LArSIM

Modeling Ionization-charge and Scintillation-light in LAr

Effects of Electric Field and Energy Loss Density

DRA Mtg - July 08, 2020

FLC, L. Paulucci, F. Marinho, D.Totani

LArSIM

Motivations, Goals and Limits

- Lack of well defined mechanism for Scintillation Light emission in LAr inside LArG4/LArSoft *[results from protoDUNE PDS data analysis proved to be sensitive to some non yet adequately simulated effects of Light from recombination]*

- Implement a unitary model for Ionization Charge AND Scintillation Light in LAr with dependance on deposited Energy density $\frac{dE}{dx}$ and Electridc Field EF

✦ Cover the range of interest for **LArTPC for Neutrino Experiments**:

$$EF = 0 \leftarrow \quad 250\frac{V}{cm} \leq EF \leq 500\frac{V}{cm} \quad \rightarrow \quad 750\frac{V}{cm}$$

$$(e \text{ at min. stopping pwr}) \quad 2\,\frac{MeV}{cm} \leq \frac{dE}{dx} \leq 40\,\frac{MeV}{cm} \text{ (p – stop)}$$

LArSIM

- T. Doke, Fundamental properties of liquid Argon, Krypton and Xenon as Radiation detector media, Portgal Phys. 12 (1981), 9.
- S. Kubota, A. Nakamoto, T. Takahashi, T. Hamada, E. Shibamura, M. Miyajima, K. Masuda and T. Doke, “ Phys. Rev. B 17 (1978) 2762.
- T. Doke, H. J. Crawford, A. Hitachi, J. Kikuchi, P. J. Lindstrom, K. Masuda, E. Shibamura and T. Takahashi: Nucl. Instrum. & Methods A 269 (1988) 291
- T.DOKE, A.HITACHI, JunKIKUCHI, K.MASUDA, H.OKADA and E.SHIBAMURA, Absolute Scintillation Yields in Liquid Argon and Xenon for Various Particles, Jpn. J. Appl. Phys. Vol. 41 (2002) pp. 1538–1545

Theoretical/Phenomenological foundations:

- Free Ionization Charge and Scintillation Light AntiCorrelated-Complementary at any dE/dx and any EF: *Charge - Light Master Equation*
- Observed Reduction of Scintillation Light in the low dE/dx region at 0-EF attributed to “*escape electrons*”, i.e. ionization charge escaping Geminate Recombination

Initial Microscopic Fast Processes

(ps-**μs**)

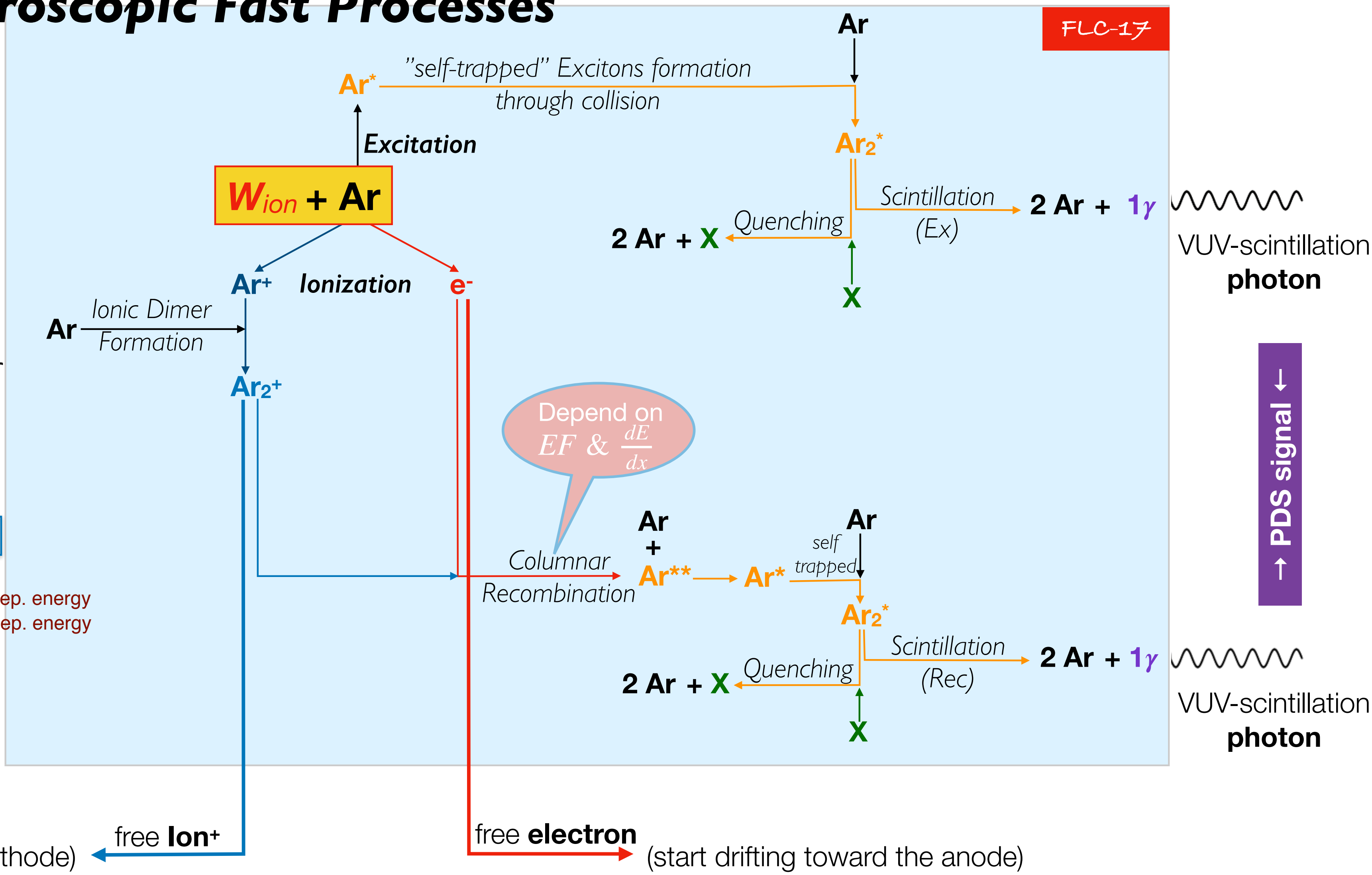
induced by

Energy release

from

charged

particles in LAr



$$W_{ion} = E_i + \epsilon_{kin} + \frac{N_{ex}}{N_i} E_{ex}$$

N_i n. of Ionizations per unit of dep. energy

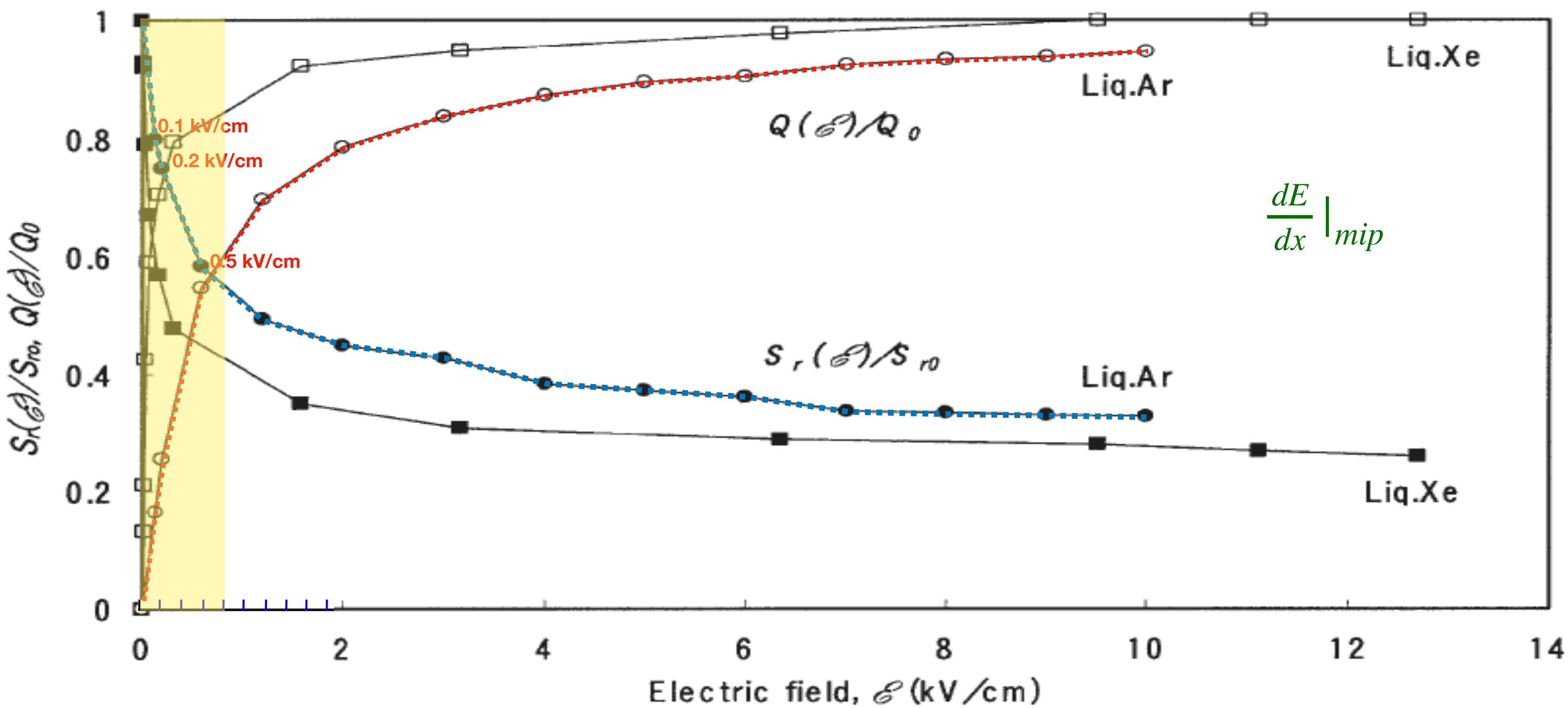
N_{ex} n. of Excitations per unit of dep. energy

Effect of Electric Field

$\left[\frac{e}{\text{MeV}}\right]$ Free Charge Yield $\left[\frac{ph}{\text{MeV}}\right]$ Light Yield

Charge - Light master equation: $QY(EF, dE/dx) + LY(EF, dE/dx) = N_i + N_{ex}$

Doke et al. Jpn. J. Appl. Phys. Vol. 41 (2002) Pt. 1, No. 3A



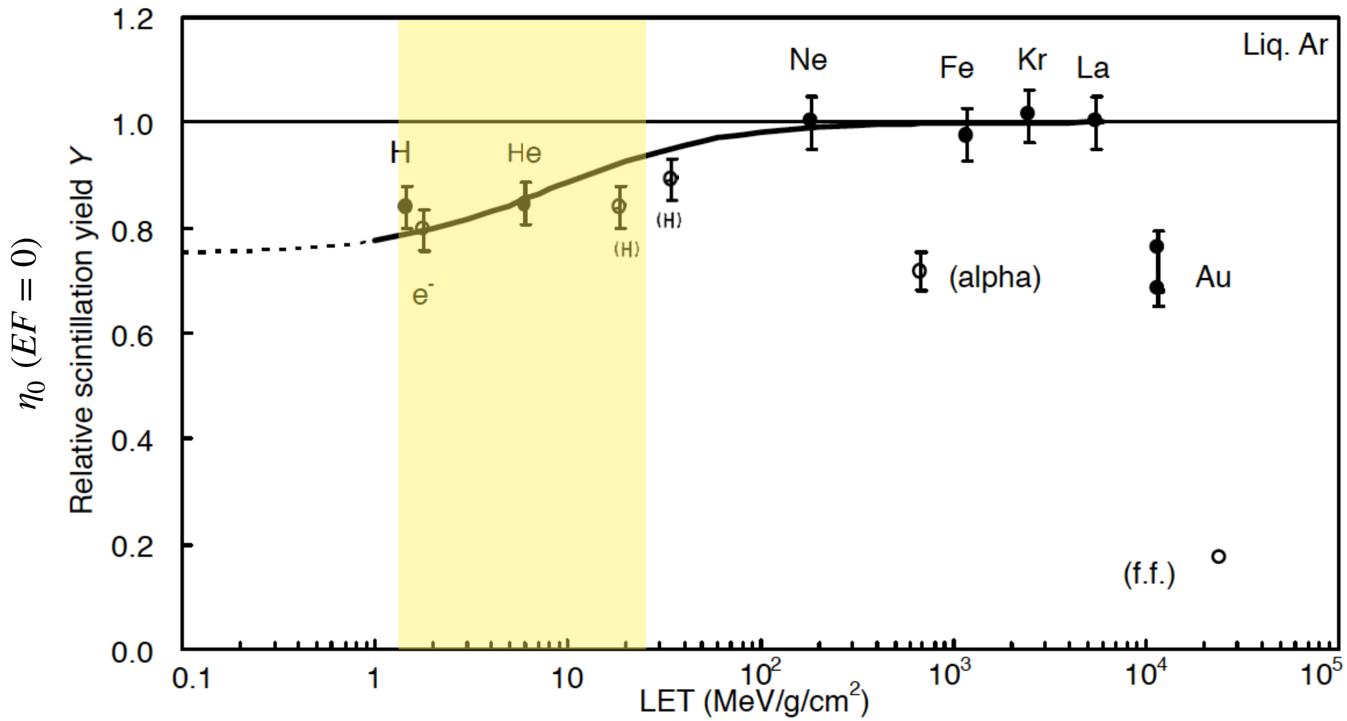
Effect of deposited Energy Density

At EF=0, observed Light reduction at low $\frac{dE}{dx}$ due to ionization electrons escaping recombination

N_0 n. of escape electrons per unit of dep. energy

η_0 - Evidence of *Light reduction at 0-EF due to escape electrons*

$$\eta_0 = \frac{N_i - N_0 + N_{ex}}{N_i + N_{ex}}$$



Measure η_0 Light Yield Reduction at low dE/dx

$[(1 - \eta_0) = \text{fraction of missing photons}] \implies \chi_0 \quad (= \frac{N_0}{N_i}\ \text{fraction of escape electrons})$

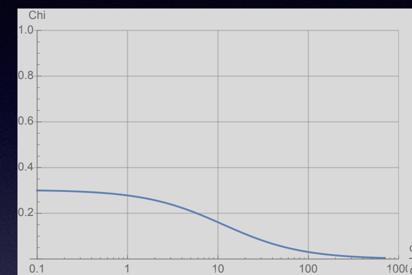
LArSIM

Set relation between Ionization Charge Yield $QY \left[\frac{e}{\text{MeV}}\right]$ and Scintillation Light Yield $LY \left[\frac{ph}{\text{cm}}\right]$

based on:

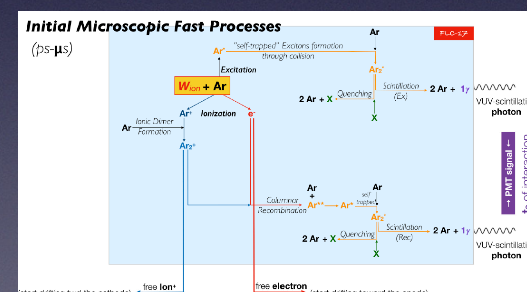
- 3 parameters (experimentally measured):

- $N_i = \frac{1}{W_{ion}}$
- $\frac{N_{ex}}{N_i}$
- $\chi_0 \left(= \frac{N_0}{N_i} \right)$ with $\chi_0(\frac{dE}{dx})$ - This accounts for escape electron charge, at given dE/dx



- Initial Ionization Energy partition:

- $W_{ion} = E_i + \epsilon_{kin} + (\frac{N_{ex}}{N_i})\, E_{ex}$



- **Charge - Light Master Equation:** $QY + LY = N_i + N_{ex}$ and thus:

Light Yield expressed through Free Charge Yield

- $LY = N_i - QY\left(\frac{dE}{dx}, EF\right) + N_{ex}$ where $N_i - QY = LY_{rec}$ n. recombined e = n. ph from Recombination

$= LY_{rec} + LY_{ex}$

Conventional Notation and nomenclature

Energy density $\frac{dE}{dx} \left[\frac{MeV}{cm}\right]$

$$\frac{dE}{dx}|_{mip} = 2.1\ \frac{MeV}{cm}$$

$$W_{ion} = 23.6\ \frac{\text{eV}}{e} = 23.6 \times 10^{-6}\ \frac{\text{MeV}}{e}$$

Charge Yield $QY = \frac{dQ^{free}}{dE} \left[\frac{e}{\text{MeV}}\right]$

Max Charge at $EF = \infty$: $QY_{\infty} = \frac{1}{W_{ion}} \left[\frac{e}{\text{MeV}}\right]$

Charge density $\frac{dQ^{free}}{dx} \left[\frac{e}{\text{cm}}\right] = \frac{dQ^{free}}{dE} \cdot \frac{dE}{dx}$

$$\frac{dQ}{dx}|_{\infty} = \frac{dE/dx}{W_{ion}} \left[\frac{e}{\text{cm}}\right]$$

A similarly for Light:

Light Yield $LY\ [\frac{ph}{MeV}]$

Max Light at $EF = 0$: LY_0

Light Density $\frac{dL}{dx} \left[\frac{ph}{\text{cm}}\right]$

$$\frac{dL}{dx}|_0$$

$$\frac{dE}{dx} \rightarrow \frac{dQ}{dx}\Big|_{\infty} = \frac{dE/dx}{W_{ion}}$$

Max Ionization Charge
(collectable at infinite EF - ie. no Recombination)

$W_{ion} = 23.6 \text{ eV}/e = 23.6 \times 10^{-6} \text{ MeV}/e, \qquad \rho_{LAr} = 1.39 \ g/cm^3$

Recombination (ie finite EF)

Electron-ion recombination in liquid argon ionization chambers has been studied since early '70s

None of the electron recombination theories developed so far (Geminate/Onsager, Columnar/Jaffe-Kramers Box Model/Thomas-Imel) is fully successful in describing experimental data in LAr at all EF and dE/dx.

In the range of interest here (low EF, lower dE/dx), Jaffe's Thory approximated by the so-called Birks Law (for quenching effects in scintillators) and Modified Box Model are used to fit data in this range.

LArSIM:

$$\frac{dE}{dx} \rightarrow \text{Mod Box Mod } \textit{or} \text{ Birks Law} \rightarrow \frac{dQ^{free}}{dx}$$

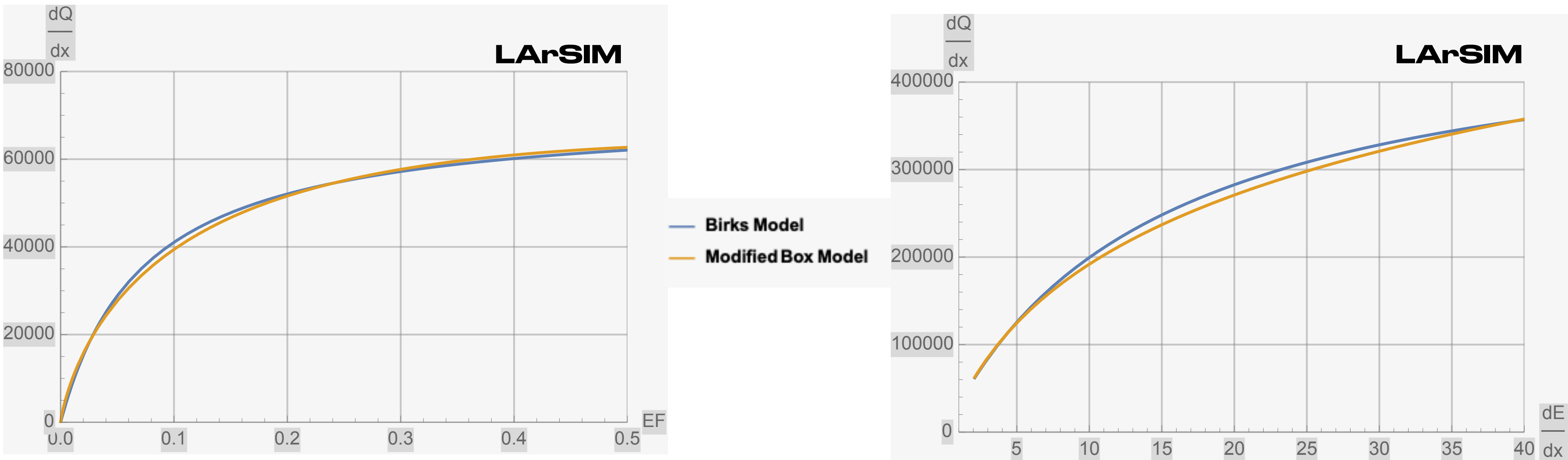
Mod Box Model:

$\alpha_{MBM} = 0.93, \quad \beta'_{MBM} = 0.212$

Birks Law

$A_B = 0.800 \pm 0.003, \ \ k_B = 0.0486 \pm 0.0006 \ \frac{\text{kV}}{\text{cm}} \frac{\text{g/cm}^2}{\text{MeV}}$

$\frac{dQ^{free}}{dx}$ as fcn. of EF $\quad\quad$ $\frac{dQ^{free}}{dx}$ as fcn. of $\frac{\text{dE}}{\text{dx}}$



Mod Box Model:

$$\alpha_{MBM} = 0.93, \quad \beta'_{MBM} = 0.212$$

Birks Model

$$A_B = 0.800 \pm 0.003, \quad k_B = 0.0486 \pm 0.0006 \ \frac{\text{kV}}{\text{cm}} \frac{\text{g/cm}^2}{\text{MeV}}$$

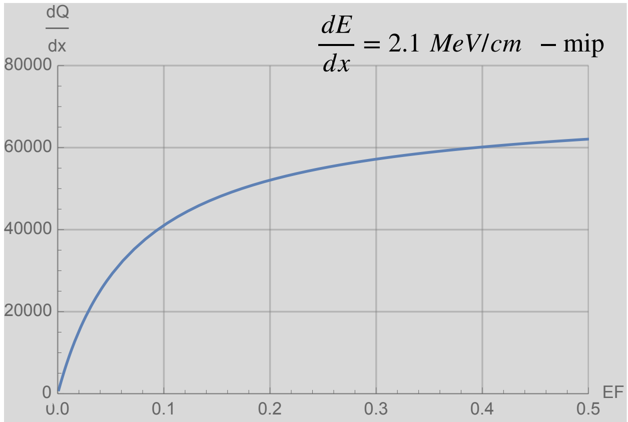
In both Charge parameterizations

$$\frac{dQ}{dx}^{free}_{Birks/Box}\left(\frac{dE}{dx}, EF \to 0\right) \to 0$$

From Birks Model:

$$\frac{dQ}{dx}^{free}_{Birks} = \frac{A_B \frac{1}{W_{ion}} \frac{dE}{dx}}{1 + \frac{k_B}{\rho_{LAr}} \frac{1}{EF} \frac{dE}{dx}}$$

$$A_B = 0.800 \pm 0.003, \quad k_B = 0.0486 \pm 0.0006 \, \frac{\text{kV}}{\text{cm}} \frac{\text{g/cm}^2}{\text{MeV}}$$

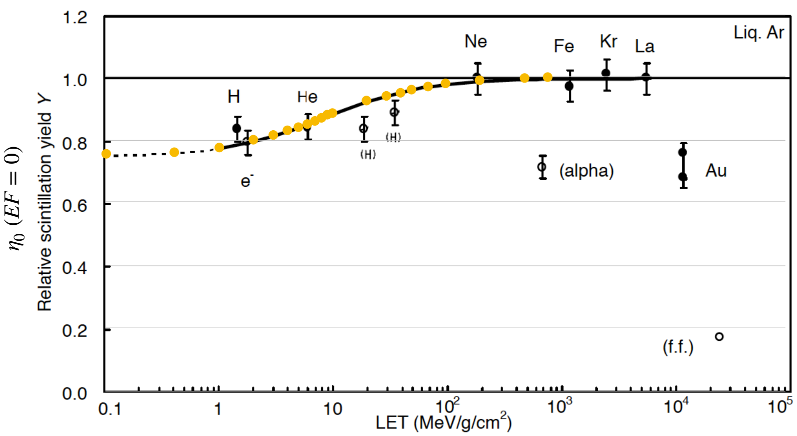


in friction with escape electron evidence

At any dE/dx <u>in our range of interest</u> (from ~2 to ~40 MeV/cm),

@EF=0 $\Rightarrow \frac{dQ}{dx}^{free}\Big|_0 = \chi_0 \cdot \frac{dQ}{dx}\Big|_\infty \neq 0$ due to escape electrons

$$\to \chi_0 \cdot \frac{dQ}{dx}\Big|_\infty \leq \frac{dQ}{dx}^{free} \leq \frac{dQ}{dx}\Big|_\infty$$



Use $\frac{N_{ex}}{N_i} = 0.29$

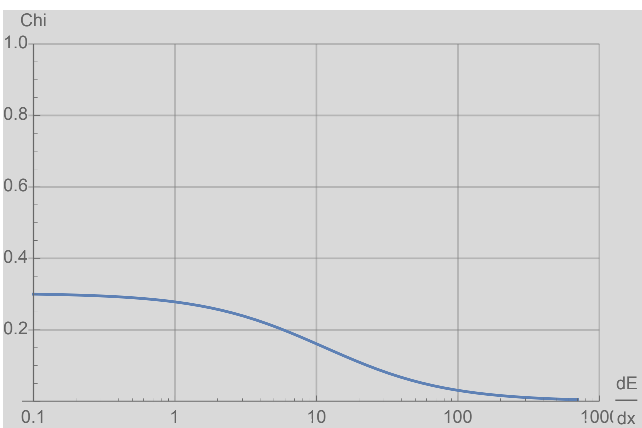
[Doke'02]

η_0, Light reduction at 0-EF, allows to infer χ_0, *free Charge rise* (escape el) *at 0-EF* (not directly measurable, *if EF=0 - no detector*) for any dE/dx in the range of our interest.

$$\eta_0 = \frac{(1 - \chi_0 + \frac{N_{ex}}{N_i})}{(1 + \frac{N_{ex}}{N_i})}$$

$$\eta_0 = \eta_0(\frac{dE}{dx})$$

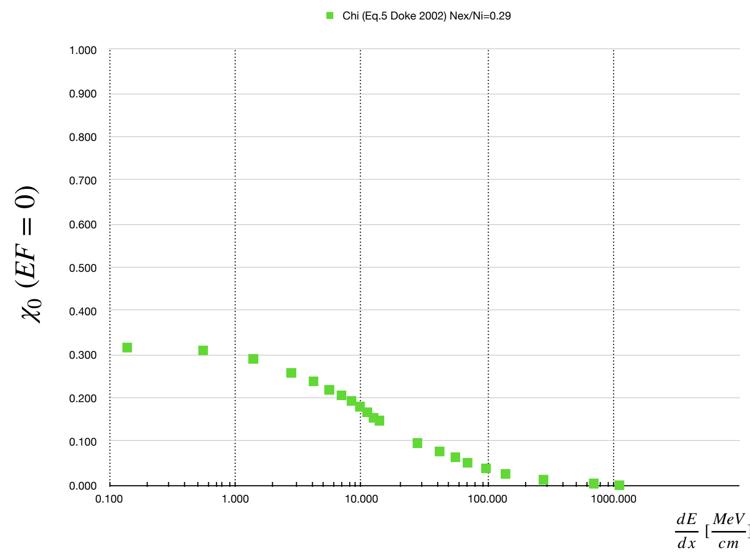
$$\chi_0 = (1 + \frac{N_{ex}}{N_i}) - (1 + \frac{N_{ex}}{N_i}) \cdot \eta_0$$



$$\chi_0\left(\frac{dE}{dx}\right) = \frac{0.00338427}{-6.57037 + exp\left[1.88418 + 0.000129379\ \frac{dE}{dx}\right]}$$

Fit w/ Sigmoid fcn

$$sig(x) = \frac{p1}{p2 + exp[p3 + p4\ x]}$$



LArSIM

Modified Birks Model

to include escape electrons at 0-EF and correction for additional charge freed at low EF

Introduce charge protection for escape el:

(i) at EF=0, require $\frac{dQ}{dx}^{free}|_0 = \chi_0 \cdot \frac{dQ}{dx}|_\infty$, *escape electrons*

(ii) at low EF (above/near EF=0), add *EF-extracted electrons* in addition to escape electrons,

(iii) at higher EF, additional electrons must decrease to 0, restoring standard behavior from Birks Model (known to be valid for EF > ~200 V/cm)

$$\chi_0 = \chi_0\left(\frac{dE}{dx}\right) \quad \rightarrow \quad \chi = \chi\left(\frac{dE}{dx}, EF\right) = \chi_0\left(\frac{dE}{dx}\right) \cdot f_{corr}(EF)$$

$$\frac{dQ}{dx}^{ee}\left(\frac{dE}{dx}, EF\right) = \chi \cdot \frac{dQ}{dx}|_\infty$$

$$\frac{dQ}{dx}^{free}_{ModBirks} = \frac{dQ}{dx}^{free}_{Birks} + \frac{dQ}{dx}^{ee} = \frac{A_B \frac{1}{W_{ion}} \frac{dE}{dx}}{1 + \frac{k_B}{\rho_{LAr}} \frac{1}{EF} \frac{dE}{dx}} + \chi_0\left(\frac{dE}{dx}\right) \cdot f_{corr}(EF) \cdot \frac{dQ}{dx}|_\infty$$

Modified Birks Model in LArSIM

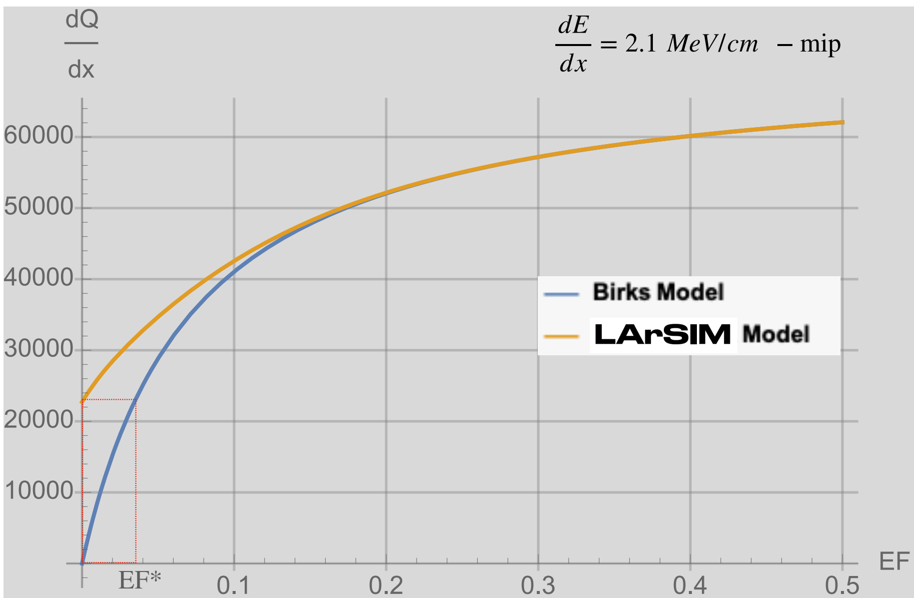
(to include escape electrons at 0-EF and correction for charge freed at very low EF)

$$\frac{dQ}{dx}^{free}_{ModBirks} = \frac{A_B \frac{1}{W_{ion}} \frac{dE}{dx}}{1 + \frac{k_B}{\rho_{LAr}} \frac{1}{EF} \frac{dE}{dx}} + \chi_0\left(\frac{dE}{dx}\right) \cdot f_{corr}(EF) \cdot \frac{dQ}{dx}\Big|_{\infty}$$

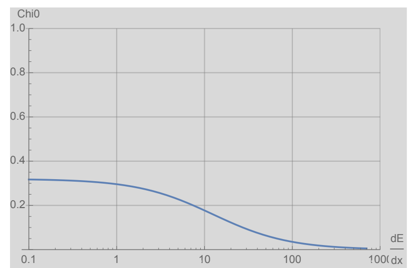
Where:

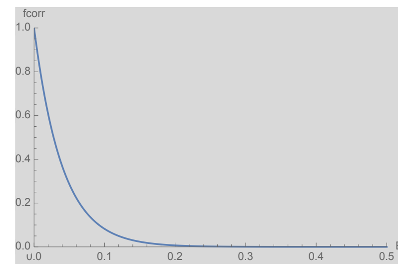
$$\chi_0\left(\frac{dE}{dx}\right) = \frac{0.00338427}{-6.57037 + exp\left[1.88418 + 0.000129379\ \frac{dE}{dx}\right]}$$

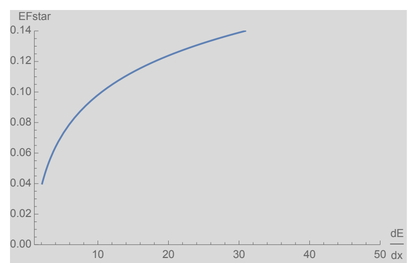
$$f_{corr} = exp\left[-\frac{EF}{EF^*}\right]$$



$EF^* = 0.038\ V/cm$







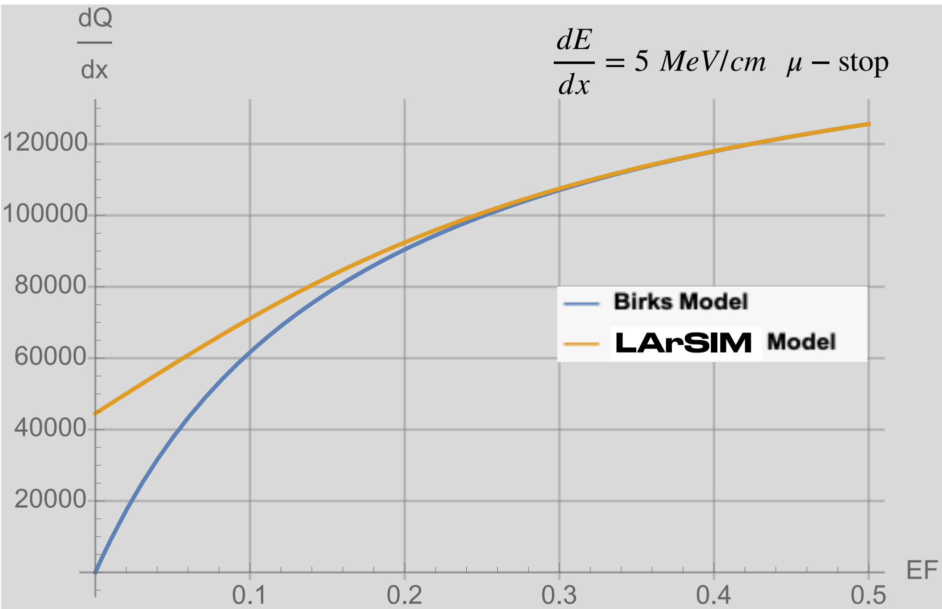
EF^* is the EF value where

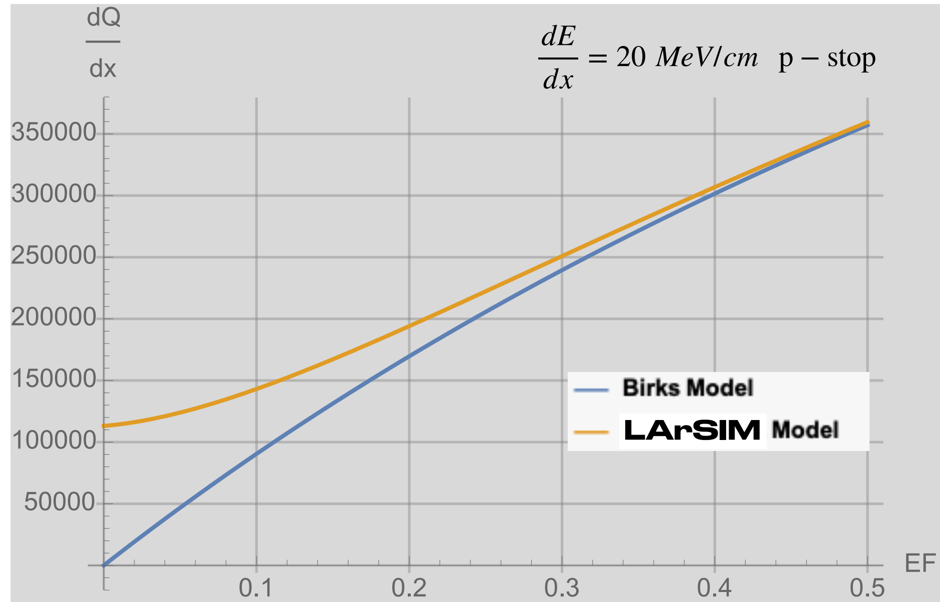
$$QY_{Birks}(EF = EF^*) = \chi_0\ QY_\infty$$

Note: EF^* depends ~logarithmically on $\frac{dE}{dx}$

$$EF^*\left(\frac{dE}{dx}\right) = 0.0372\ \ln\left[\frac{dE}{dx}\right] + 0.0124$$

Fit EF* data point by Logarithmic fcn.





Charge Sector:

LArSIM: from Birks Law → Modified Birks Model (to extend Recombination effects at very low EF/null-EF).

Deviations from current Birks Law expectation only for LArTPC operating at low E, for heavily ionizing particle (stopping p's)

LArSIM

Implementation in MC simulation

(starting from energy deposited in G4 step):

$$\frac{dQ}{dx}\Big|_\infty = \frac{1}{W_{ion}}\frac{dE}{dx}$$

$$\frac{dE}{dx} \rightarrow \text{(STD) Birks Law} \rightarrow \frac{dQ}{dx}^{free}_{Birks} \rightarrow \text{Mod Birks Mod} \rightarrow \frac{dQ}{dx}^{free}_{ModBirks} \rightarrow \frac{dL}{dx}$$

$$\frac{dQ}{dx}\Big|_\infty \left(1 + \frac{N_{ex}}{N_i}\right) - \frac{dQ}{dx}^{free}_{ModBirks} = \frac{dL}{dx}$$

$$\frac{dQ}{dx}_{ModBirks} = \frac{dQ}{dx}_{Birks} + \chi\left(\frac{dE}{dx}, EF\right) \cdot \frac{dQ}{dx}\Big|_\infty$$

$$\frac{dQ}{dx}\Big|_\infty \left(1 + \frac{N_{ex}}{N_i} - \chi\right) - \frac{dQ}{dx}^{free}_{Birks} = \frac{dL}{dx}$$

Where:

$$\chi_0\left(\frac{dE}{dx}\right) = \frac{0.00365337}{-5.46204 + exp\left[1.70003 + 0.000194084\ \frac{dE}{dx}\right]}$$

$$f_{corr} = exp\left[-\frac{EF}{EF^*}\right]$$

$$EF^*\left(\frac{dE}{dx}\right) = 0.0318\ \ln\left[\frac{dE}{dx}\right] + 0.0133$$

$$\frac{dL}{dx} = \frac{1}{W_{ion}}\frac{dE}{dx}\left[1 + \frac{N_{ex}}{N_i} - \chi_0\left(\frac{dE}{dx}\right) f_{corr}(EF) - \frac{A_B}{1 + \frac{k_B}{\rho_{LAr}}\frac{1}{EF}\frac{dE}{dx}}\right]$$

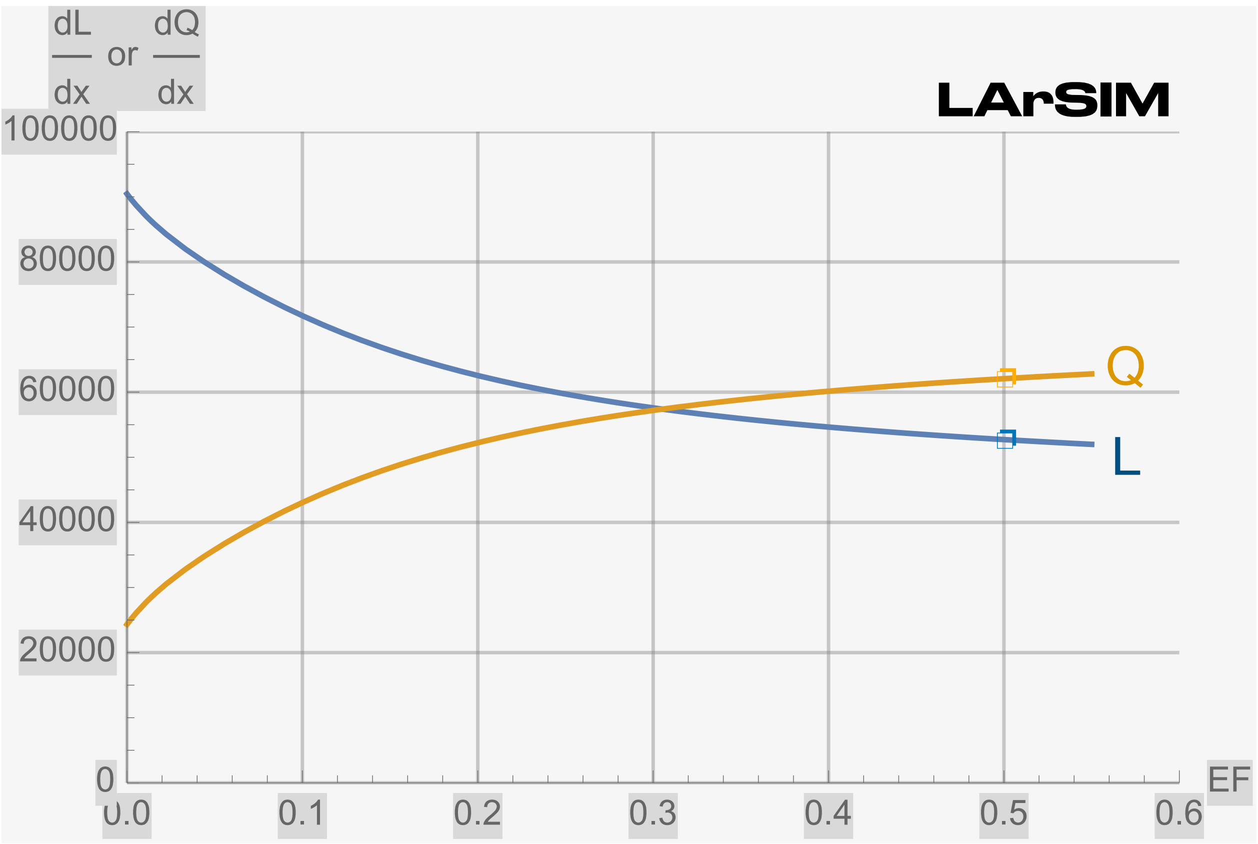
N. of primary Ionizations

N. of excitation ph's

N. of escaping e's

N. of free (not recombined) e's

$$\frac{dE}{dx} = 2.1\ MeV/cm \quad - \text{mip}$$



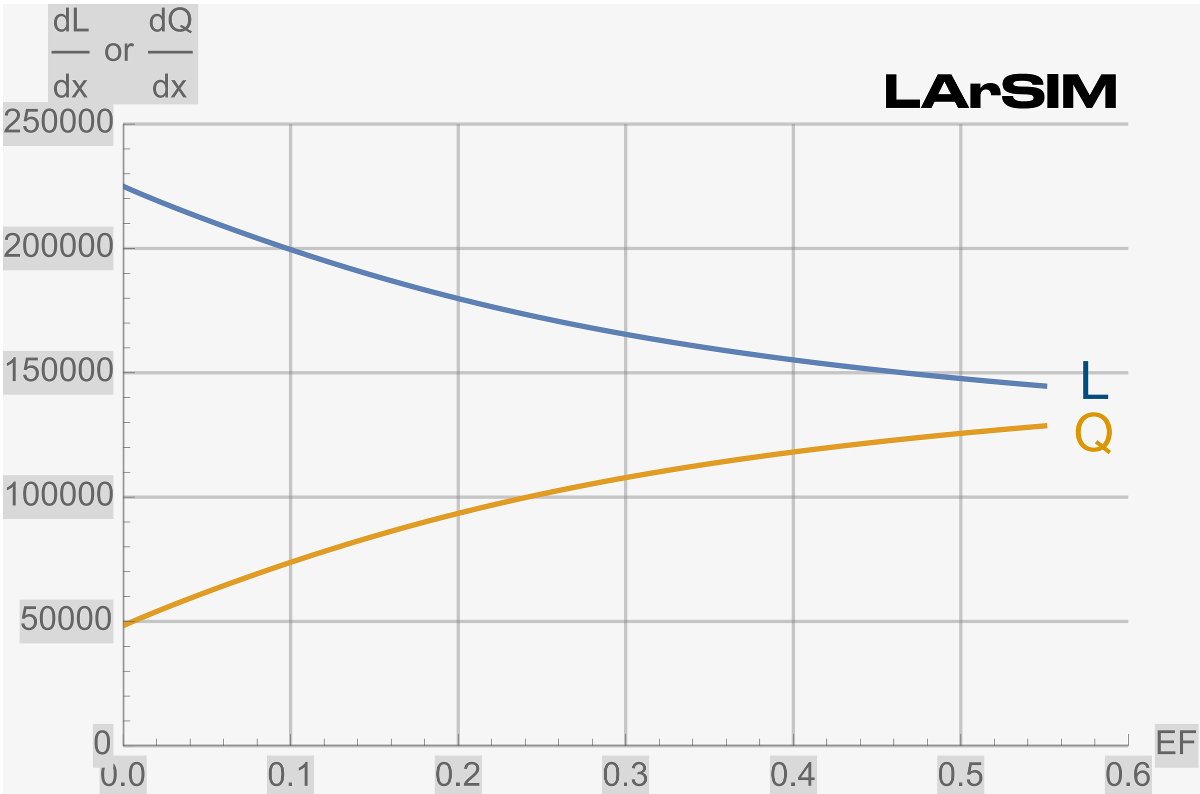
Q+L = const

$$= \frac{1}{W_{ion}}\left(1+\frac{N_{ex}}{N_i}\right)\cdot\frac{dE}{dx}$$

At $EF = 0.5\ \frac{kV}{cm}, \frac{dE}{dx} = 2.1\ \frac{MeV}{cm}$

$L = 52700\ \frac{ph}{cm},\ Q = 62000\frac{e}{cm}$

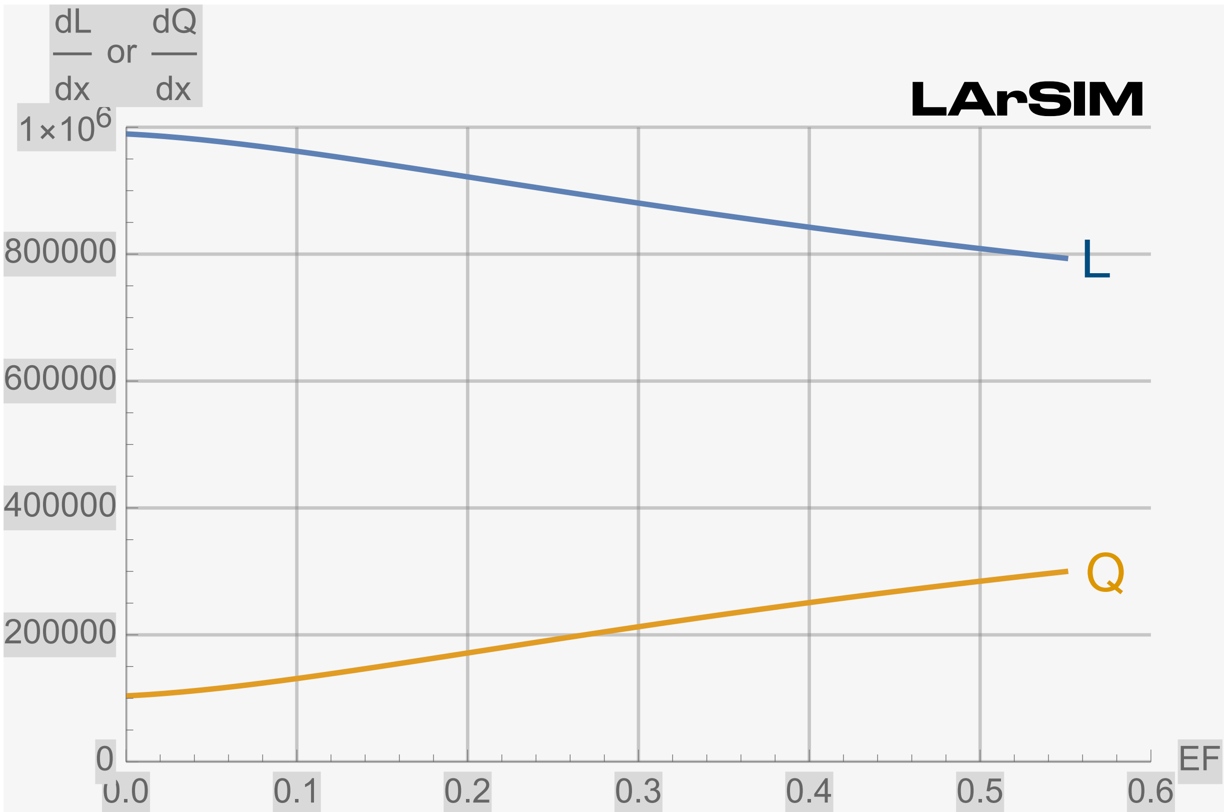
$$\frac{dE}{dx} = 5\ MeV/cm \qquad \mu - \text{stop}$$



Q+L = const

$$= \frac{1}{W_{ion}}\left(1+\frac{N_{ex}}{N_i}\right)\cdot\frac{dE}{dx}$$

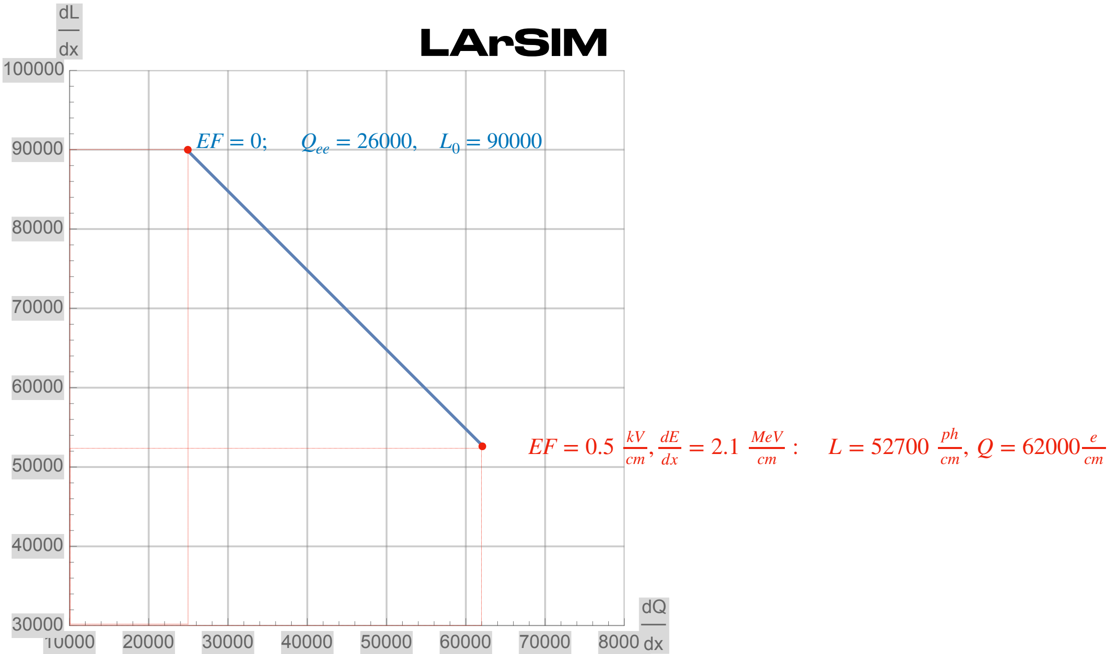
$$\frac{dE}{dx} = 20\ MeV/cm \qquad \text{p} - \text{stop}$$

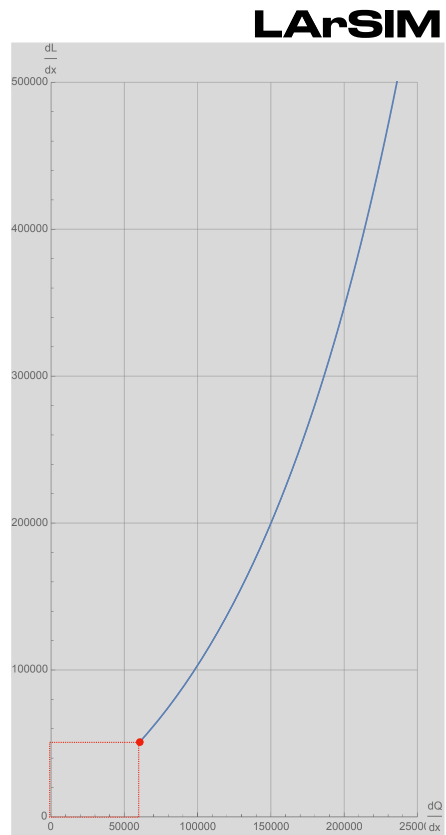


Q+L = const

$$= \frac{1}{W_{ion}} \left(1 + \frac{N_{ex}}{N_i}\right) \cdot \frac{dE}{dx}$$

$$\frac{dL}{dx} \quad \text{vs.} \quad \frac{dQ^{free}}{dx}$$





$$\frac{dL}{dx} \quad \text{vs.} \quad \frac{dQ^{free}}{dx}$$

Varying EF: $0 \leq EF \leq 0.5\ \frac{kV}{cm}$

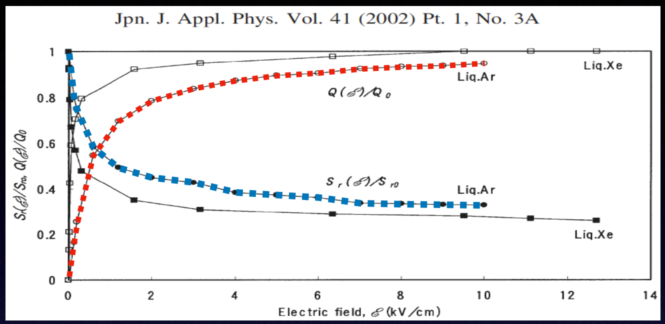
at $\frac{dE}{dx} = 2.1\ \frac{MeV}{cm} \quad (mip)$

Varying $\frac{dE}{dx}$: $2.1 \leq \frac{dE}{dx} \leq 40\ \frac{MeV}{cm}$

at $EF = 0.5\ \frac{kV}{cm} \quad (LArTPC\ nominal)$

LArSIM

predictions to Data Comparison



Relative Charge *[rel. to Max Free Charge Yield at* $EF = \infty$*]:* $RQ = \frac{QY(EF)}{QY_\infty}$ (*)

and

Relative Light *[rel. to Max Light Yield at* $EF = 0$*]:* $RL = \frac{LY(EF)}{LY_0}$

(*) RQ *aka Charge Recombination Factor*

Charge - Light master relation: $QY(EF) + LY(EF) = N_i + N_{ex}$

$$LY = N_i - QY\left(\frac{dE}{dx}, EF\right) + N_{ex} \;=\; LY_{rec} \;+\; LY_{ex}$$

$N_i = \frac{1}{W_{ion}} = QY_\infty$ by definition

At $EF = 0$:

$$LY_0 = N_i - QY_0\left(\frac{dE}{dx}\right) + N_{ex}$$

$QY_0 = \chi_0 \cdot QY_\infty$

$$= \; N_i - \chi_0 \cdot QY_\infty + \; N_{ex}$$

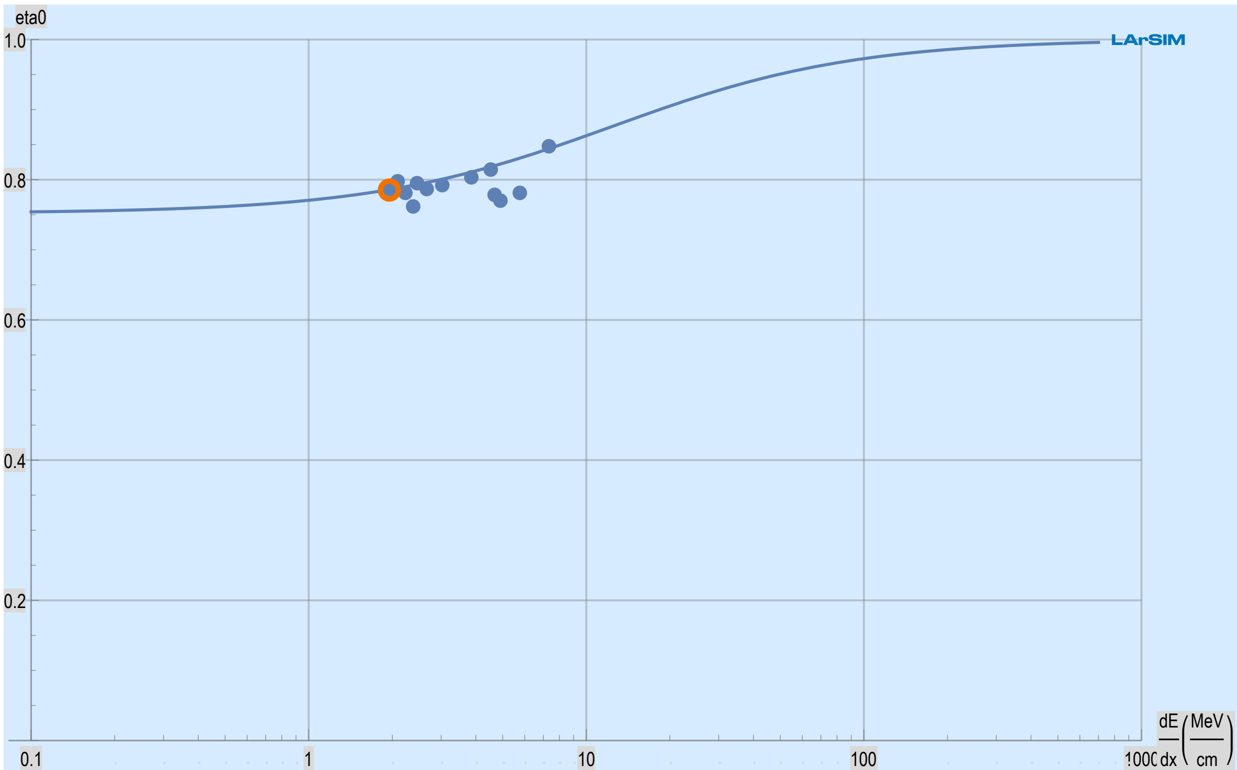
$$= \; QY_\infty \left(1 \; - \; \chi_0 \; + \; \frac{N_{ex}}{N_i}\right)$$

And correspondingly, by dividing all by $\frac{dE}{dx} \Rightarrow \left(\frac{dL}{dx}\right)_0$

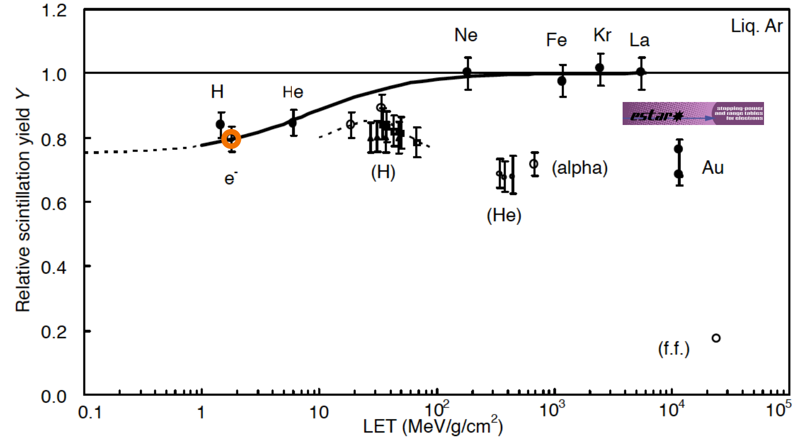
$$\left(\frac{dL}{dx}\right)_0 \; = \; \left(\frac{dQ}{dx}\right)_\infty \left(1 \; - \; \chi_0 \; + \; \frac{N_{ex}}{N_i}\right)$$

EF=0

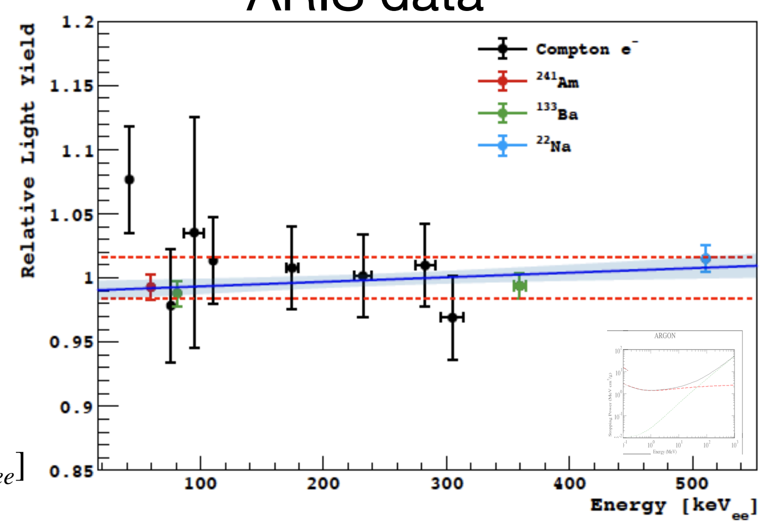
η_0, *Light reduction at 0-EF*, due to escape el.

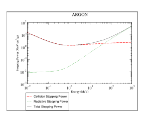


Doke data



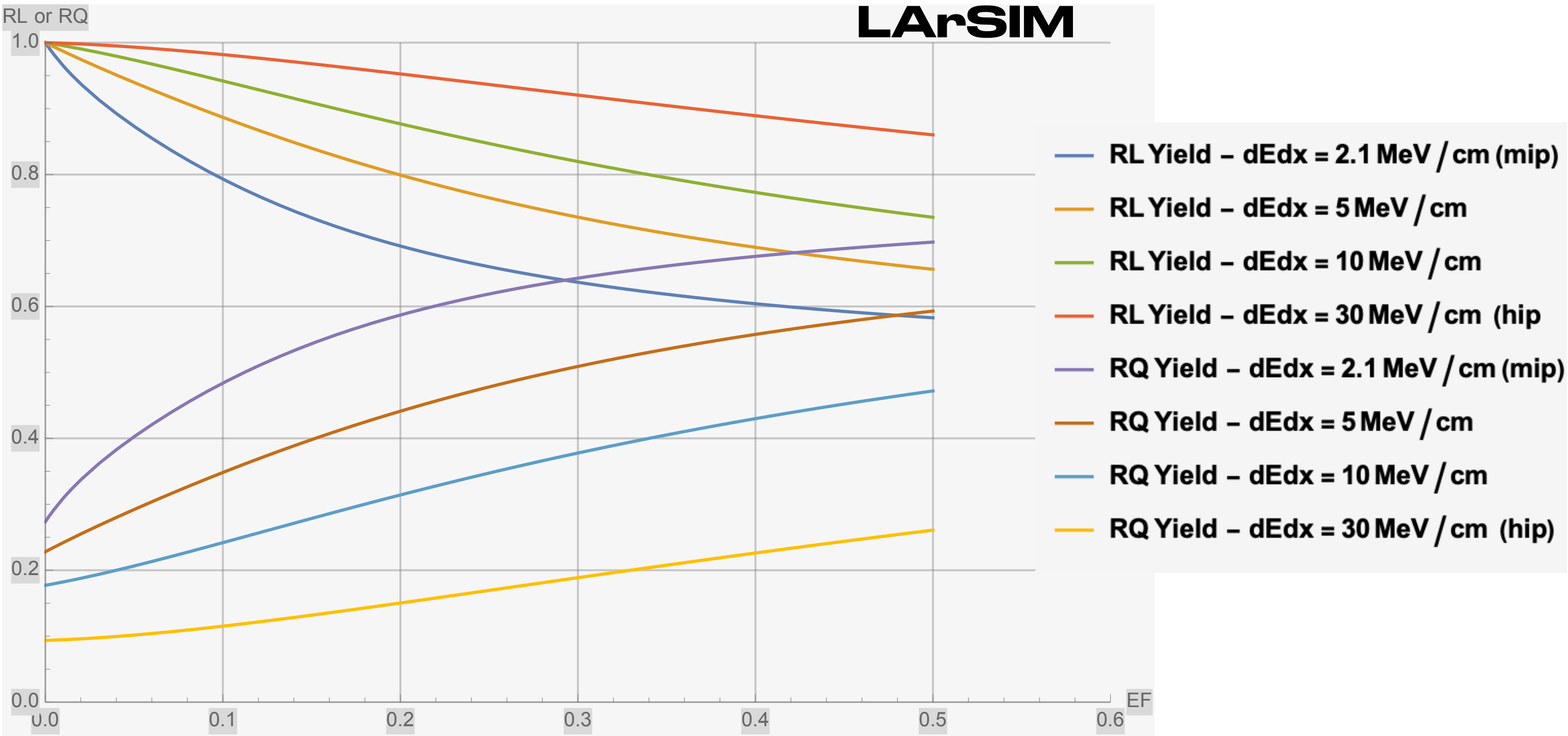
ARIS data





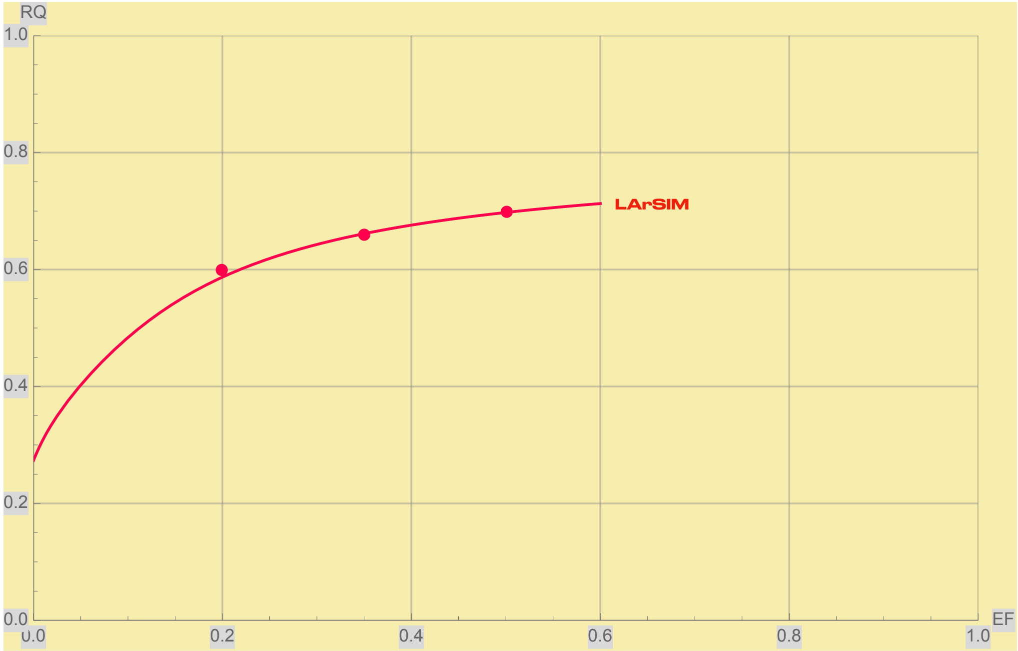
$\frac{dE}{dx}\left[\frac{MeV}{cm}\right] \Leftarrow$ Energy $[keV_{ee}]$

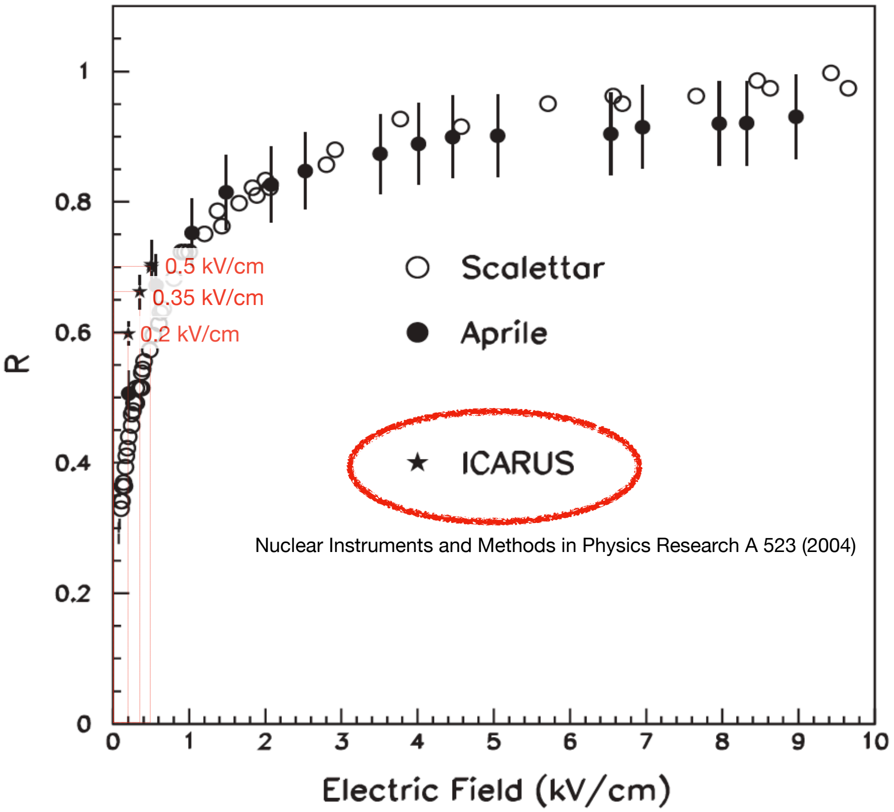
LArSIM: RL and RQ as fcn of EF



LArSIM: free Charge RQ as fcn of EF

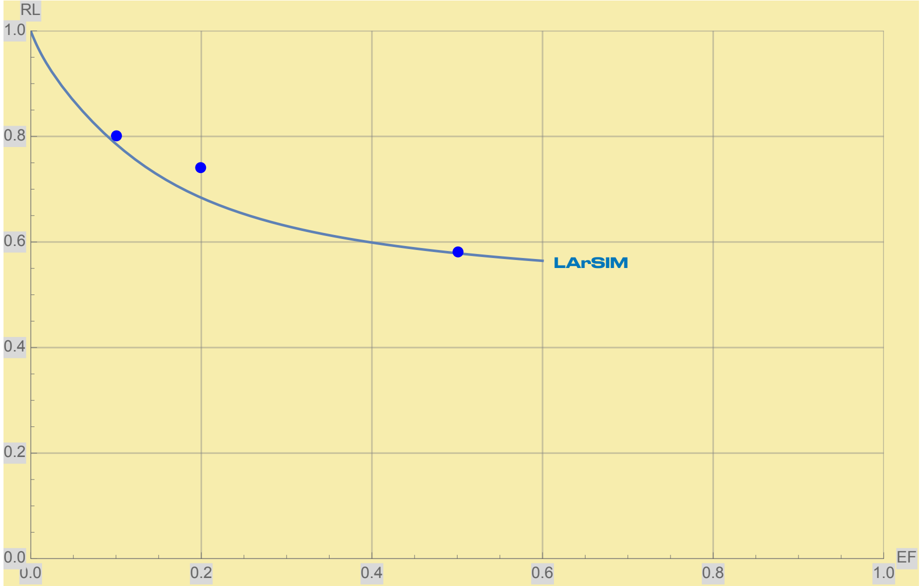
vs. ICARUS Data



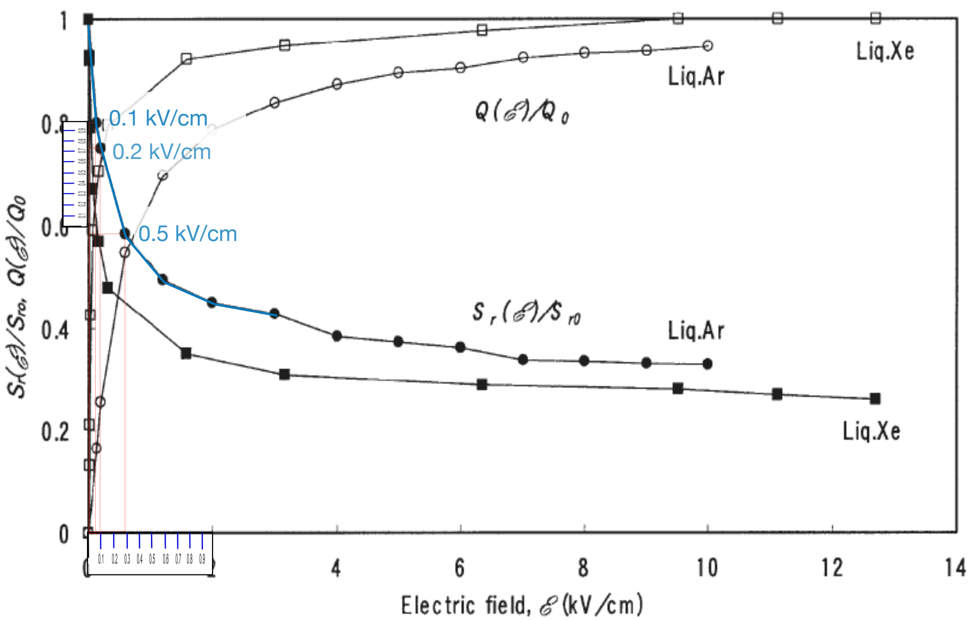


LArSIM: Light RL as fcn of EF

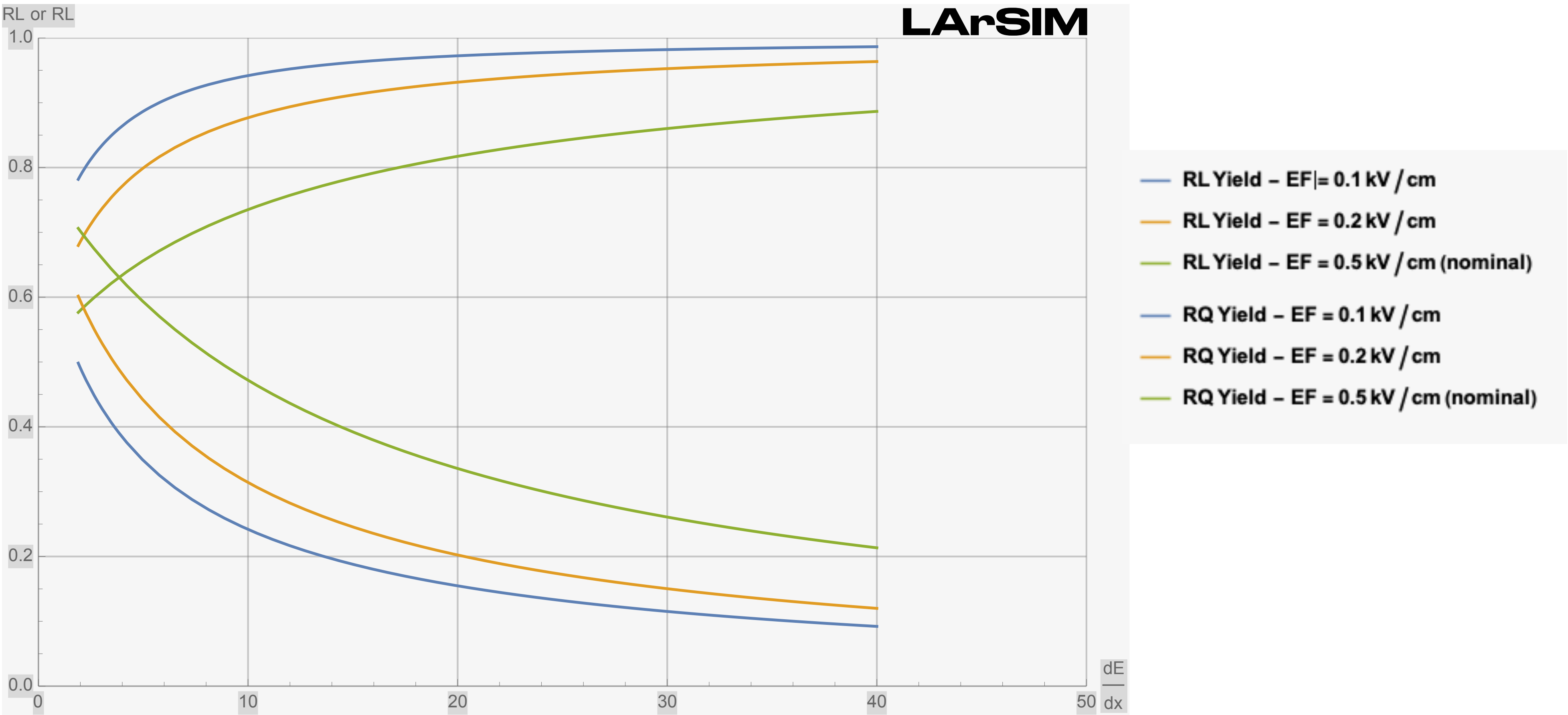
vs. Doke et al. Data



Jpn. J. Appl. Phys. Vol. 41 (2002) Pt. 1, No. 3A



SIM: RL and RQ as fcn of Stopping Pwr $\frac{dE}{dx}$



LArSIM: free Charge RQ as fcn of Stopping Pwr

vs. ICARUS Data

Nuclear Instruments and Methods in Physics Research A 523 (2004)

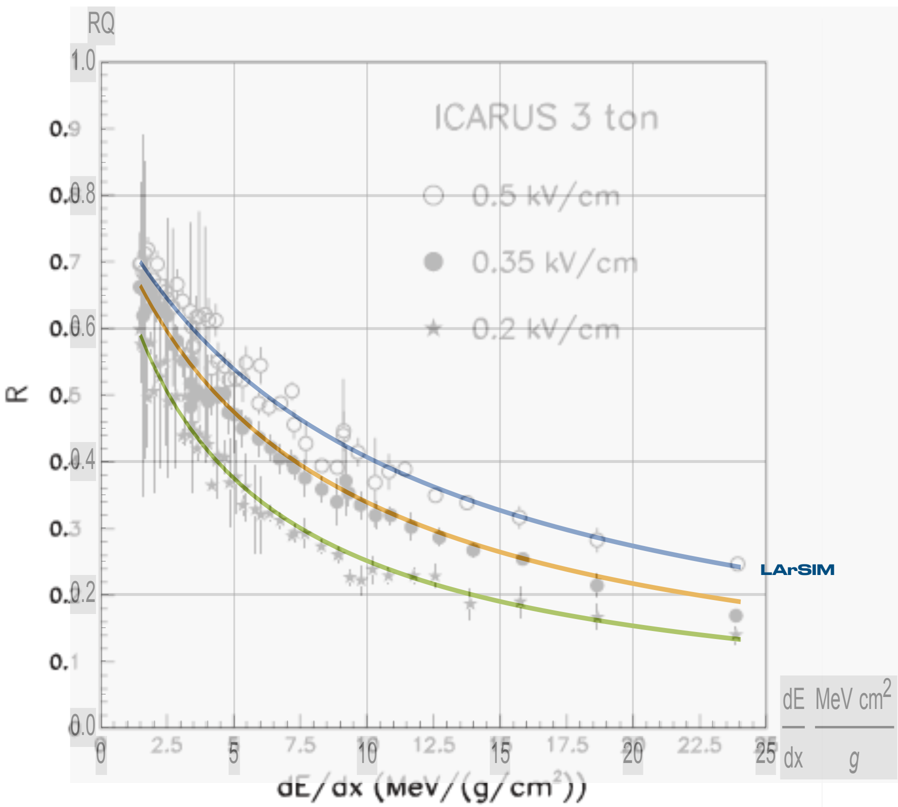


Fig. 1. Recombination factors measured with the 3 ton ICARUS prototype as a function of the theoretical particle stopping power, for different electric field values.

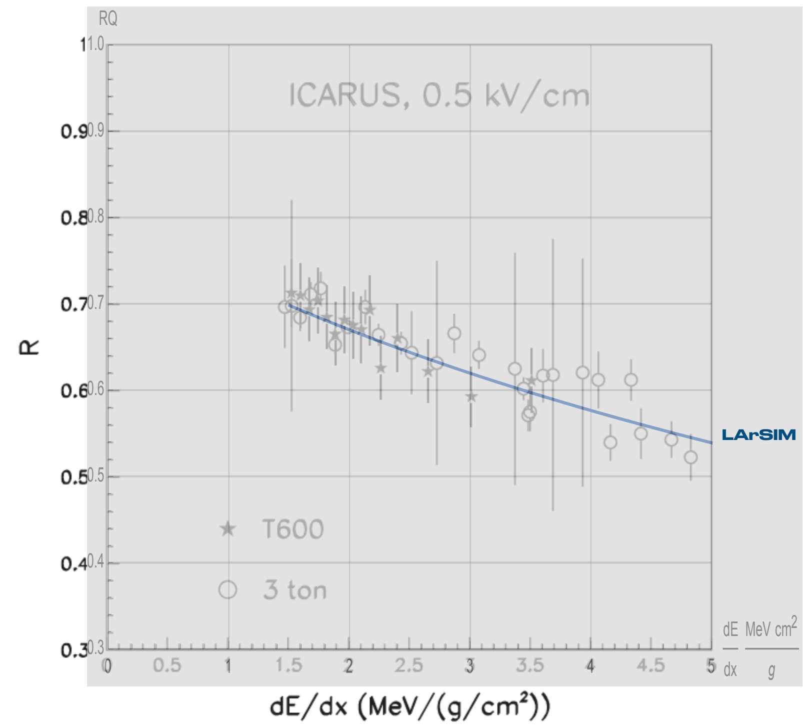
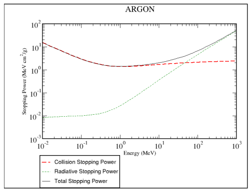


Fig. 2. Recombination factors measured with the ICARUS T600 and 3 ton detectors at 500 V/cm as a function of the theoretical particle stopping power. The errors on T600 data include a 5% systematics from the transparency correction.

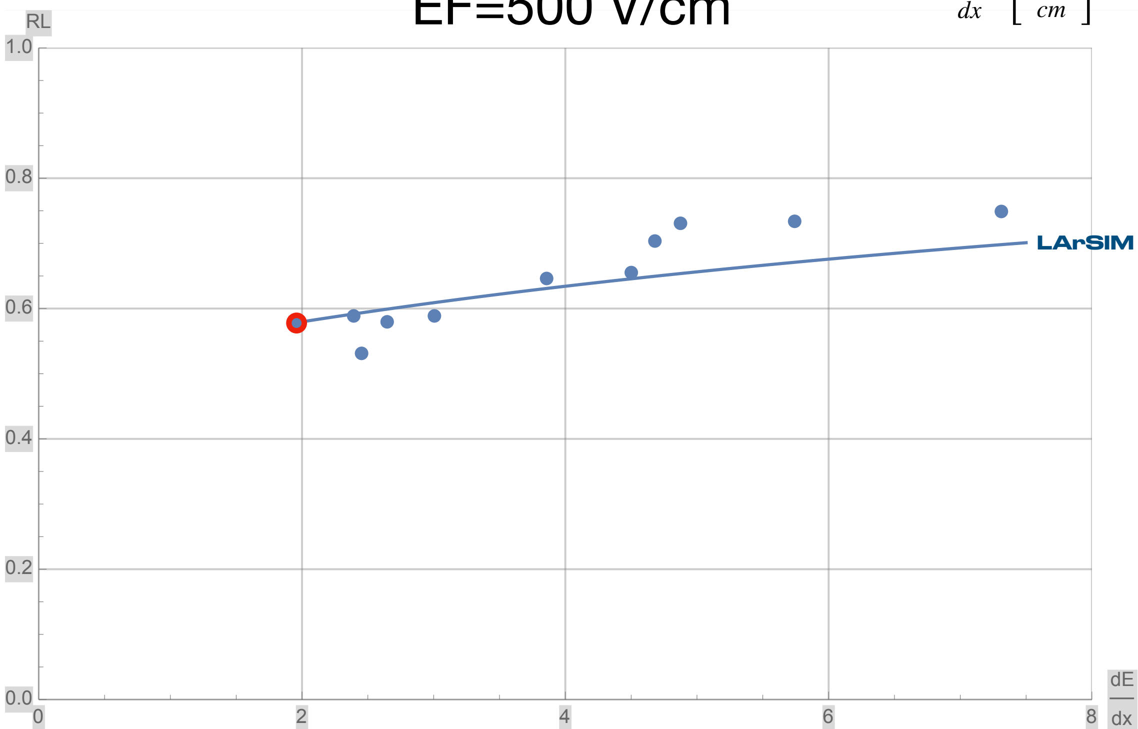
LArSIM: Light RL as fcn of Stopping Pwr

vs. Doke et al. Data ●, and ARIS Data ●



EF=500 V/cm

$\frac{dE}{dx}\left[\frac{MeV}{cm}\right] \Leftarrow$ Energy $[keV_{ee}]$



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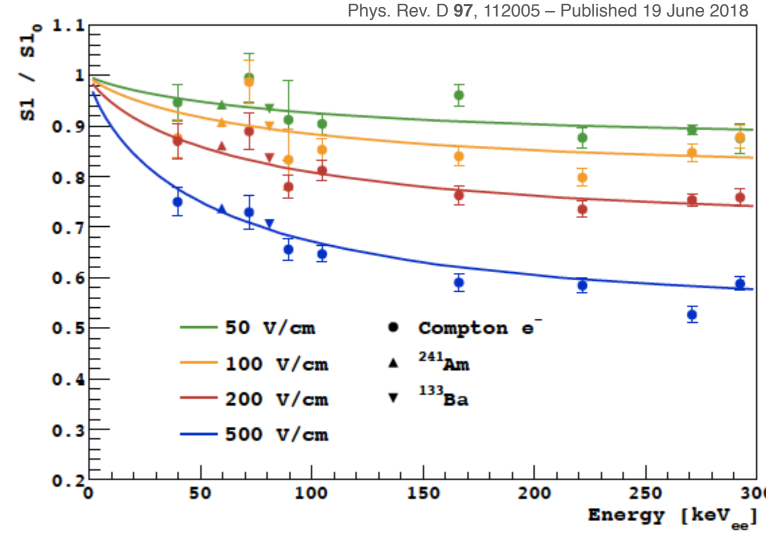
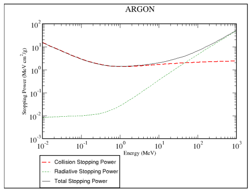
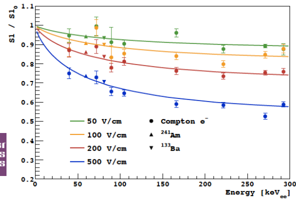


FIG. 16. Field induced quenching of S1 for ERs at different drift fields, fit with the Doke-Birks model.

LArSIM: Light RL as fcn of Stopping Pwr

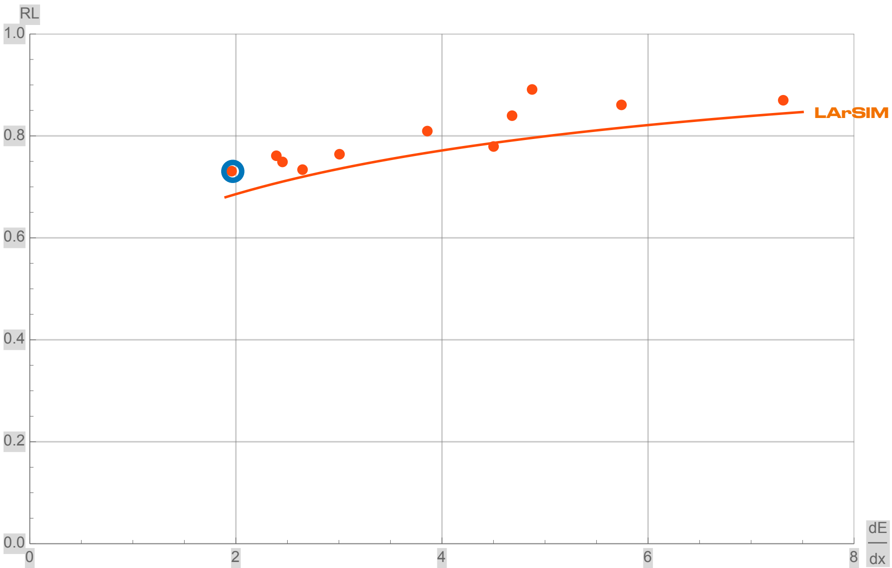
vs. Doke et al. Data ●, and ARIS Data ●



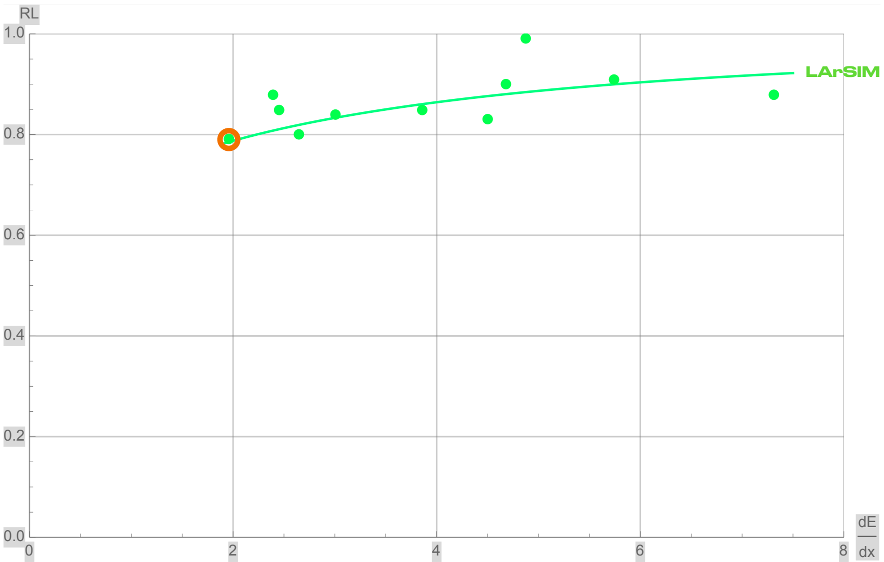


$\frac{dE}{dx}\left[\frac{MeV}{cm}\right] \Leftarrow$ Energy $[keV_{ee}]$

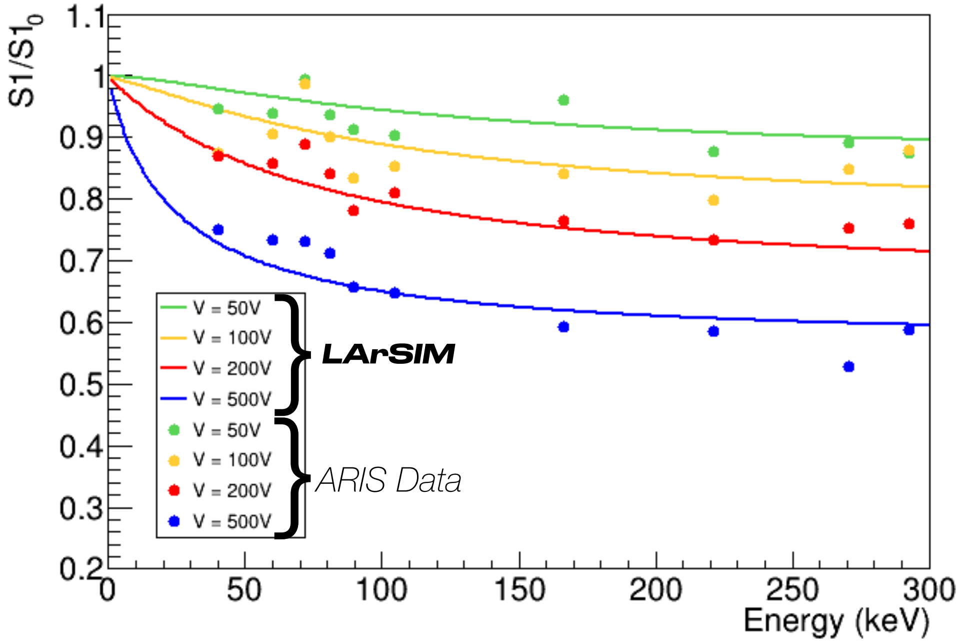
EF=200 V/cm



EF=100 V/cm



$$\frac{dE}{dx}\left[\frac{MeV}{cm}\right] \Rightarrow \text{Energy } [keV_{ee}]$$



ARIS Data + ARIS Model

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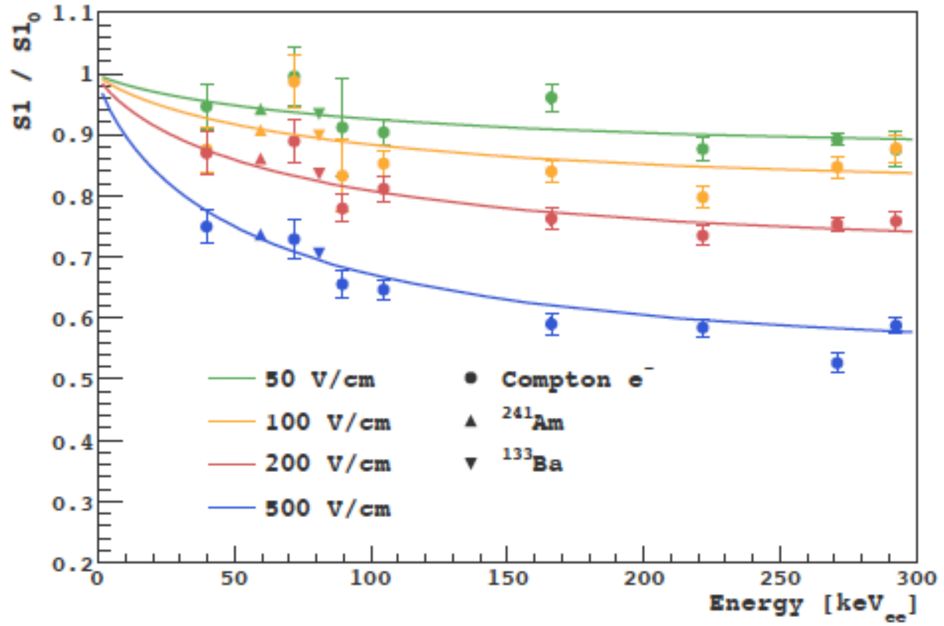
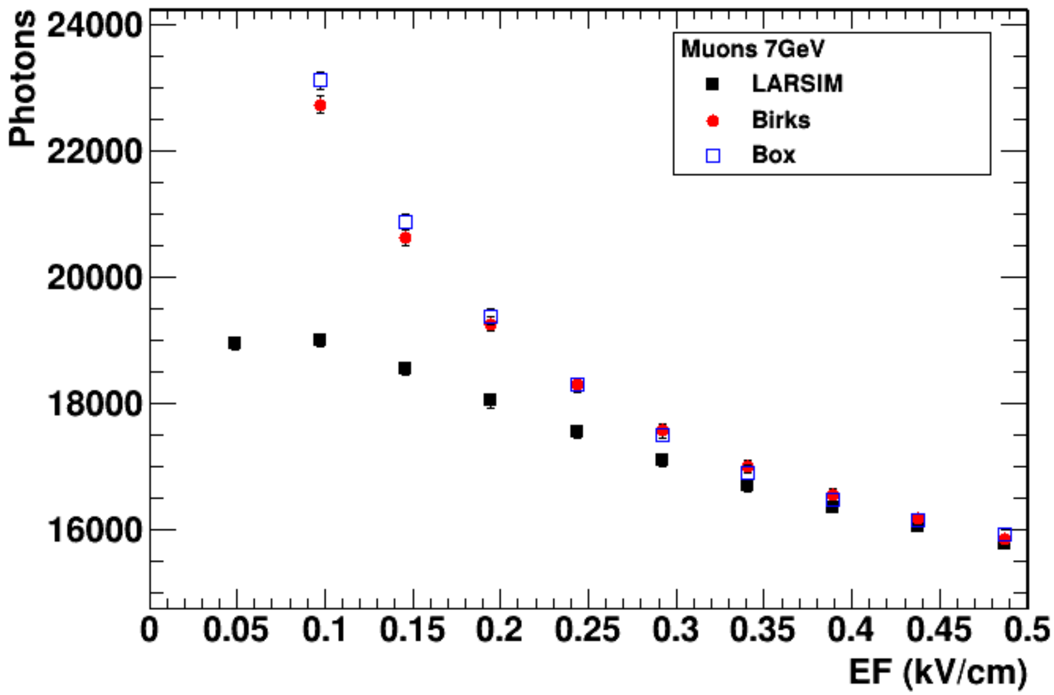
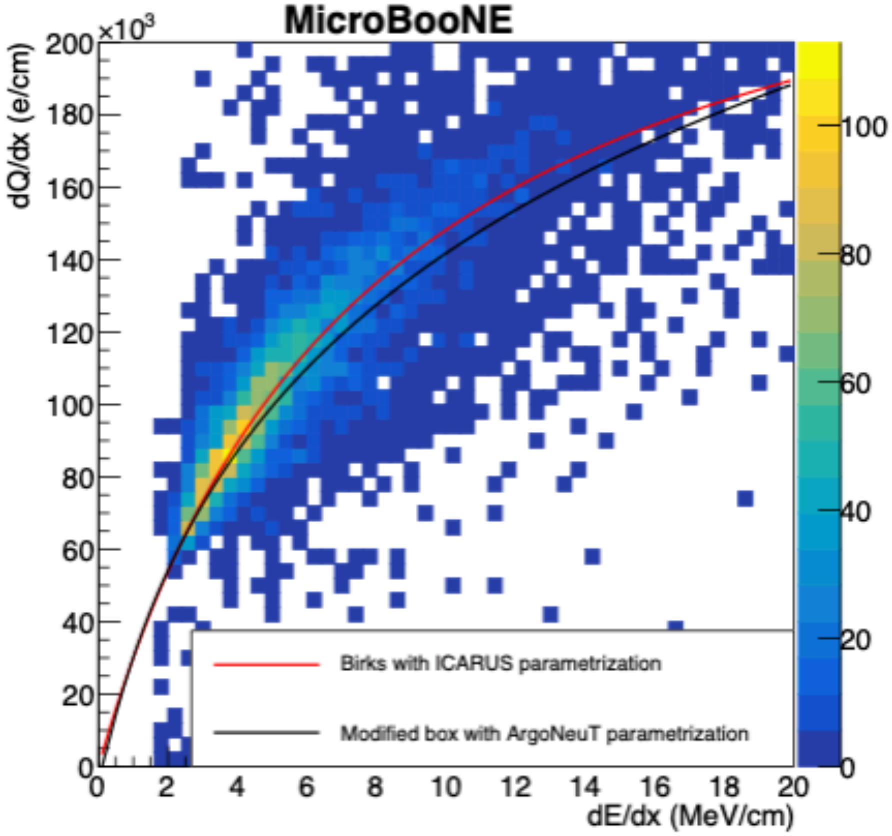


FIG. 16. Field induced quenching of S1 for ERs at different drift fields, fit with the Doke-Birks model.

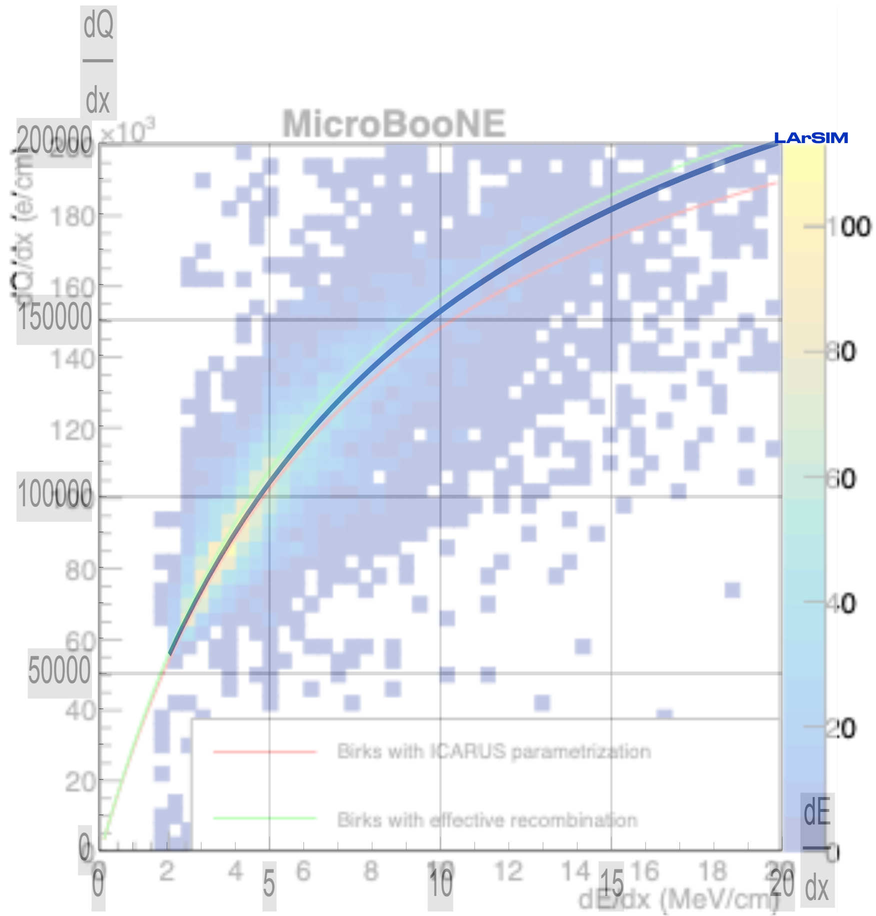
LArSIM implemented in LArSoft for scintillation light emission from Charged particle energy deposition.

First simulation of 7 GeV/c Muons in protoDUNE





(a) Data



(b) Comparison with Birks' law

LArSIM

- Motivations, Goals and Limits
- Theoretical/Phenomenological foundations
- Implementation in MC simulation
- Predictions to Data Comparison

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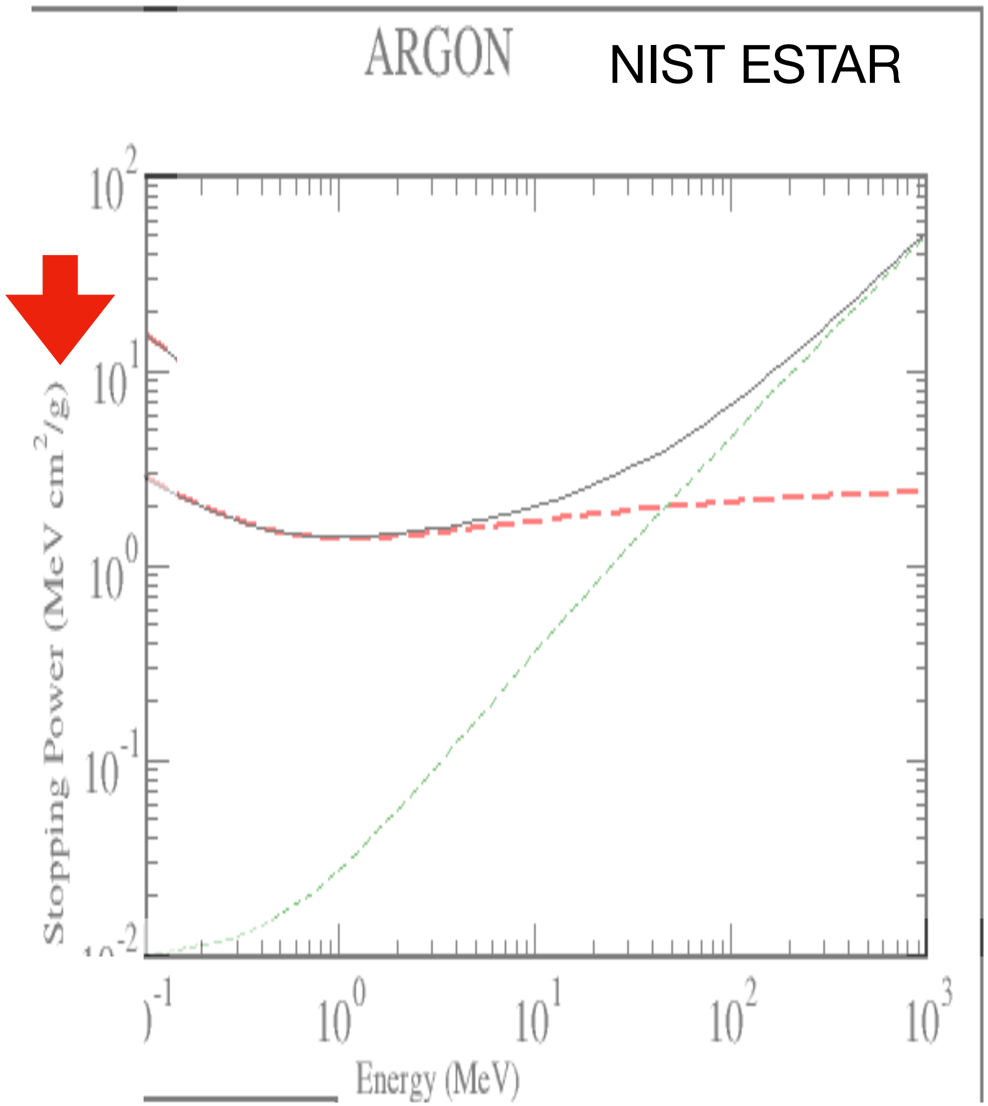

D. Caratelli dE/dx for el.