.75$ (Ionization process only)
  determined in correspondence of $\alpha = \frac{d}{E_o}\sqrt{\frac{n^i_{pair}}{\epsilon_o \epsilon_r \mu_+}} = 1.2$
  Final value: $\beta = 0.79$ (Ionization + A + MN + VR)

Solution: Electric Field Distortion from Space Charge

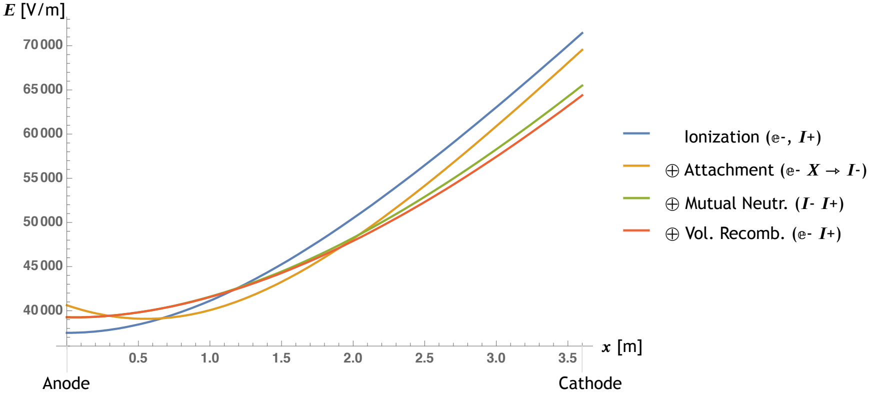


Figure: Electric Field Distortion

Solution: Ar_2^+ Ion-density distribution

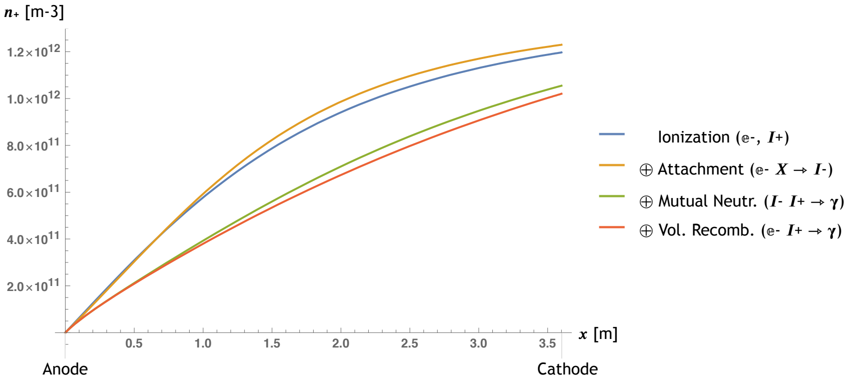


Figure: Positive Ion Density

Solution: el-density distribution

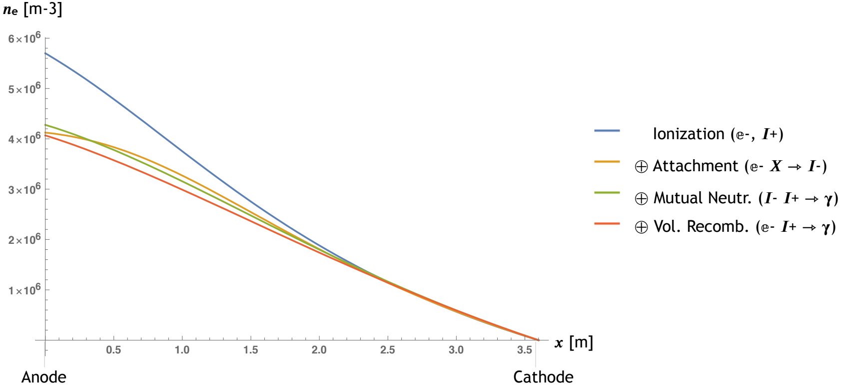


Figure: Electrons Density

Solution: X^- Ion-density distribution

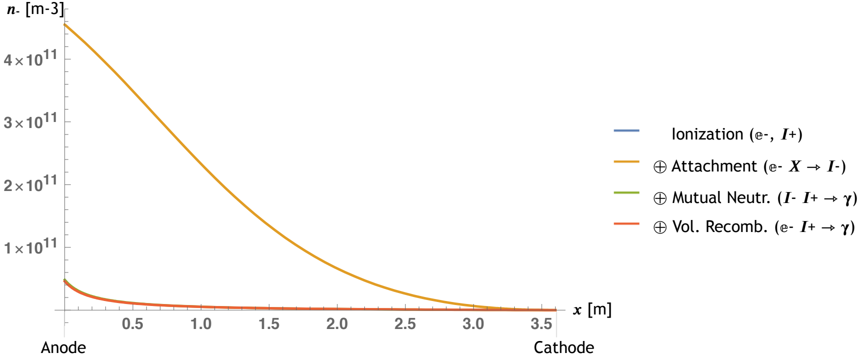


Figure: Negative Ions Density

Photon Emission during Ion Transport

Assuming One VUV Photon (γ) emitted per interaction process:

- Photon Emission Rate from Volume Recombination Process:
  $S^{R}_{Gen}(\gamma) \; = \; k_R \; n_e \; n_+ \;\; [m^{-3} \; s^{-1}]$

- Photon Emission Rate from Mutual Neutralization Process:
  $S^{MN}_{Gen}(\gamma) \; = \; k_{MN} \; n_- \; n_+ \;\; [m^{-3} \; s^{-1}]$

Total Photon emission rate in the protoDUNE TPC Volume:

$$R^{\gamma}_{Tot} \;\; \left[s^{-1}\right] \; = \; \int (S^{R}_{Gen}(\gamma) + S^{MN}_{Gen}(\gamma)) \, dV \; = \; \Delta z \Delta y \int_0^d (S^{R}_{Gen}(\gamma) + S^{MN}_{Gen}(\gamma)) \, dx \tag{8}$$

Solution: photon rate distribution

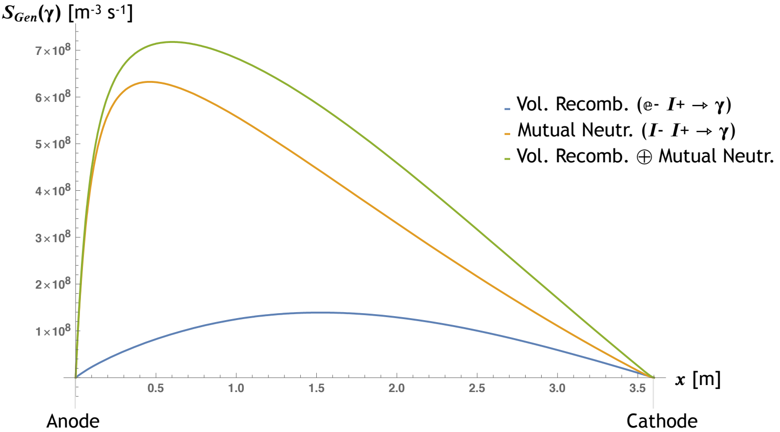


Figure: Photon Rate per Unit Volume

Total Rate $R_{tot}^{\gamma} \;=\; 6.7 \times 10^{10}\ \gamma/s$

BACK-UP

e^- Charge Survival probability along drift distance

- e^- Charge Generation rate per unit Volume:
  $S^i_{Gen}(e^-) \;=\; n^i_{Pairs} \;\; [\mathrm{m}^{-3}\ \mathrm{s}^{-1}]$

- e^- Charge Loss rate per unit Volume due to Attachment:
  $S^A_{Loss}(e^-) \;=\; -\; k_A\ n_e\ n^0_X \;\; [\mathrm{m}^{-3}\ \mathrm{s}^{-1}]$

- e^- Charge Loss rate per unit Volume due to Volume Recombination:
  $S^R_{Loss}(e^-) \;=\; -\; k_R\ n_e\ n_+ \;\; [\mathrm{m}^{-3}\ \mathrm{s}^{-1}]$

- e^- Charge Survival rate per unit Volume:
  $S^i_{Gen}(e^-) \;+\; S^A_{Loss}(e^-) \;+\; S^R_{Loss}(e^-) \;=$
  $n^i_{Pairs} \;-\; k_A\ n_e\ n^0_X \;-\; k_R\ n_e\ n_+ \;\; [\mathrm{m}^{-3}\ \mathrm{s}^{-1}]$

- e^- Charge Survival Probability:
  $\frac{S^i_{Gen}(e^-) \;+\; S^{A,R}_{Loss}(e^-)}{S^i_{Gen}(e^-)} \;=\; \frac{n^i_{Pairs} \;-\; k_A\ n_e\ n^0_X \;-\; k_R\ n_e\ n_+}{n^i_{Pairs}} \;=\; \mathbf{P}^{Surv}_e(x)$

Solution: e^- Charge Survival Probability

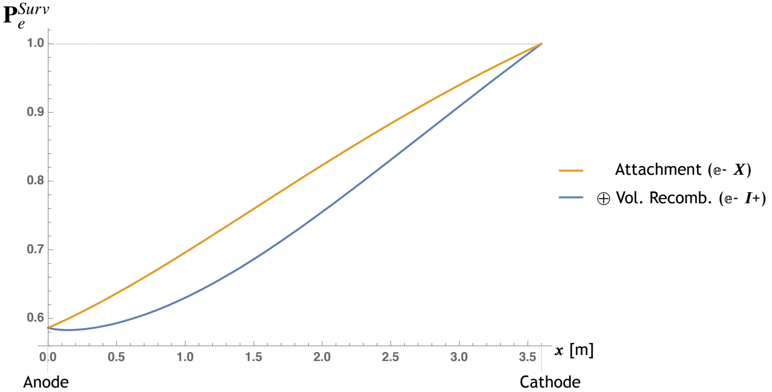
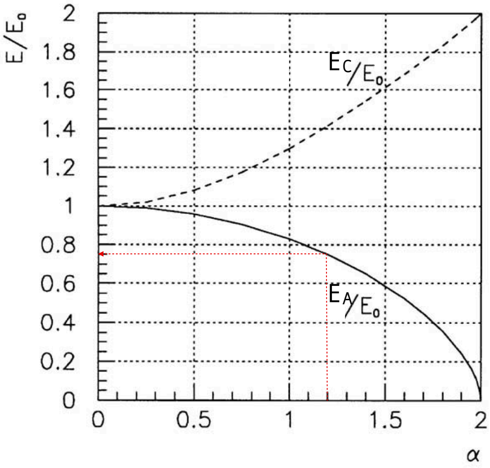


Figure: e^- Charge Survival probability

The α Parameter and the E Field boundary Condition



$$\alpha = \frac{d}{E_0}\sqrt{\frac{n^i_{pair}}{\mu_+ \ \epsilon_0 \epsilon_r}}$$

$$= 0.33\ d = 1.2$$

$$\frac{E_A}{E_0} = \beta$$

$$= 0.75$$