Microscopic simulation of Xenon-based optical TPCs in the presence of additives

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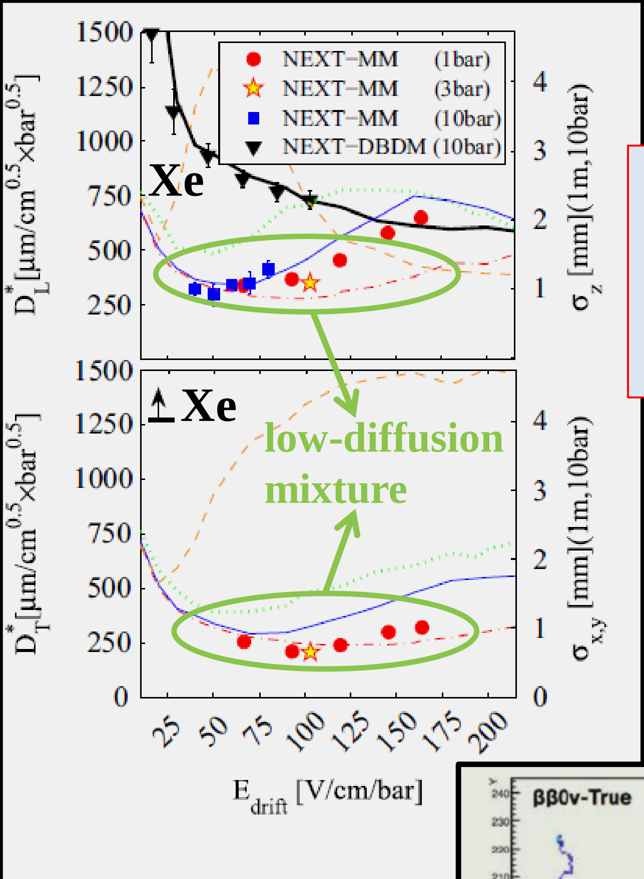
and the NEXT collaboration

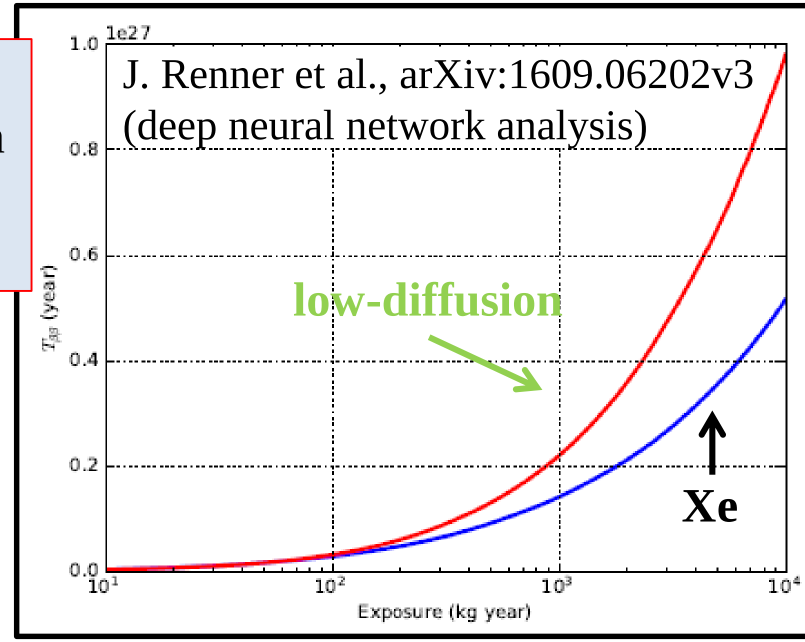
@Paris (05/12/2016)

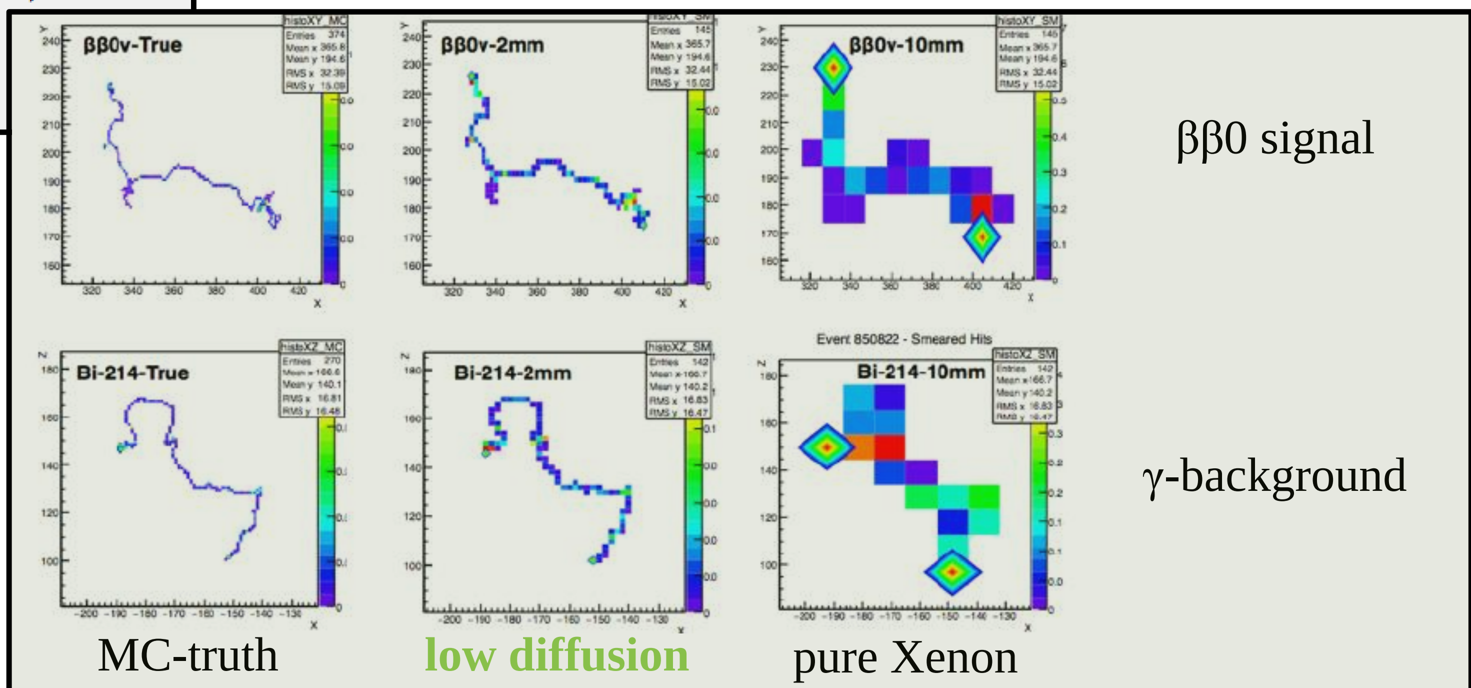
I. The problem

The importance of the ‘topological’ information in NEXT



but what happens to the Xenon scintillation when diffusion is reduced??





From TPC conference 2014!

A ‘conceptual’ magic mixture

(Penning)-Fluorescent

(2 candidate molecules identified)

1. Able to **reduce electron diffusion** in gas.
2. **Recombination small.**

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3. Strongly **fluorescent at higher λ** and self-transparent.
4. Allows for **EL at lower field** due to low-lying excited states of the additive.
5. Suitable for **Penning** transfer. Can potentially reduce Fano factor.

~’low IP/high-reactive type’

Low diffusion/light preserving

(6+ candidate molecules identified)

1. Able to **reduce electron diffusion** in gas.
2. **Recombination small.**

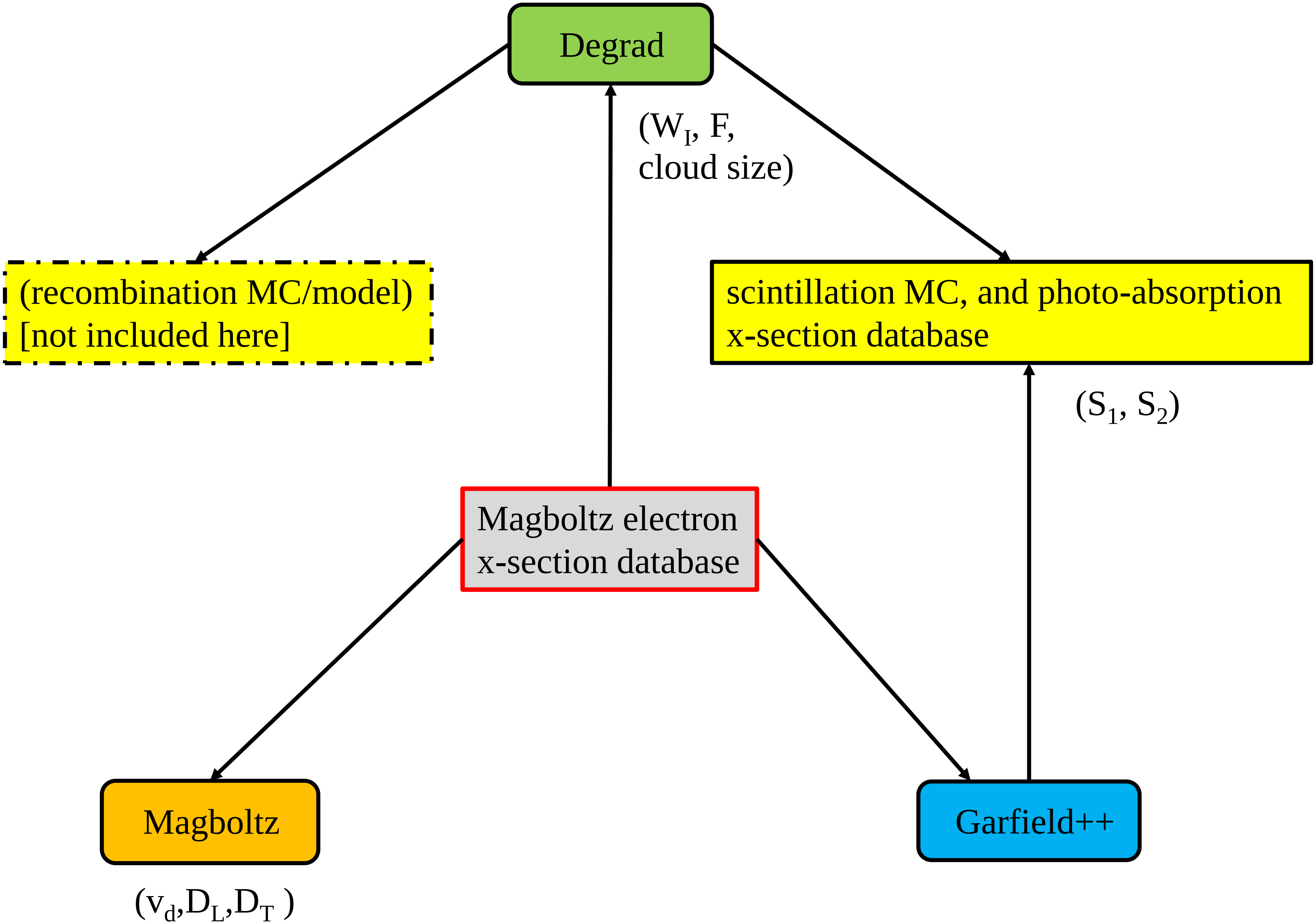
---

3. Light mechanisms unaffected.
   a) **Highly transparent** to Xenon-light.
   b) **Small quenching for S_1, S_2 and small fluctuations in EL**.

~’high IP/low-reactive type’

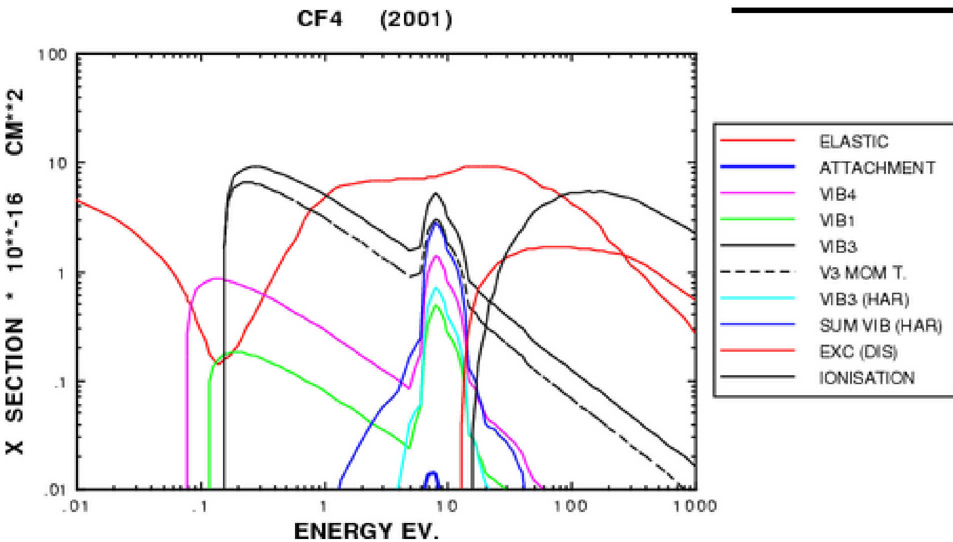
II. The tool

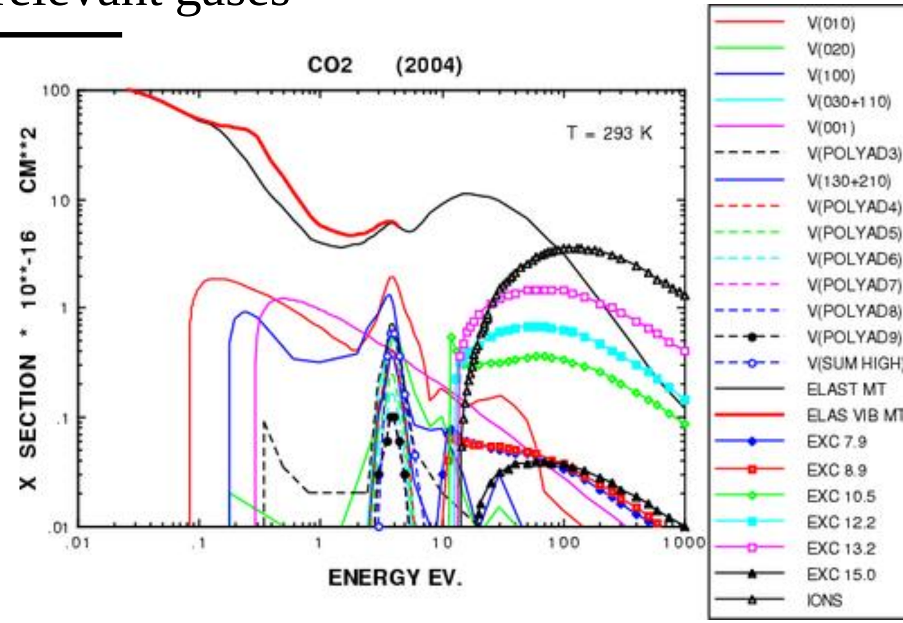
A microscopic software for electron and photon transport in gas

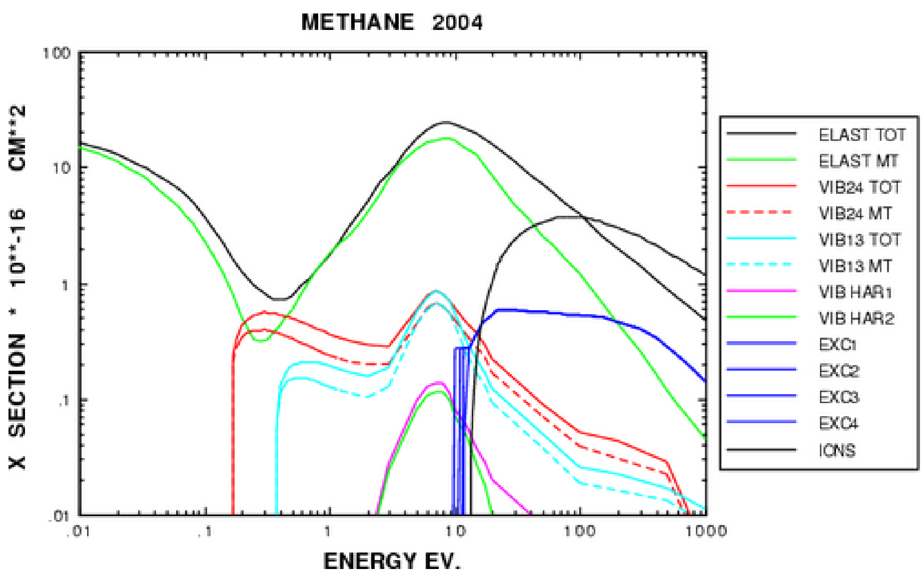


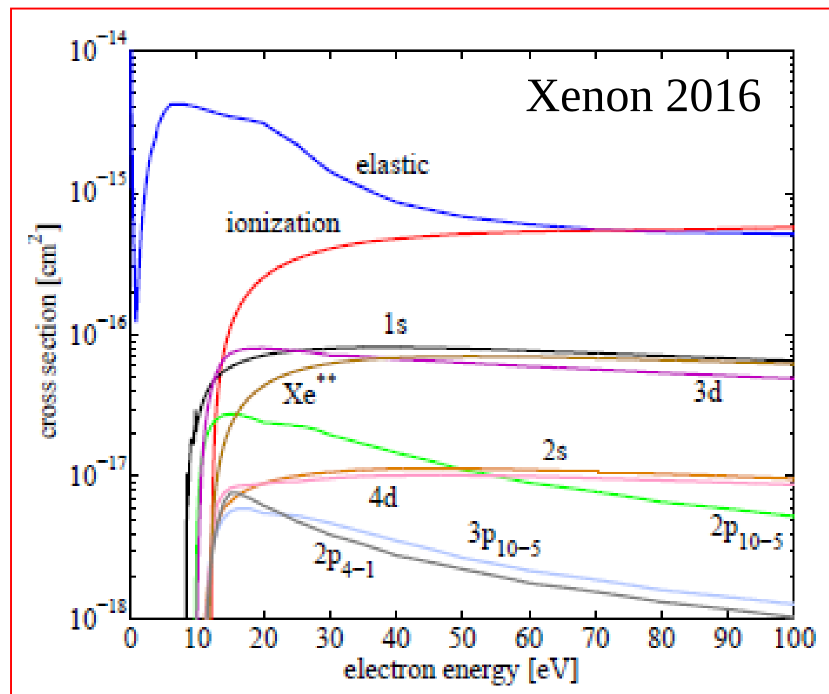
III. Basic considerations and input

Electron x-sections of relevant gases









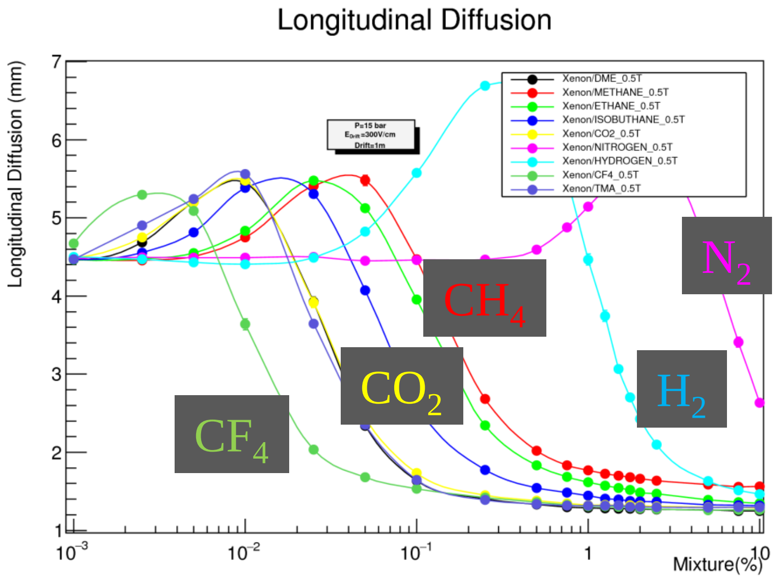
x-sections for molecules that are plot here are actually old ones (just illustrative!)

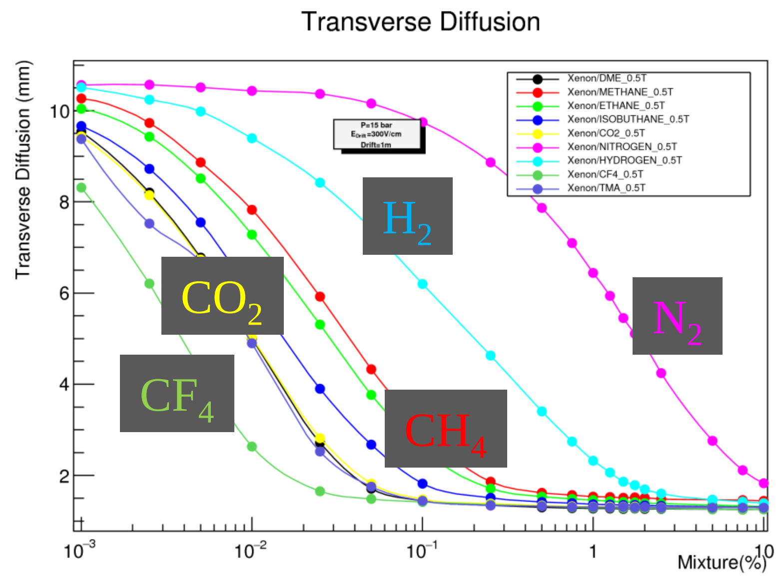
I

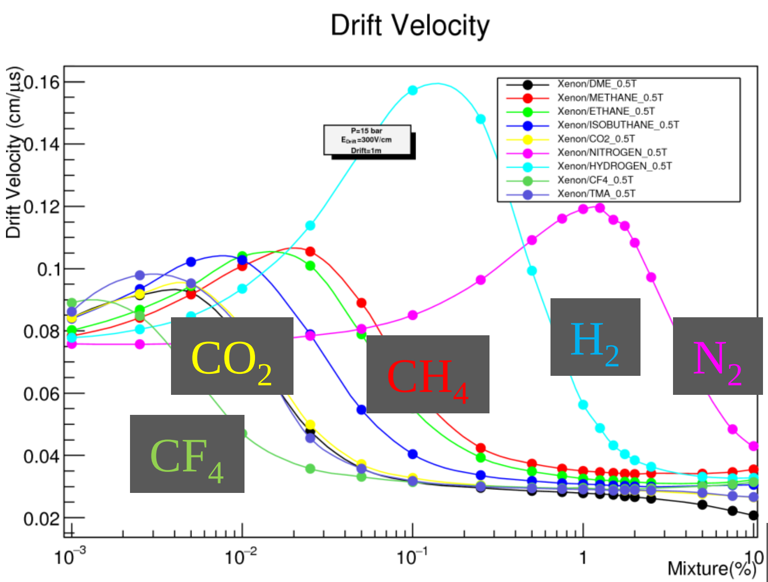
Ionization transport characteristics (v_d, D_L, D_T)

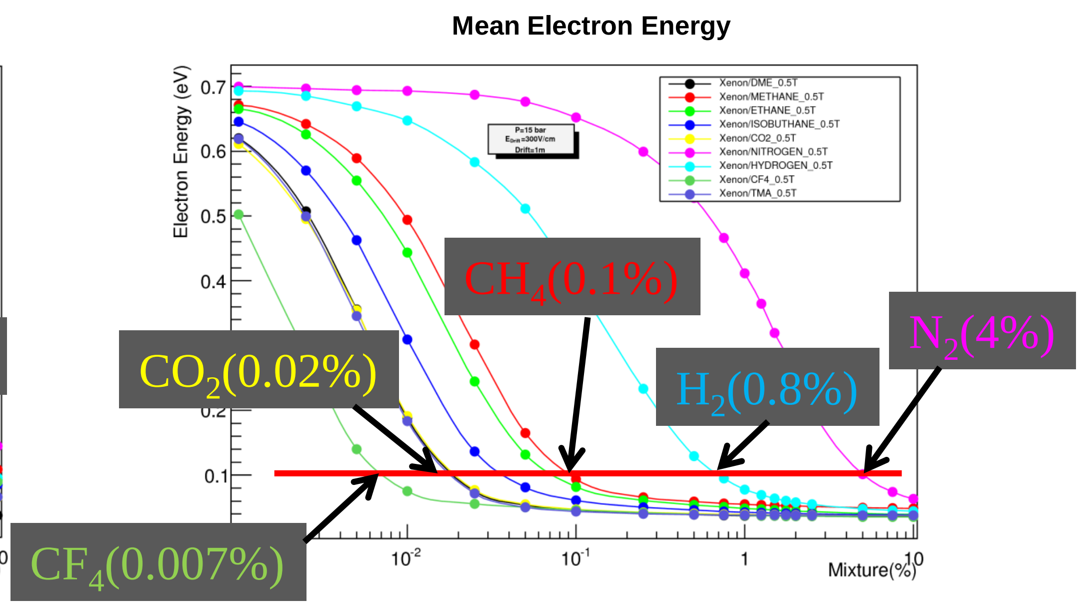
Outside 20-30V/cm/bar it performs generally worse

E_d=20 V/cm/bar, P=15bar









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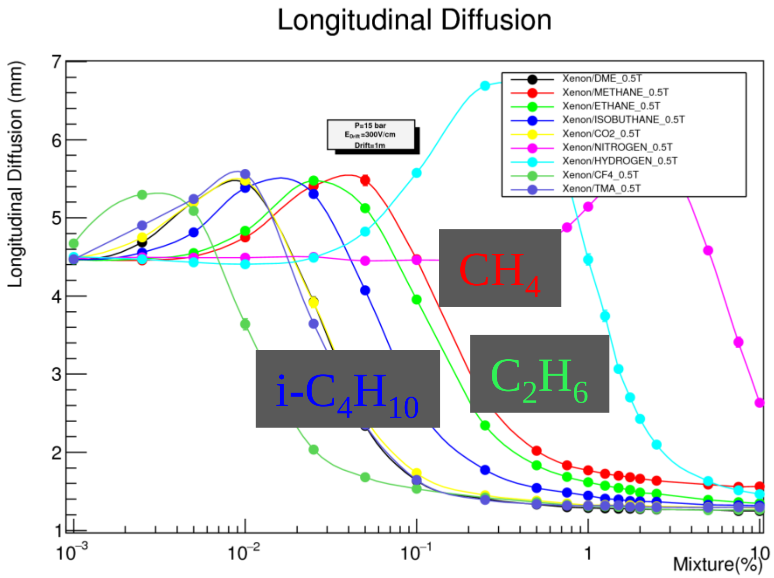
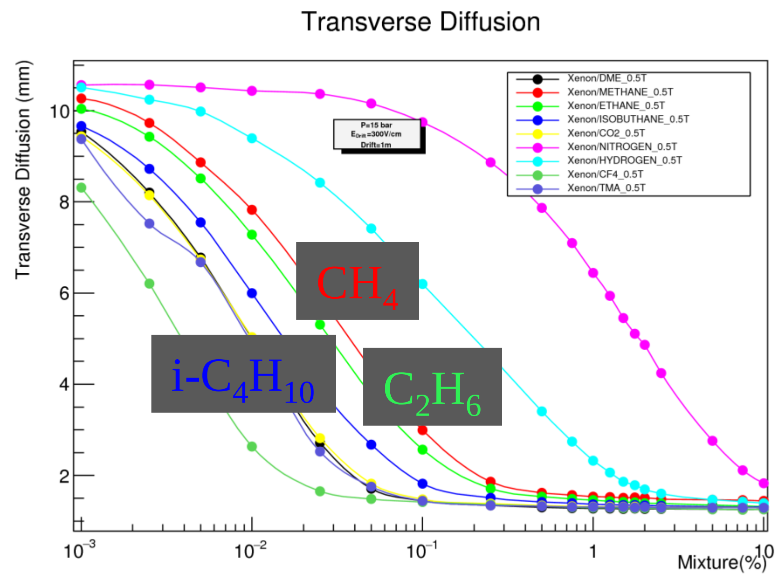
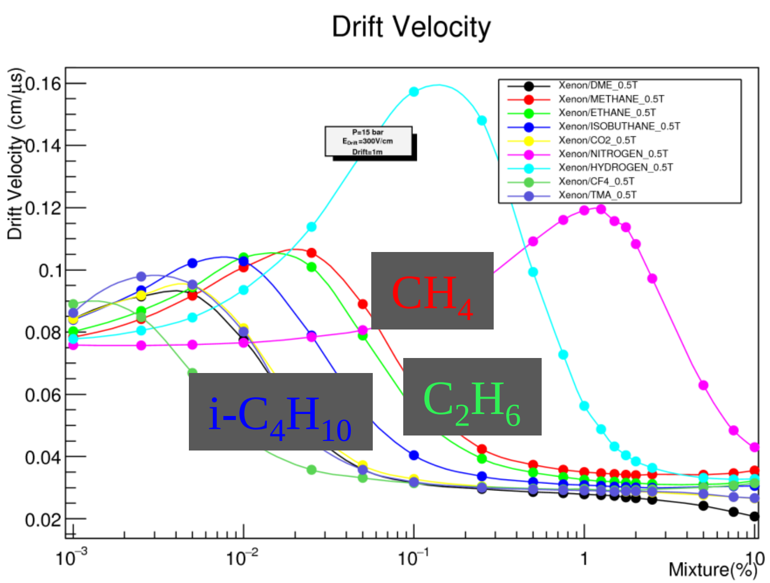
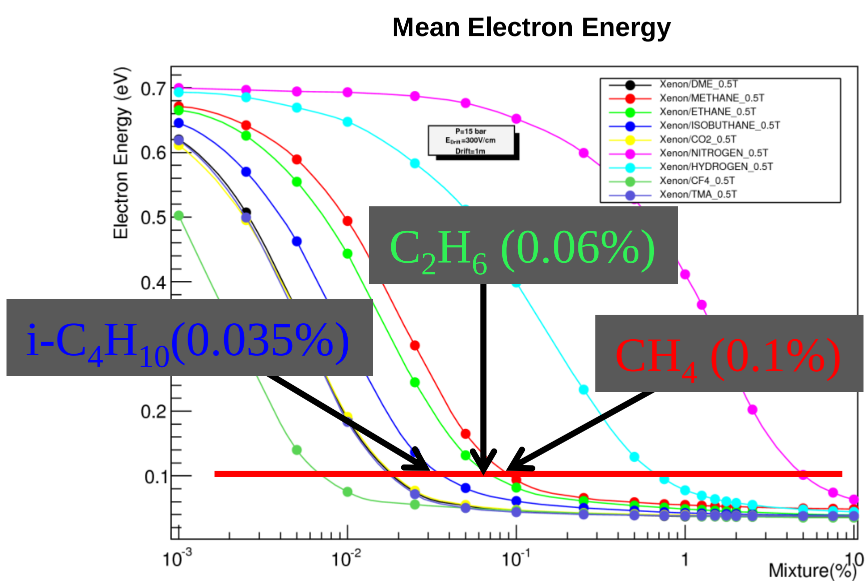








Light transparency

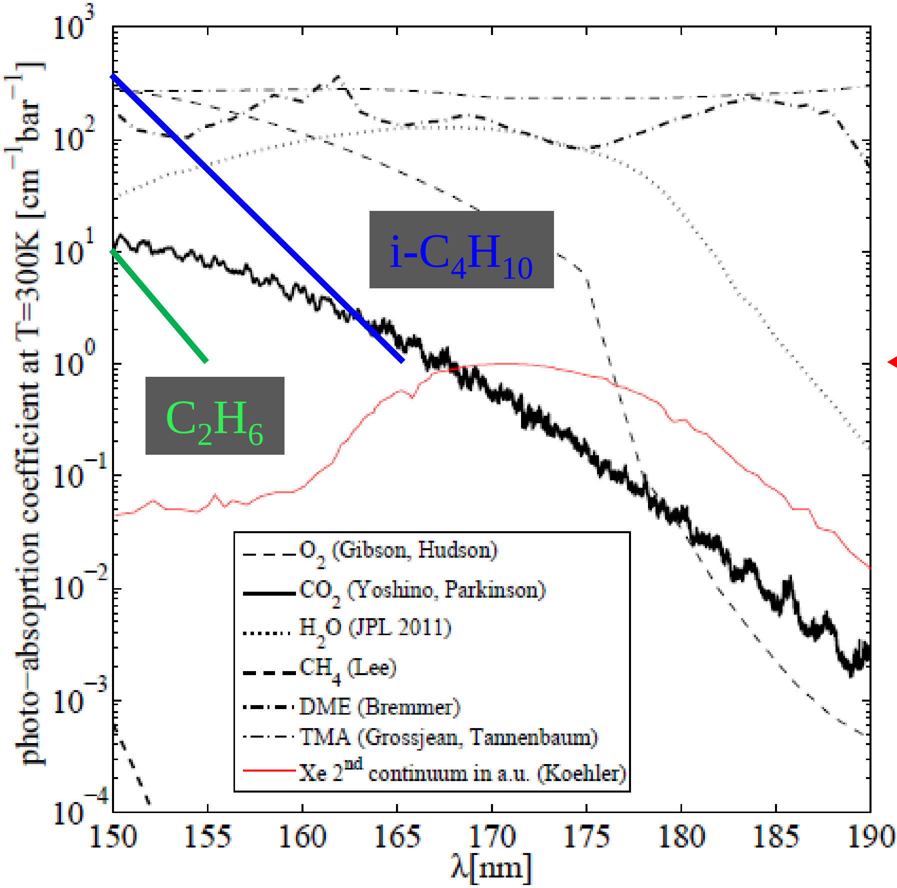


Fig. 1. Compilation of photo-absorption coefficients of some relevant TPC admixtures at around $T = 300$K in the region corresponding to the Xenon 2nd continuum, [9–18]. The reference spectrum from Koehler has been overlaid as a thin continuous line [2]. For H_2, N_2 and CF_4 there is no data in the region shown, and their cross-sections are plausibly orders of magnitude below that of CH_4.

$$\Pi = \frac{1}{P_o} N_o \sigma_a(\lambda)$$

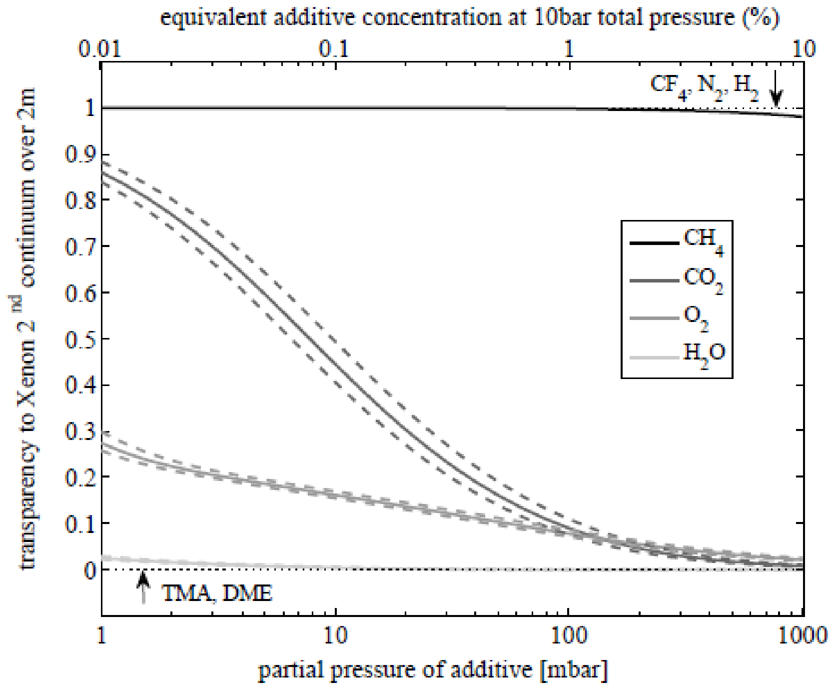
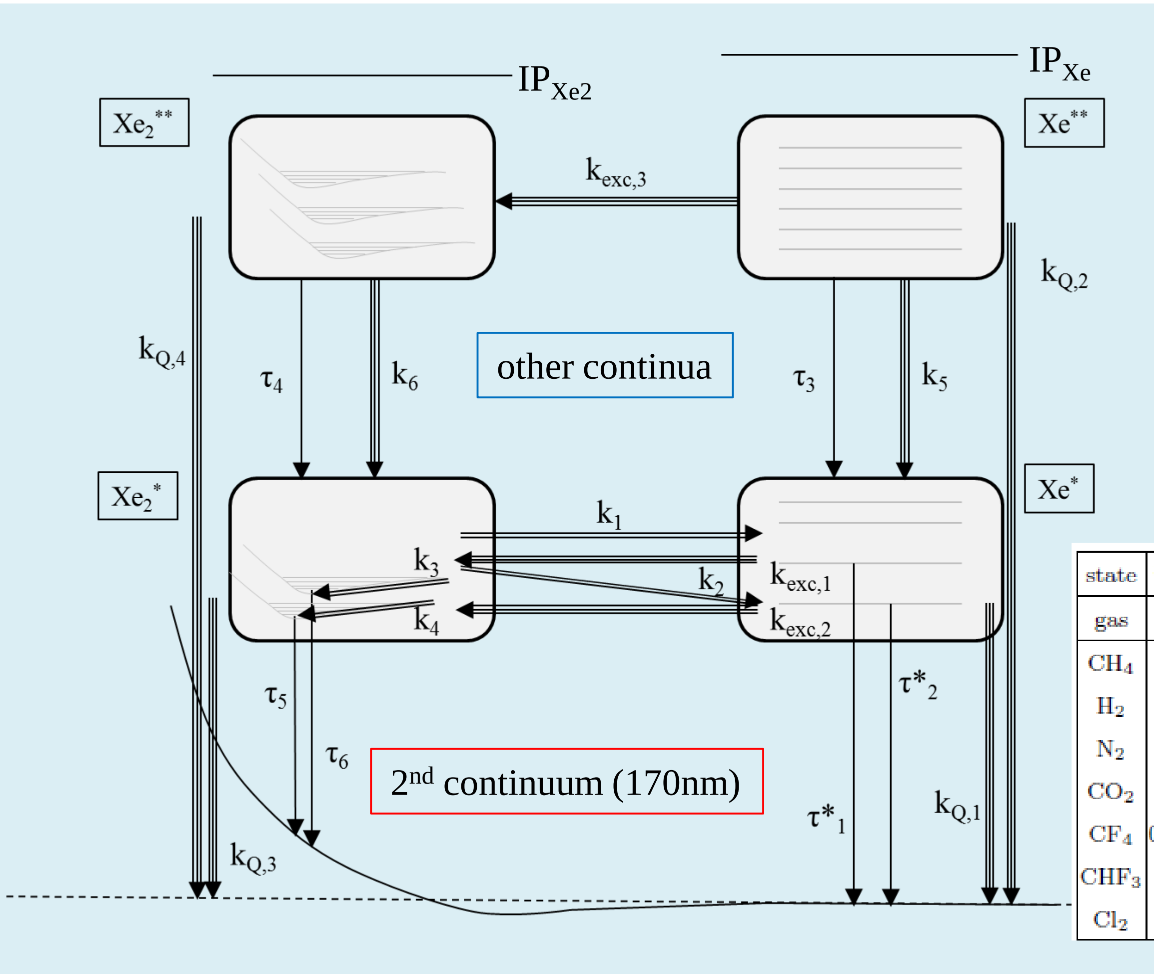


Fig. 2. Estimated transparency to scintillation from Xenon 2nd continuum as a function of partial pressure of the additive, over a 2 meter-long TPC. Dashed lines are obtained assuming 20% errors in the cross-sections.

$$\mathcal{T} \equiv \frac{\int_o^\infty \frac{dN}{d\lambda}\Big|_{2^{nd}} e^{-N\sigma_a(\lambda)L}\, d\lambda}{\int_o^\infty \frac{dN}{d\lambda}\Big|_{2^{nd}}\, d\lambda}$$

Light quenching (generic pathway diagram)



3body

2body

decay

example of main (atomic) quenching reactions

relevant for S$_2$

relevant for S$_1$

state	$^3P_1$(2b)	$^3P_2$(2b)	Xe**(2b)	$^3P_1$(3b)	$^3P_2$(3b)	Xe**(3b)
gas	-	-	-	$k_{Q,1}$	$k_{Q,1}$	$k_{Q,2}$
CH_4	8.3[24]	8.0[25]	87.3^{*4}	81.4^{*3}	81.5[25]	1770^{*5}, 888^{*3}
H_2	0.40[24]	0.40^{*2}	4.21^{*4}	4.07^{*3}	4.07^{*3}	85^{*5}, 43^{*3}
N_2	0.48[24]	0.48^{*2}	5.05^{*4}	4.88^{*3}	4.88^{*3}	102^{*5}, 51^{*3}
CO_2	11.3[24]	11.2[25]	118.4^{*4}	114.0^{*3}	119.0[25]	2400^{*5}, 1200^{*3}
CF_4	0.025[24]	0.025^{*2}	0.26^{*4}	0.25^{*3}	0.25^{*3}	5.27^{*5}, 2.64^{*3}
CHF_3	0.50[24]	0.50^{*2}	5.26[26]	5.1^{*3}	5.1^{*3}	106.6[26]^{*3}
Cl_2	18.0[24]	18.0^{*2}	189.4^{*4}	76.5^{*1},183.1^{*3}	76.5^{*1},183.1^{*3}	3840^{*5}, 1900^{*3}

Most serious difficulties related to **S$_1$**:
- **Distribution of initial excited states?.**
- **Quenching/decay of Xe**, Xe$_2^{**}$ not fully known.**

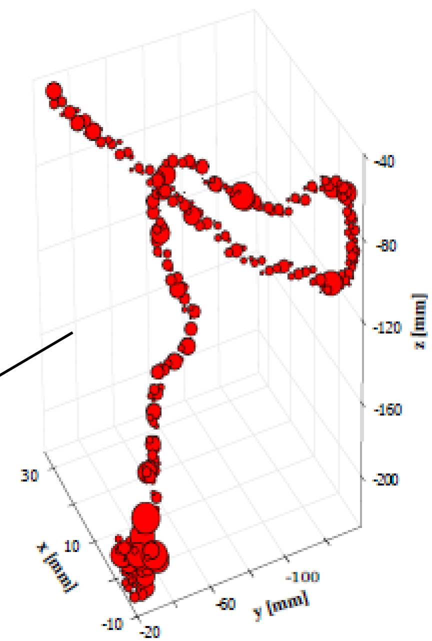
S$_2$ much more robust (dominated by low-lying states):
- **Measurements exist.**

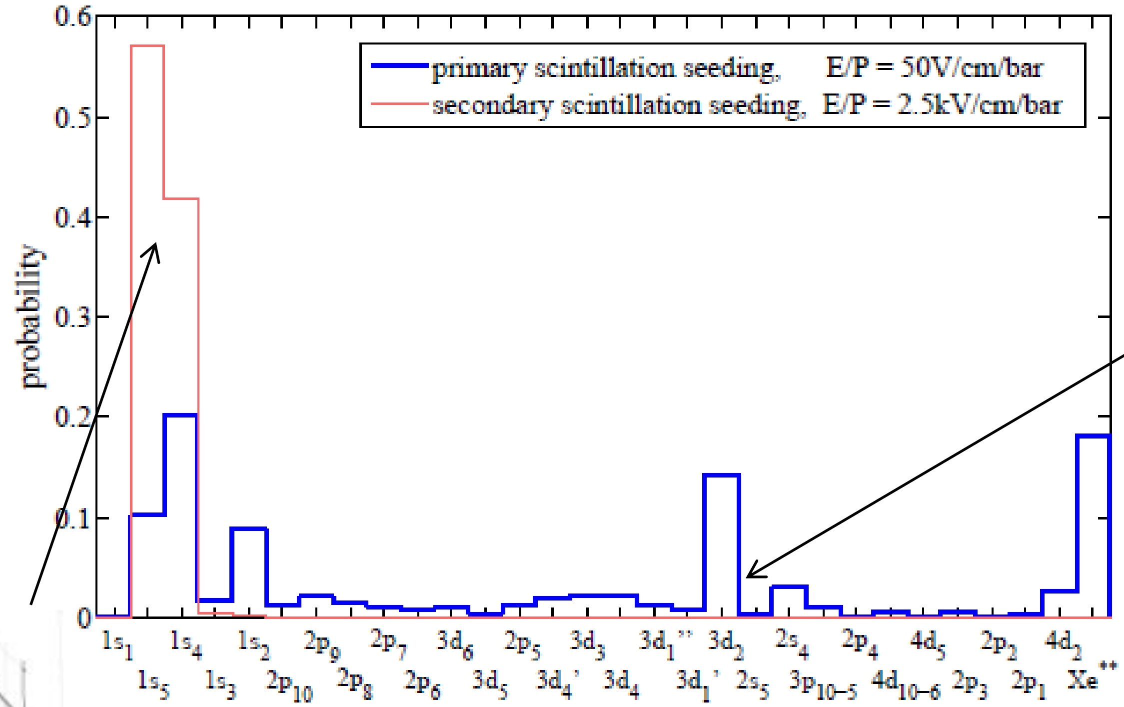
IV. Electron transport + scintillation model

I

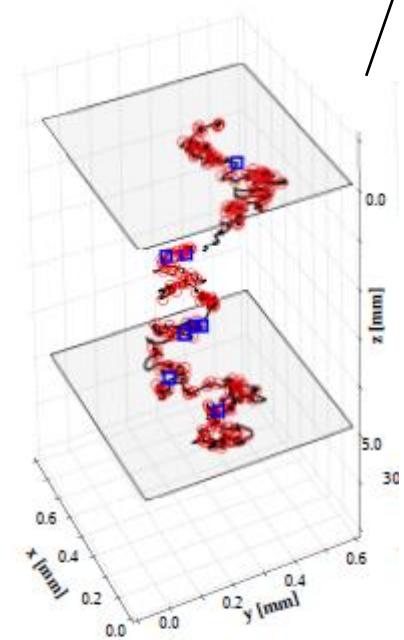
Computation of probability distribution of excited states

Degrad





Garfield++



Computation of atomic cascade

II

decay constant

2-body collision rates

3-body collision rates

state (Paschen)	state (Racah)	energy [eV]	$\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]	K_3@1bar [ns^{-1}]
$1s_1$	-	0.000	-	-	-
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}	0.1465
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	-	0.0855
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224	-
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	2.4954	-
$2p_{10}$	$6p[1/2]_1$	9.580	0.026	3.7802	-
$2p_9$	$6p[5/2]_2$	9.686	0.027	2.7425	-
$2p_8$	$6p[5/2]_3$	9.721	0.031	1.8036	-
$2p_7$	$6p[3/2]_1$	9.789	0.028	4.3979	-
$2p_6$	$6p[3/2]_2$	9.821	0.036	2.0062	-
$3d_6$	$5d[1/2]_0$	9.890	4.36×10^{-3}	9.7649	-
$3d_5$	$5d[1/2]_1$	9.917	$0.015/n_H$	4.8328	-
$2p_5$	$6p[1/2]_0$	9.933	0.031	0.1599	0.4273
$3d'_4$	$5d[7/2]_4$	9.943	4.34×10^{-3}	4.8676	-
$3d_3$	$5d[3/2]_2$	9.959	8.16×10^{-3}	4.8664	
$3d_4$	$5d[7/2]_3$	10.039	7.34×10^{-3}	4.8510	
$3d''_1$	$5d[5/2]_2$	10.157	1.21×10^{-3}	4.8649	
$3d'_1$	$5d[5/2]_3$	10.220	1.39×10^{-3}	4.8639	
$3d_2$	$5d[3/2]_1$	10.401	$3.04\times10^{-3}/n_H$	1.3637	
$2s_5$	$7s[3/2]_2$	10.562	0.018	4.9415	
$2s_4$	$7s[3/2]_1$	10.593	$0.178/n_H$	4.9415	
$3p^*_{10-5}$	-	10.902	0.010	12.6008	
$2p_4$	$6p[3/2]_1$	10.958	0.024	10.3277	
$4d^*_{10-6,4,3}$	-	10.971	0.014	5.9298	-
$4d_5$	$6d[1/2]_1$	10.979	0.018	4.8426	-
$2p_3$	$6p[3/2]_2$	11.055	0.036	11.6125	-
$2p_2$	$6p[1/2]_1$	11.069	0.033	10.3277	-
$2p_1$	$6p[1/2]_0$	11.141	0.027	10.4018	-
$4d_2$	$6d[3/2]_1$	11.163	$0.716/n_H$	4.8674	-
Xe^{**}	-	11.7	-	12.35	-

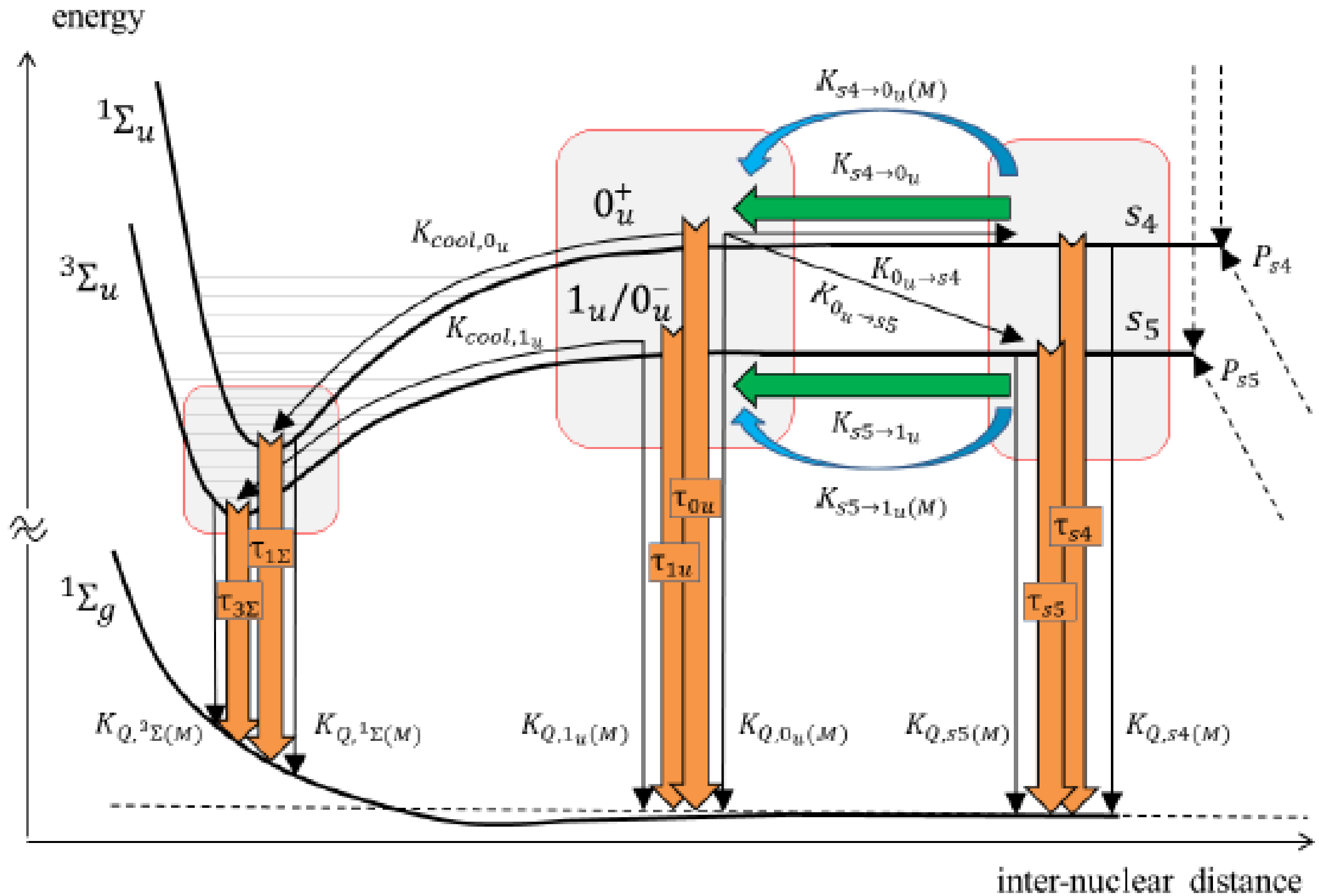
each value represents a vector!

-	$1s_1$	$1s_5$	$1s_4$	$1s_3$	$1s_2$	$2p_{10}$	$2p_9$	$2p_8$	$2p_7$	$2p_6$
$1s_1$	-	0	0	0	0	0	0	0	0	0
$1s_5$	$1^{(1)}$	-	0	0	0	0	0	0	0	0
$1s_4$	0	0	-	0	0	0	0	0	0	0
$1s_3$	0	$0.11^{(2,3)}$	$0.89^{(2,3)}$	-	0	0	0	0	0	0
$1s_2$	0	$0.010^{(2,3)}$	$0.079^{(2,3)}$	$0.247^{(3)}$	-	$0.663^{(4)}$	0	0	0	0
$2p_{10}$	0	$0.014^{(3)}$	$0.116^{(3)}$	$0.216^{(4)}$	$0.654^{(4)}$	-	0	0	0	0
$2p_9$	0	0	0	$0.3604^{(4)}$	$0.1351^{(3)}$	$0.405^{(4)}$	-	$0.099^{(4)}$	0	0
$2p_8$	0	0	0	$0.178^{(3)}$	$0.110^{(3)}$	$0.245^{(3)}$	$0.466^{(3)}$	-	0	0
$2p_7$	0	0	0	$0.348^{(3)}$	$0^{(2)}$	$0.011^{(2)}$	$0.067^{(2)}$	$0.539^{(2)}$	-	$0.034^{(3)}$
$2p_6$	0	0	0	$0.234^{(3)}$	$0.001^{(2)}$	$0.001^{(2)}$	$0.345^{(3)}$	$0.259^{(3)}$	$0.161^{(3)}$	-

III

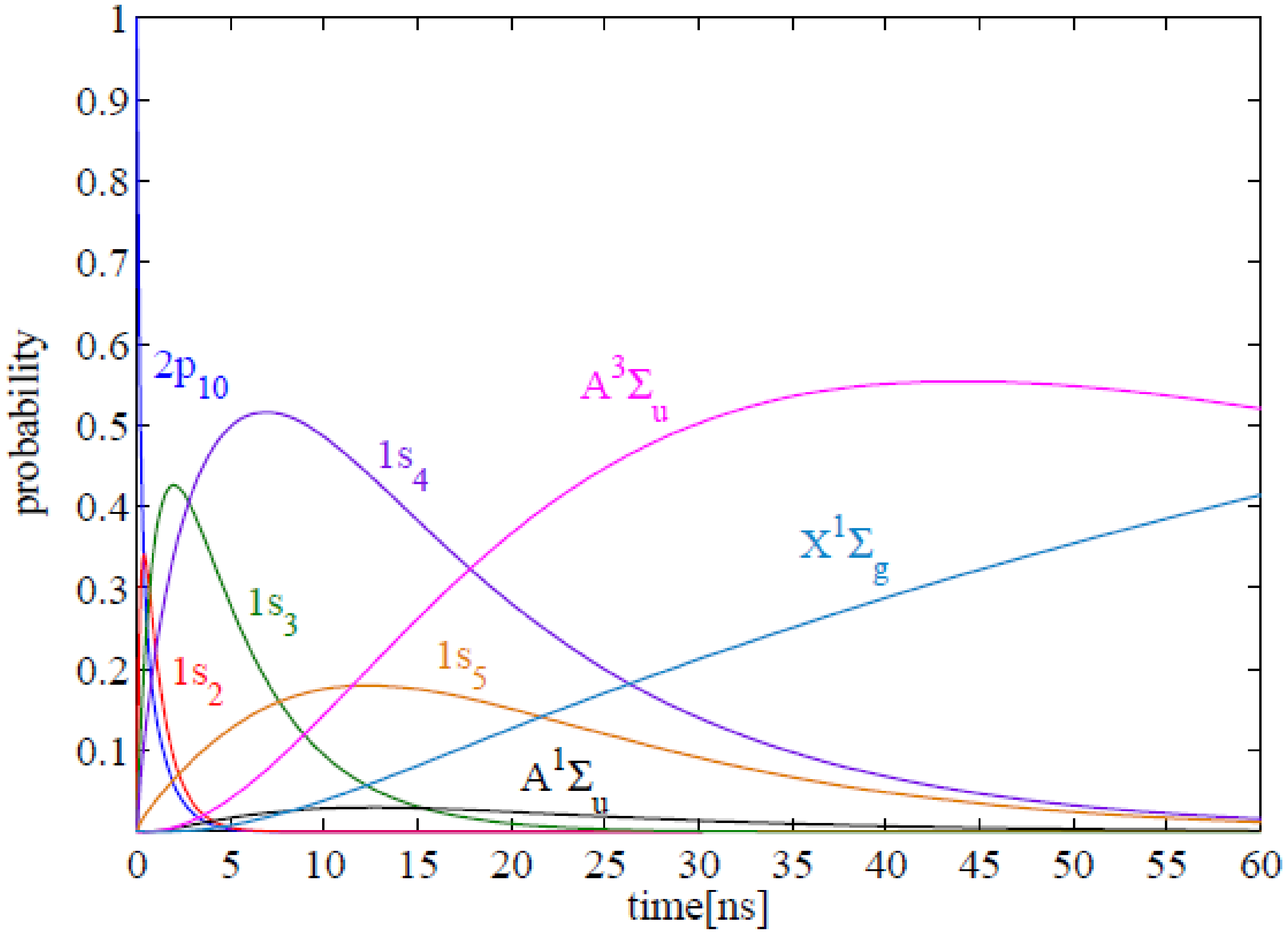
Excimer pathways

(analogous for $2p_5$ and Xe**)



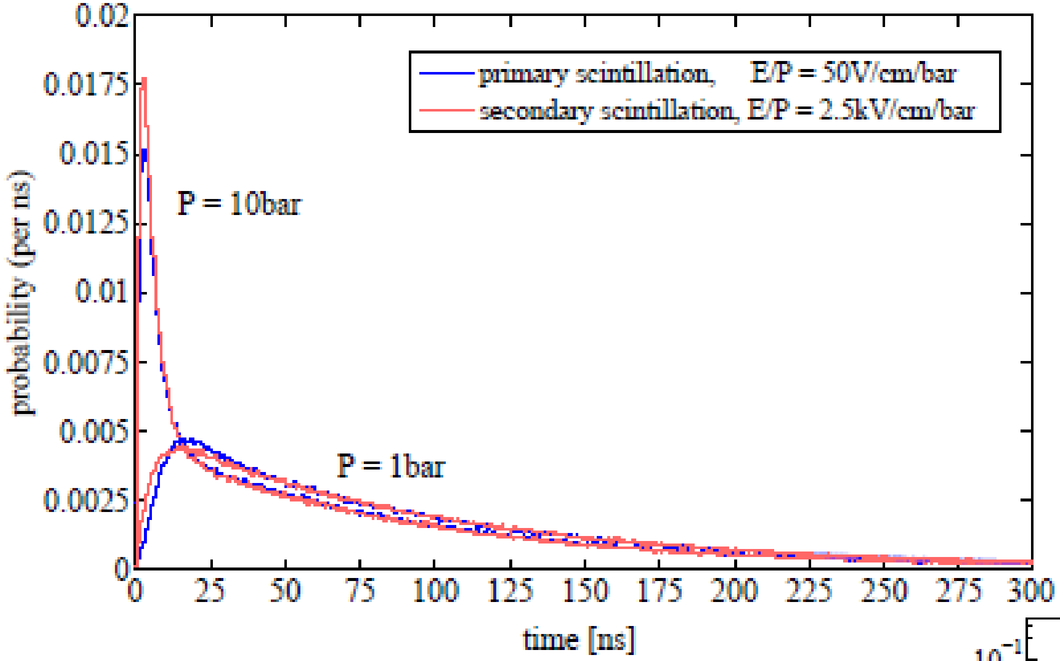
$\tau_{^3\Sigma}$	100 ns [1]	$K_{Q,^3\Sigma(M)}$	$11.12\ \mathrm{ns}^{-1}$	$K_{s_5\to 1_u}$	$0.1465\ \mathrm{ns}^{-1}$ [1]	$K_{s_5\to 1_u(M)}$	$116\ \mathrm{ns}^{-1}$
$\tau_{^1\Sigma}$	4.55 ns [1]	$K_{Q,^1\Sigma(M)}$	$12.85\ \mathrm{ns}^{-1}$	$K_{s_4\to 0_u}$	$0.0855\ \mathrm{ns}^{-1}$ [1]	$K_{s_4\to 0_u(M)}$	$116\ \mathrm{ns}^{-1}$ [6]
τ_{1_u}	40 ns [1]	$K_{Q,1_u(M)}$	$11.12\ \mathrm{ns}^{-1}$	$K_{0_u\to s_4}$	$1.43\ \mathrm{ns}^{-1}$ [1]		
τ_{0_u}	5 ns [1]	$K_{Q,0_u(M)}$	$12.85\ \mathrm{ns}^{-1}$	$K_{0_u\to s_5}$	$6.42\ \mathrm{ns}^{-1}$ [1]		
τ_{s_5}	42 s [2]	$K_{Q,s_5(M)}$	$11.12\ \mathrm{ns}^{-1}$ [4]	$K_{cool,0_u}$	$1.72\ \mathrm{ns}^{-1}$ [1]		
τ_{s_4}	$3.56 \times n_H$ ns [3]	$K_{Q,s_4(M)}$	$12.85\ \mathrm{ns}^{-1}$ [5]	$K_{cool,1_u}$	$1.72\ \mathrm{ns}^{-1}$ [1]		

Example of light production code (population evolution from $2p_{10}$)

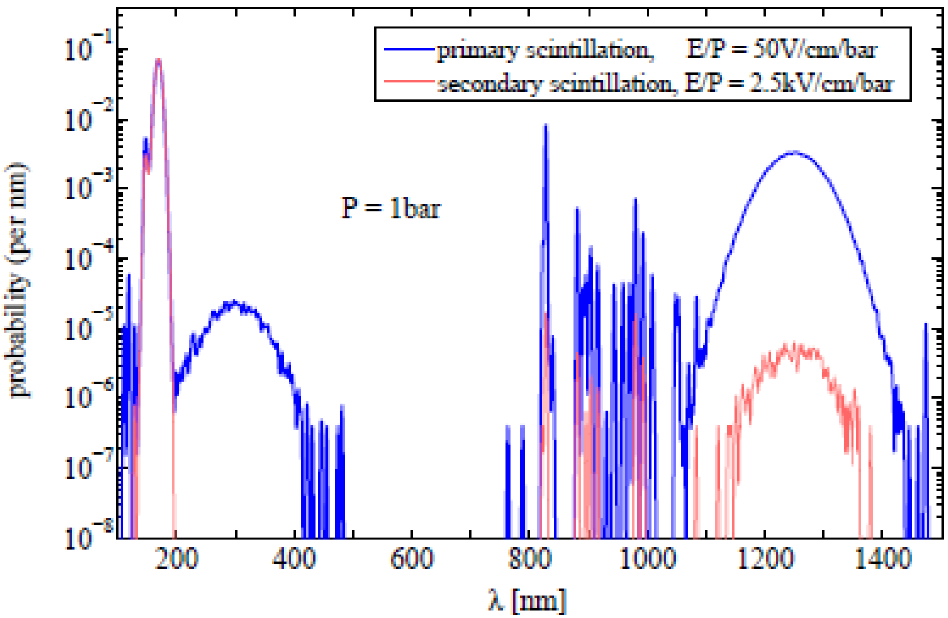


Example of electron transport + light production code

time distributions

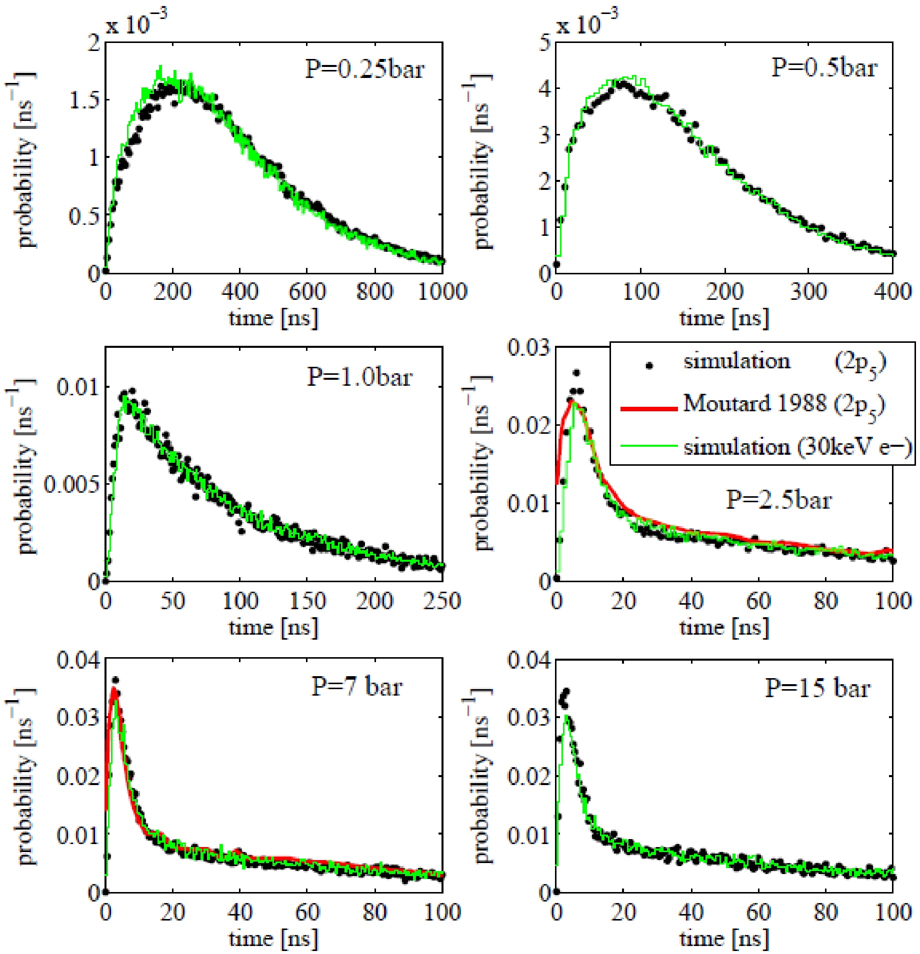


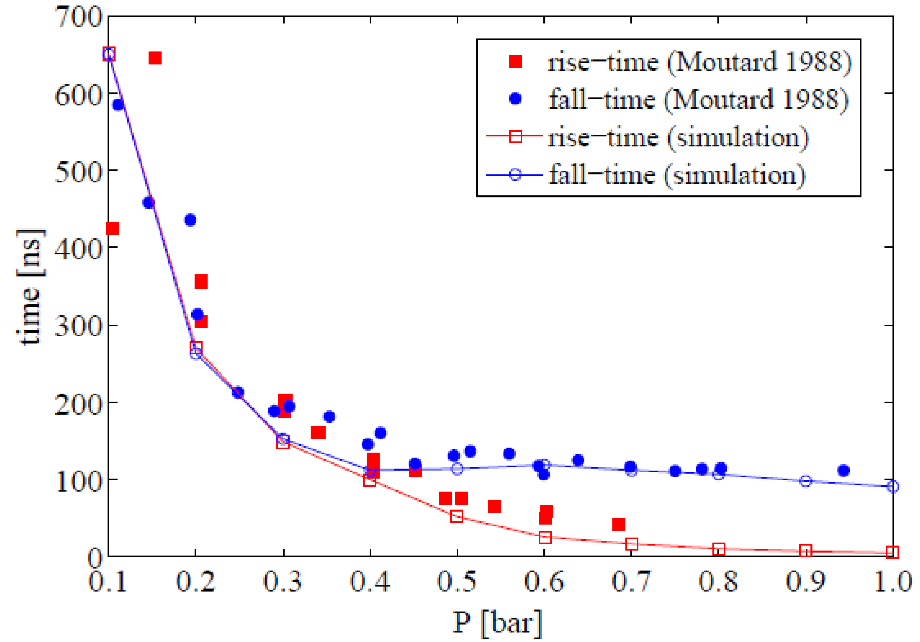
energy spectra



V. Comparison with pure xenon data

Time distributions



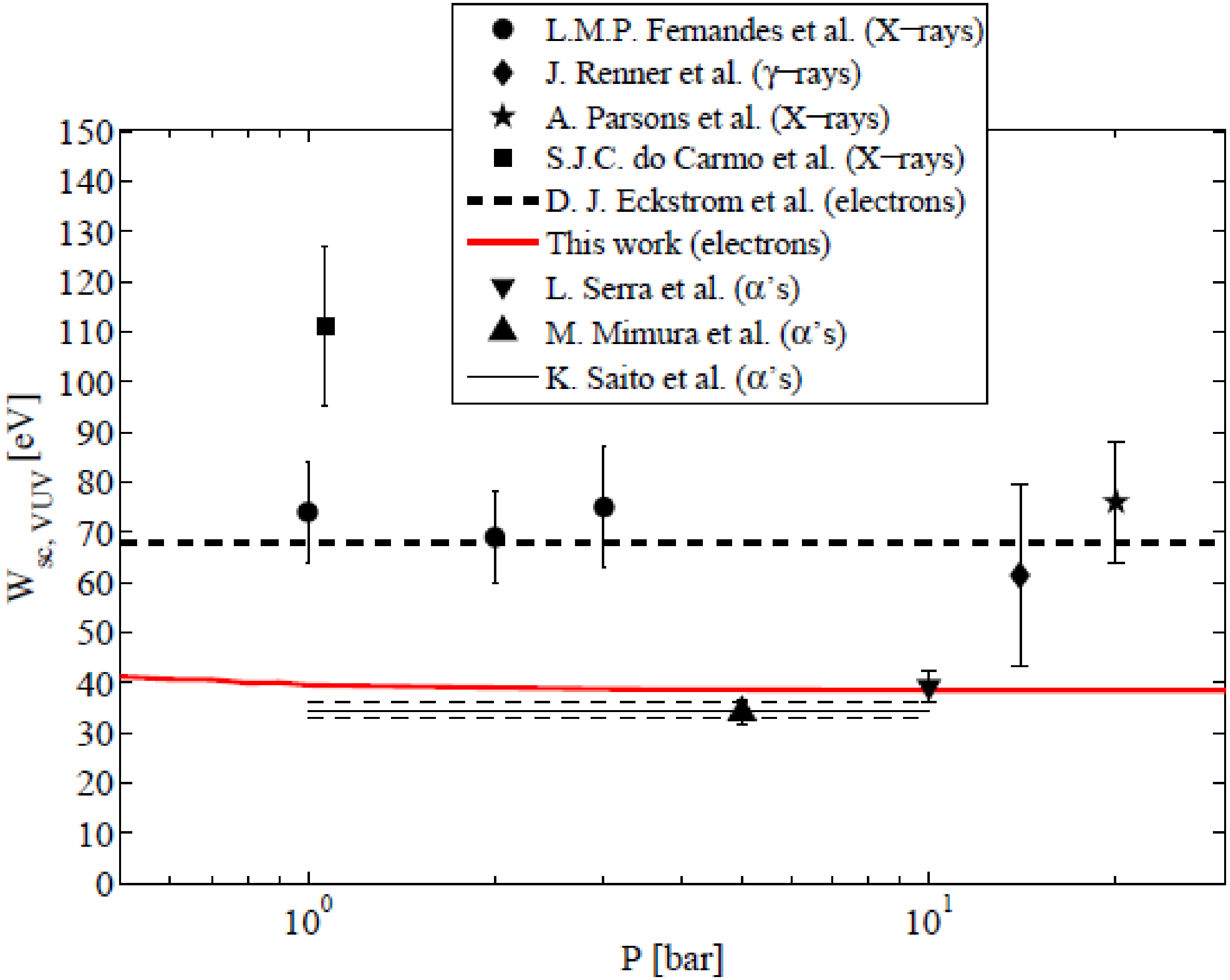


$$\left.\frac{dN_\gamma}{dt}\right|_{2^{\mathrm{nd}}} \simeq a e^{-t/t_f} - b e^{-t/t_r}, \qquad (P \lesssim 0.8 \text{ bar})$$

$$\left.\frac{dN_\gamma}{dt}\right|_{2^{\mathrm{nd}}} \simeq a e^{-t/t_{f,fast}} + b e^{-t/t_{f,slow}}, \qquad (P \gtrsim 2.5 \text{ bar})$$

Yields

VUV region



IR region

simulated

$W_{sc,IR} = 86\text{eV at } 2.5\text{bar}$

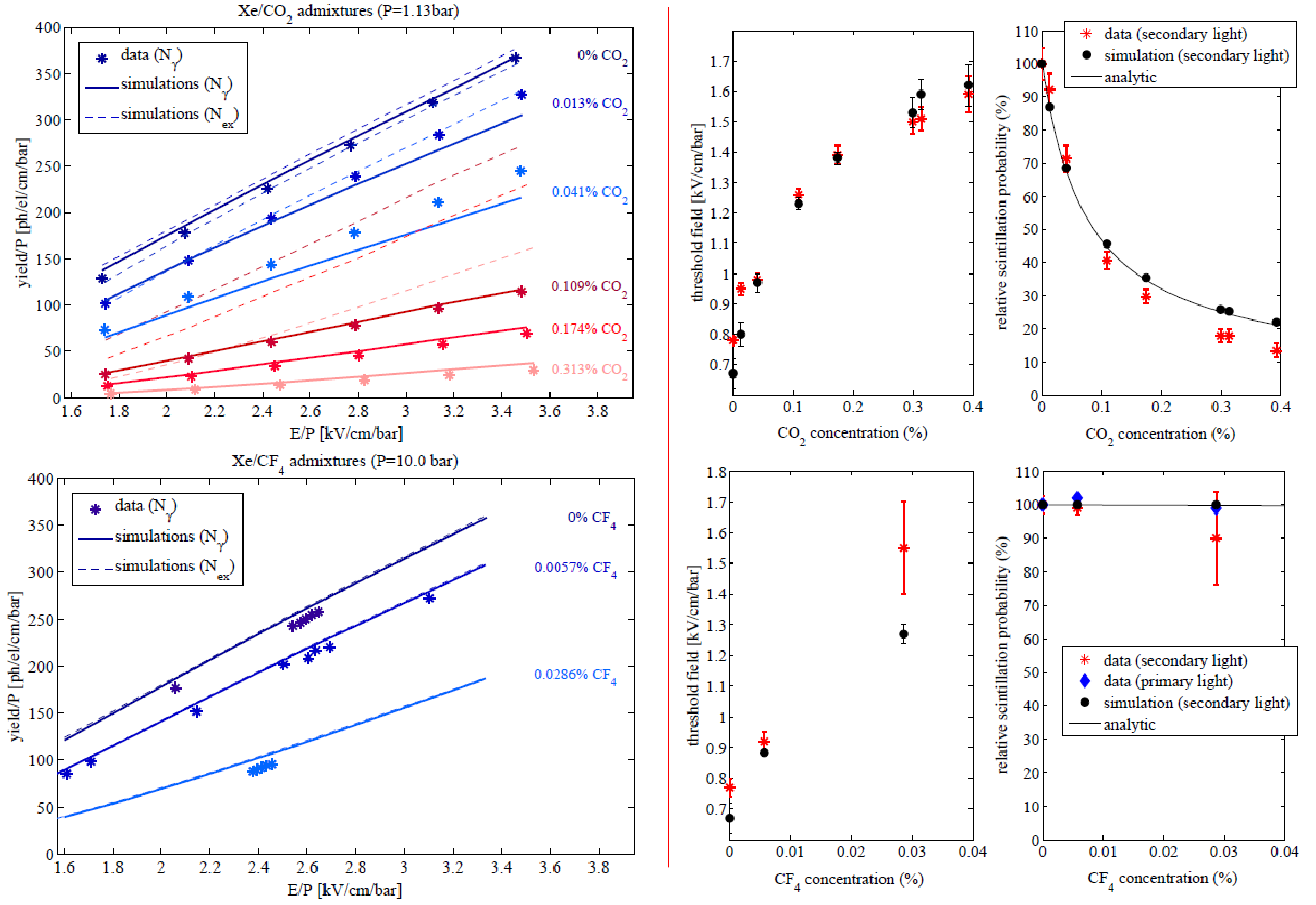
measured (α's)

$W_{sc,IR} < 48 \pm 7 \text{ eV}$

VI. Comparison with xenon + additives

Electroluminescence (yield)

$$\mathcal{P}_{scin} = 1 - \mathcal{P}_Q = \frac{N_\gamma}{N_{ex}}$$



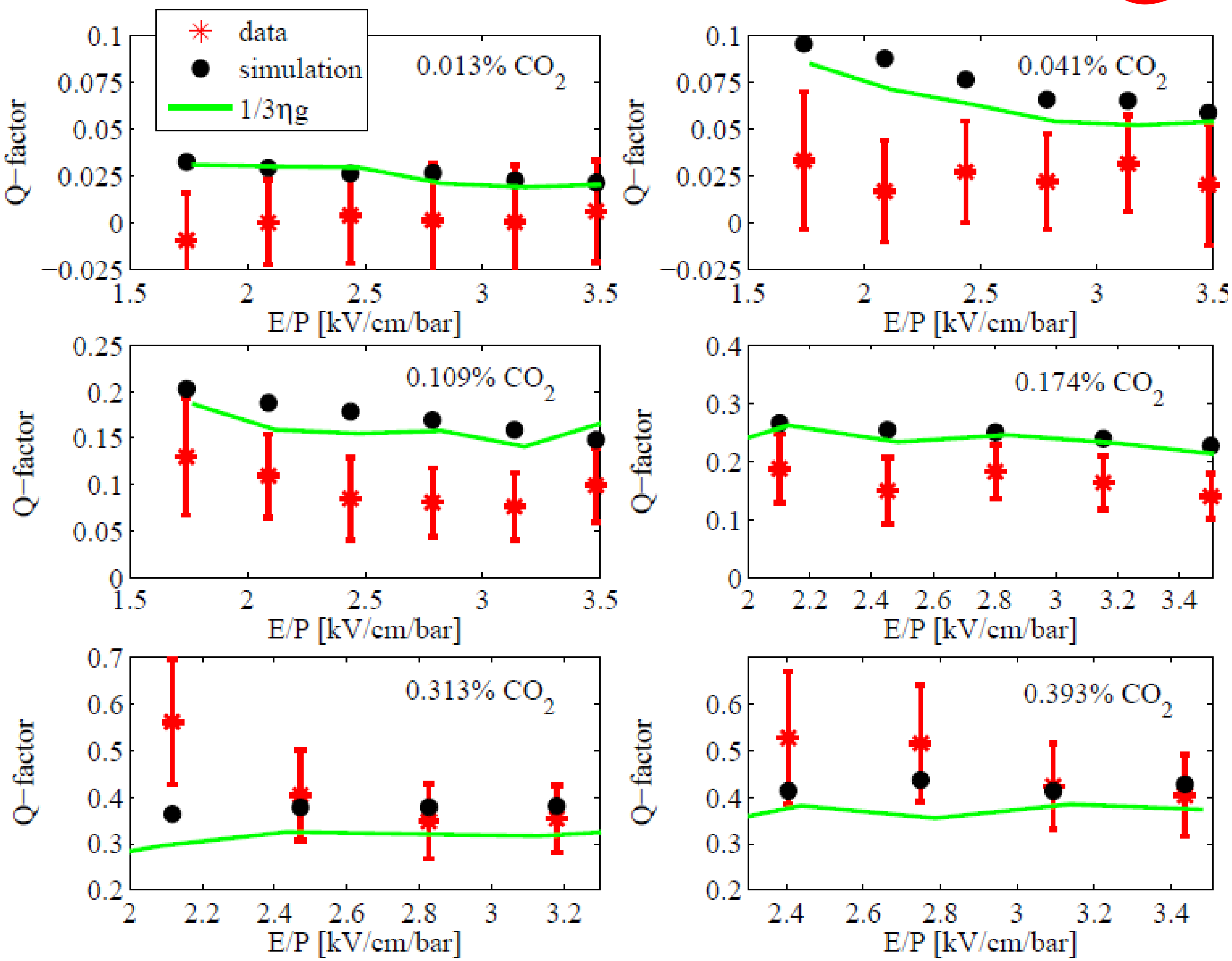
Electroluminescence (light fluctuations, Q)

$$resolution = 2.35\sqrt{F + Q\frac{W_I}{\varepsilon}}$$

$$Q = Q_{ex} + Q_{\mathcal{P}_{scin}} + Q_{att}$$

$$Q_{att} \simeq \frac{1}{3}\eta g$$

$$Q_{\mathcal{P}_{scin}} = \frac{1}{N_\gamma}\mathcal{P}_{scin}(1-\mathcal{P}_{scin})$$



Conclusions

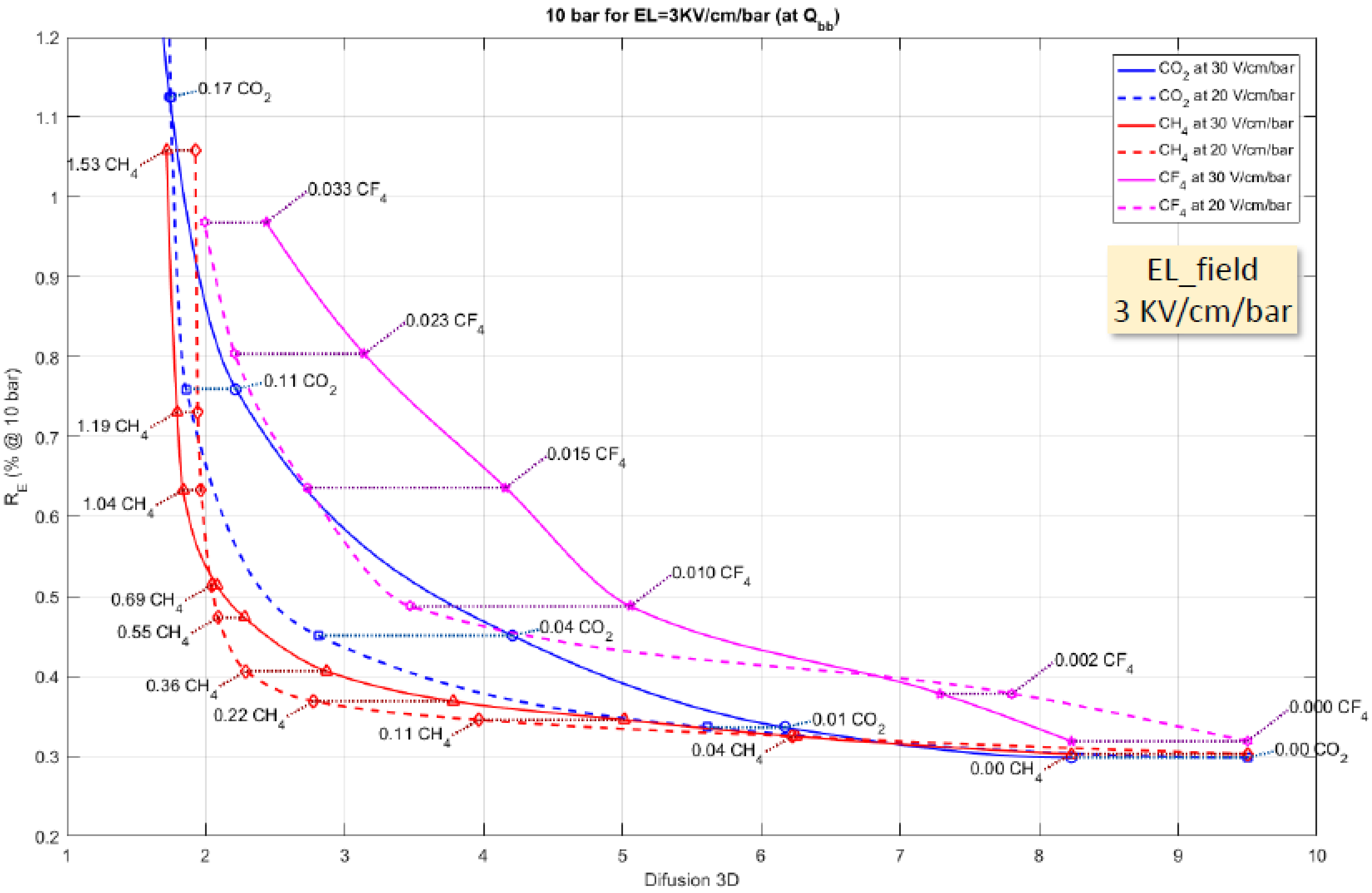
- A new microscopic simulation for photon and electron transport in gaseous Xenon has been developed inside the NEXT collaboration.
- It can compute the primary and secondary scintillation stemming from X, γ-ray and high energy electron interactions (1keV to several MeV).
- It provides the time and spectral characteristics, in the range 150nm-1500nm.
- It can describe the effect of molecular additives and its impact on the light yield.
- It has shown to be a formidable tool for the R&D on low-diffusion gases within NEXT.

Outlook

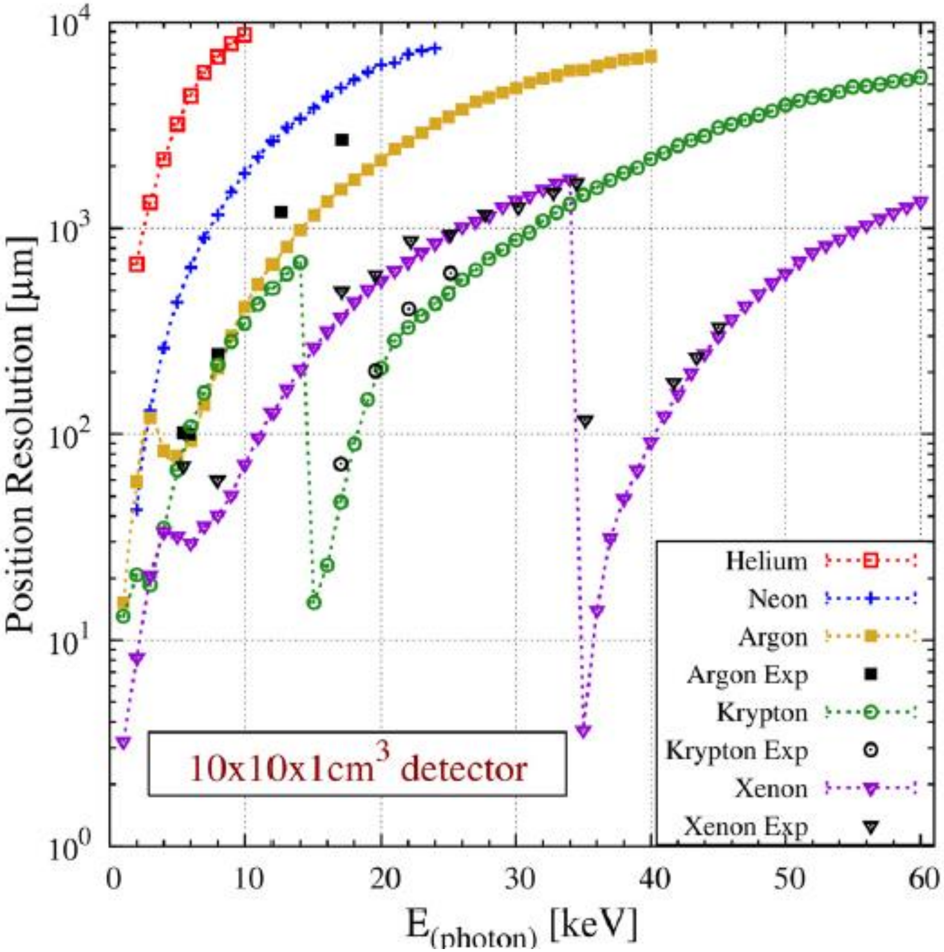
- This framework was developed to solve a concrete technological problem…
- But the authors are interested in tackling a variety of other admixtures used for optical TPC. The new landscape is enormous, so work will continue depending on the interest and the available resources.

VI. Appendix

A low diffusion/light-preserving gas in action



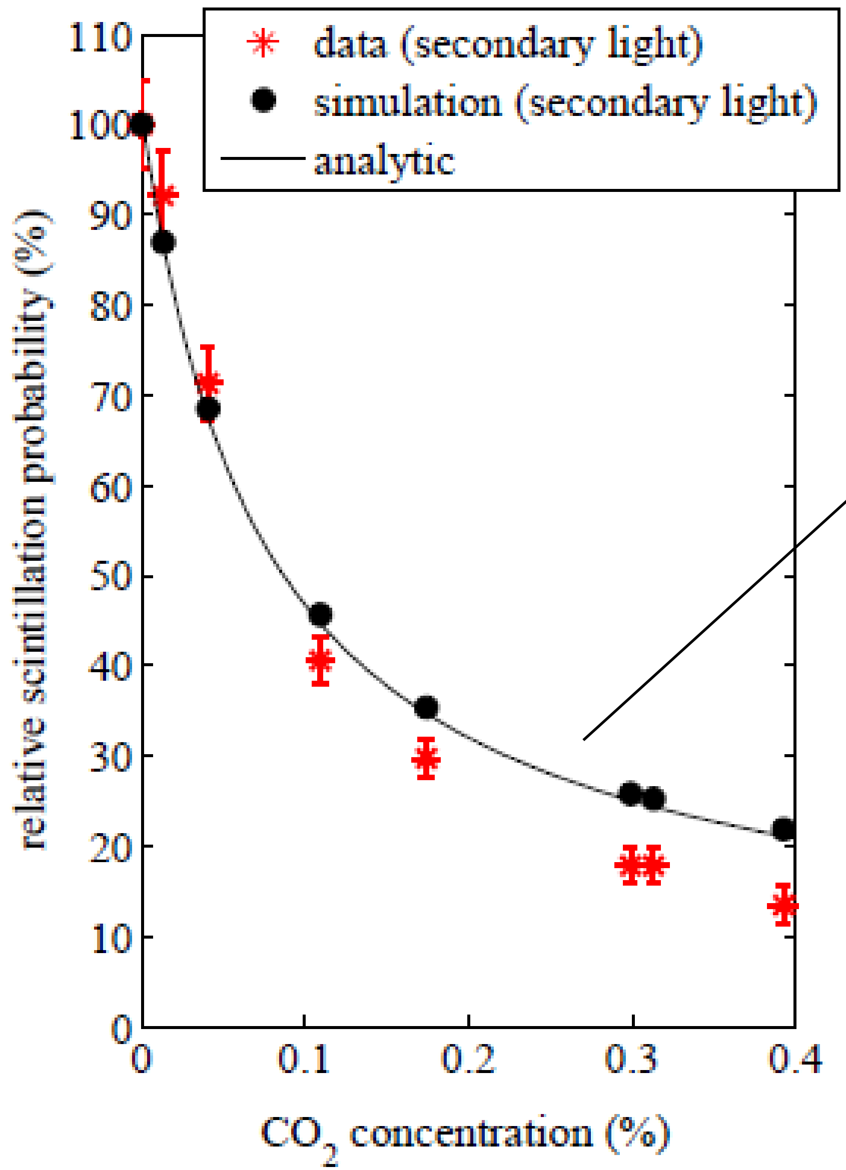
Electron cloud size in Degrad



Physics Letters B 741 (2015) 272–275

arXiv:1605.06256v3 [physics.ins-det]

Xe-CO_2



$\sim 1/(1+\tau K_2 f)$!

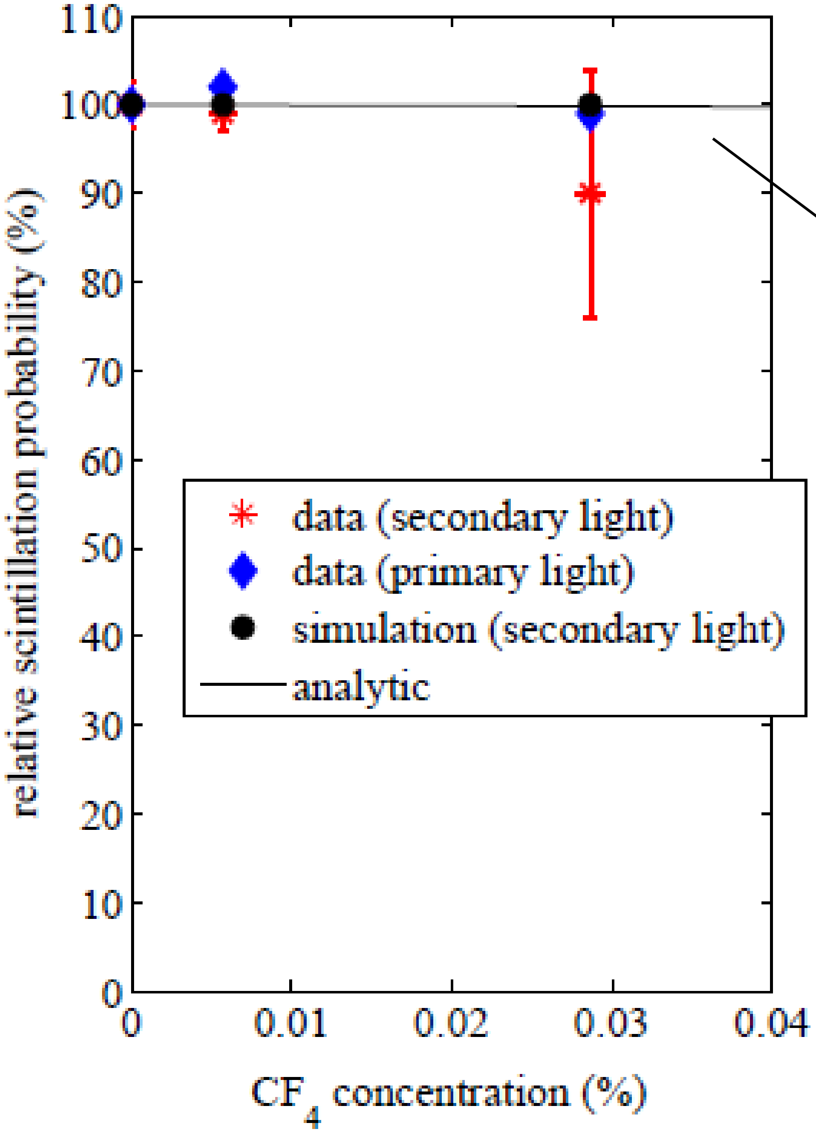
if assuming $\tau = \tau_{3\Sigma}$

a fit gives: $K_2 = 11.20 \pm 1.0 \text{ ns}^{-1}$

The quenching rate of s_5 state in CO_2 is:

$K_{Q,s_5(M)} = 11.12 \text{ ns}^{-1}$!

Xe-CF_4



$$\sim 1/(1+\tau K_2 f)\ !$$

if assuming $\tau = \tau_{3\Sigma}$

and the quenching rate of s_5 state in CF_4:

$$K_{Q,s_5(M)} = 0.074 \text{ ns}^{-1}$$

Predicts a 0.3% scintillation drop in the range of concentrations shown…

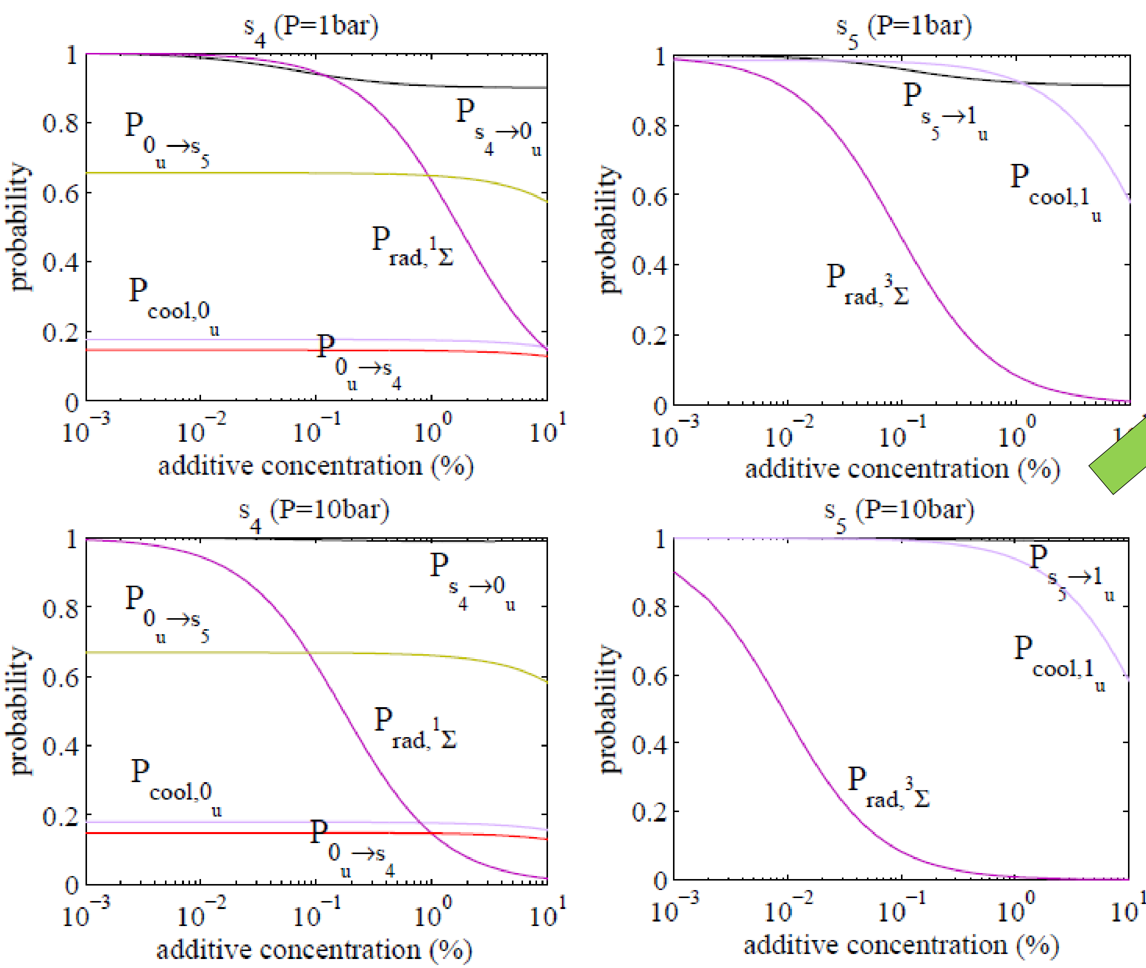
An analytic picture… and a simple one (I)

$$\mathcal{P}_{scin,s_4} = \frac{\mathcal{P}_{pop,s_4} \cdot \mathcal{P}_{s_4\to 0_u}}{1 - \mathcal{P}_{s_4\to 0_u} \cdot \mathcal{P}_{0_u\to s_4}} \times$$

$$\left(\mathcal{P}_{cool,0_u} \cdot \mathcal{P}_{rad,{}^1\Sigma} + \mathcal{P}_{0_u\to s_5} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,{}^3\Sigma}\right)$$

$$\mathcal{P}_{scin,s_5} = \mathcal{P}_{pop,s_5} \cdot \mathcal{P}_{s_5\to 1_u} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,{}^3\Sigma}$$

$$\mathcal{P}_{scin} = \mathcal{P}_{scin,s_4} + \mathcal{P}_{scin,s_5}$$



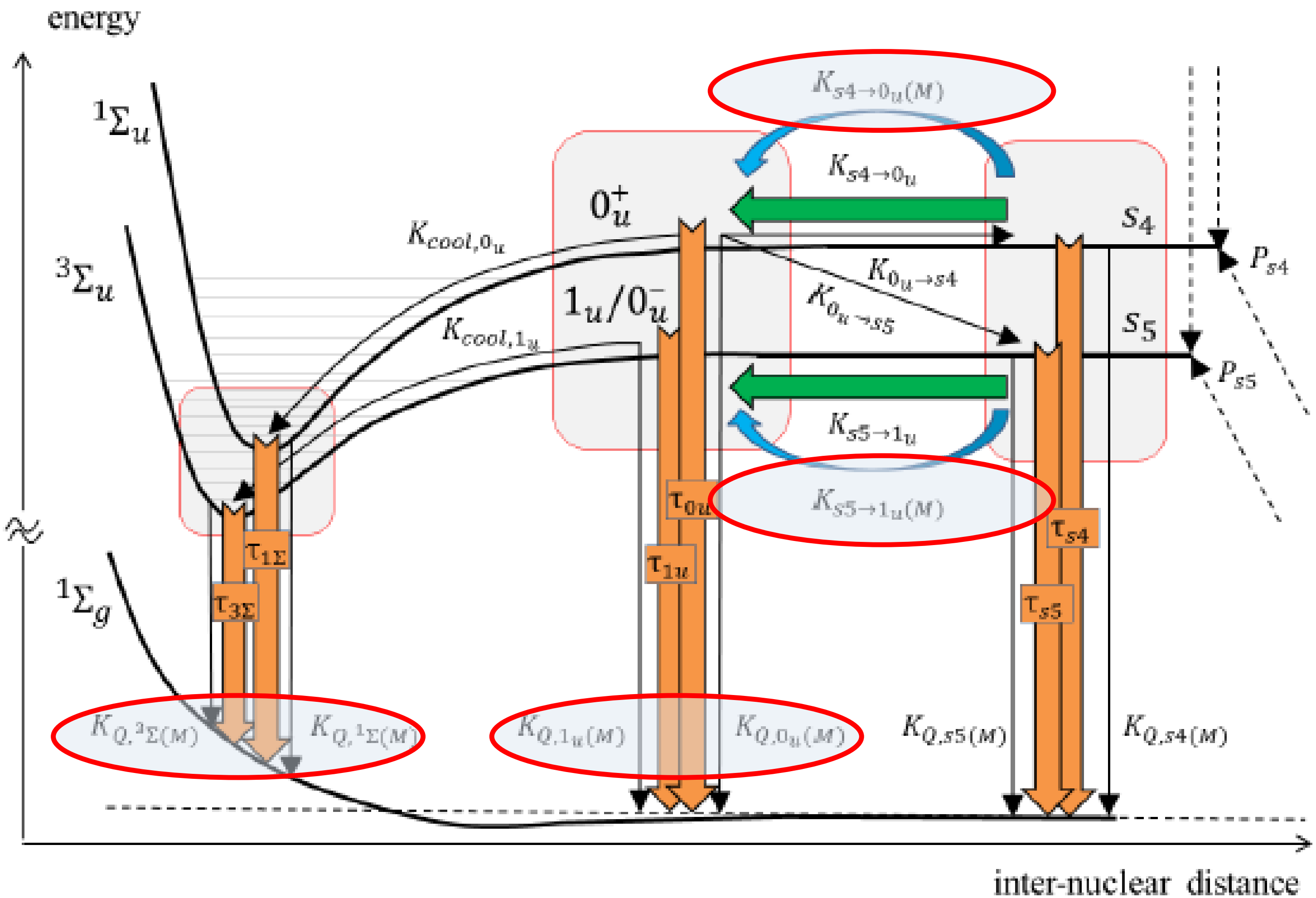
$$F_1 \simeq 0.1 \qquad F_3 \simeq 0.9$$

$$\boxed{\mathcal{P}_{scin} \simeq \frac{F_1}{1 + f n \tau_{{}^1\Sigma} K_{Q,{}^1\Sigma}} + \frac{F_3}{1 + f n \tau_{{}^3\Sigma} K_{Q,{}^3\Sigma}}}$$

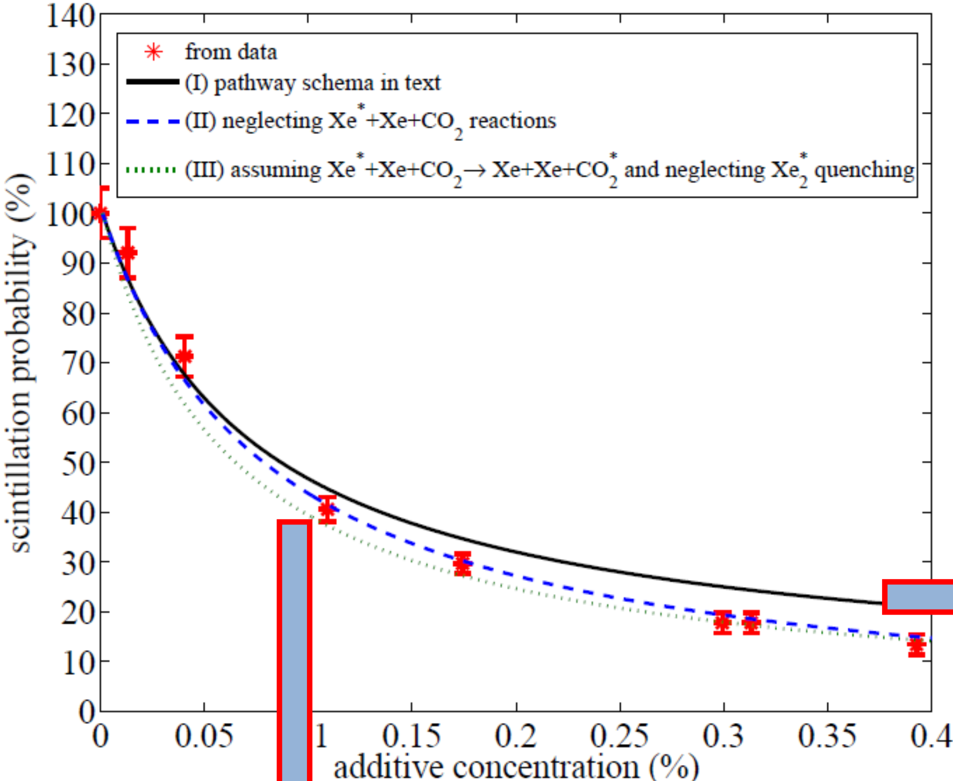
$$n = P/P_o$$

Indeed: dominance of triplet state scintillation above 1bar!

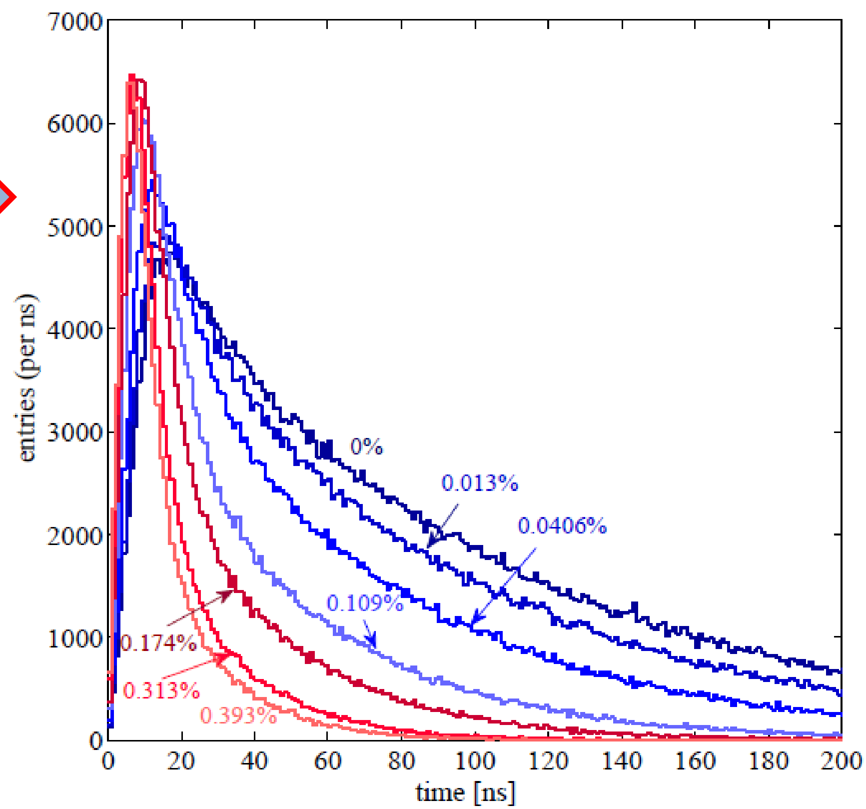
Ambiguities in the scintillation model (I)



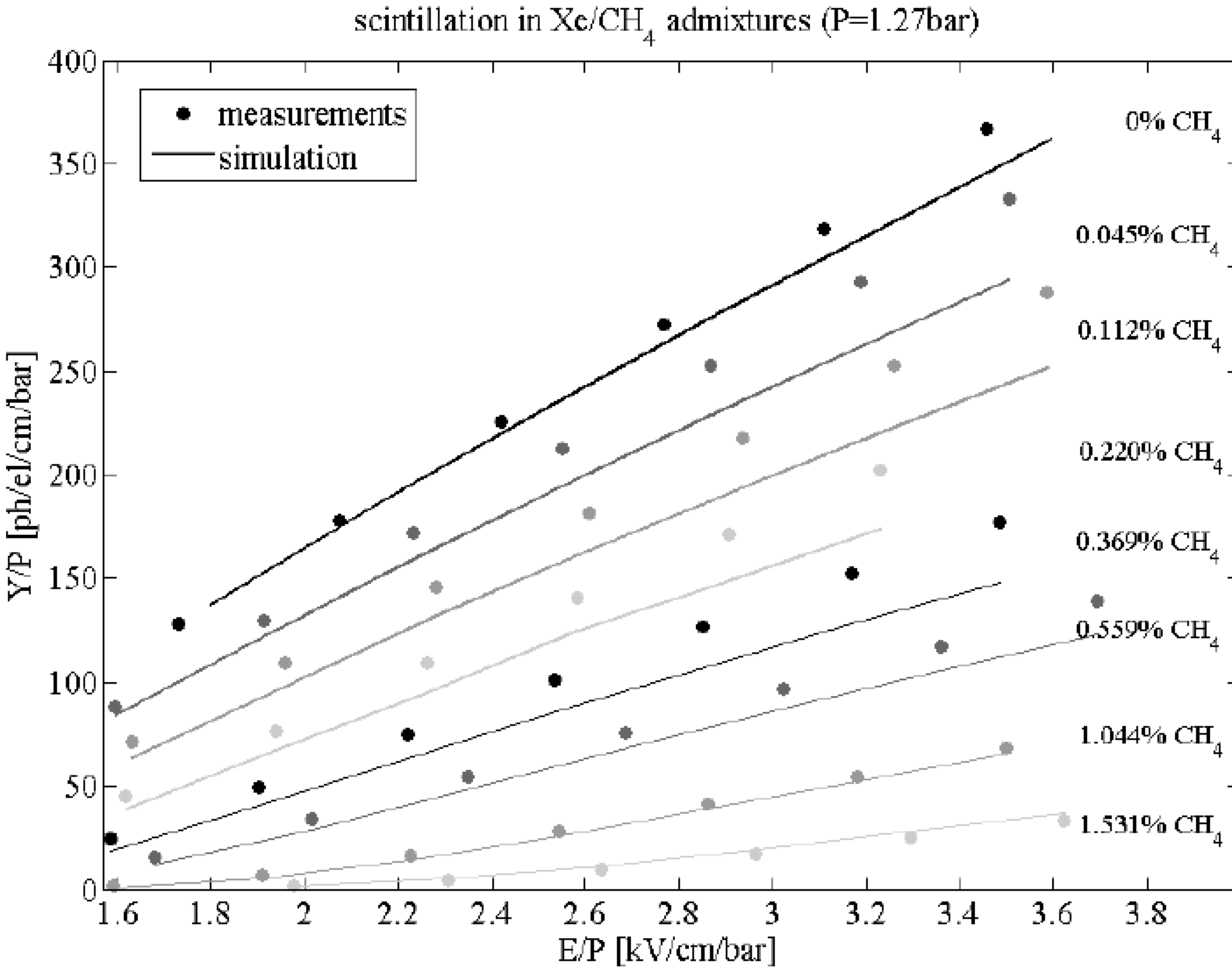
Ambiguities in the scintillation model (II)



default model used in simulations



model by J. Escada
(predicts no pressure dependence of time spectra!, just a global yield drop)



scintillation in Xe/CH4 admixtures (P=1.27bar)
measurements
simulation
0% CH4
0.045% CH4
0.112% CH4
0.220% CH4
0.369% CH4
0.559% CH4
1.044% CH4
1.531% CH4
Y/P [ph/el/cm/bar]
E/P [kV/cm/bar]
0
50
100
150
200
250
300
350
400
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
3.6
3.8
4

Extrapolations for primary and secondary light for $CO_2/CH_4/CF_4$