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

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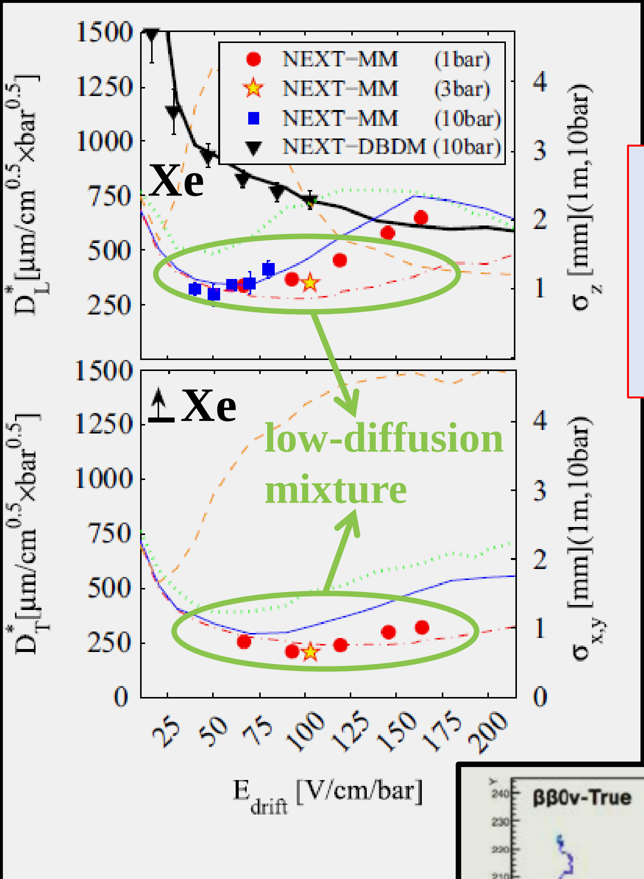
D. Gonzalez-Diaz
and the NEXT collaboration

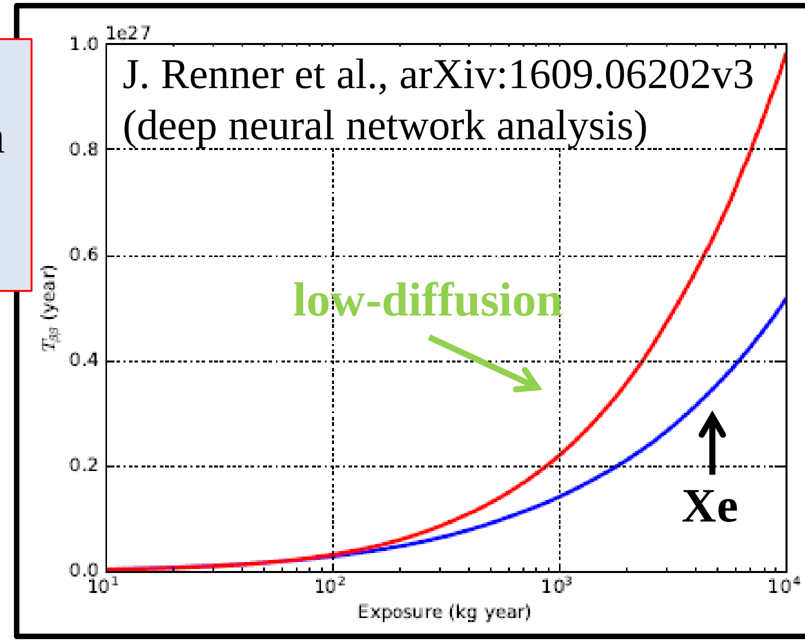
@RD51 (14/12/2016)

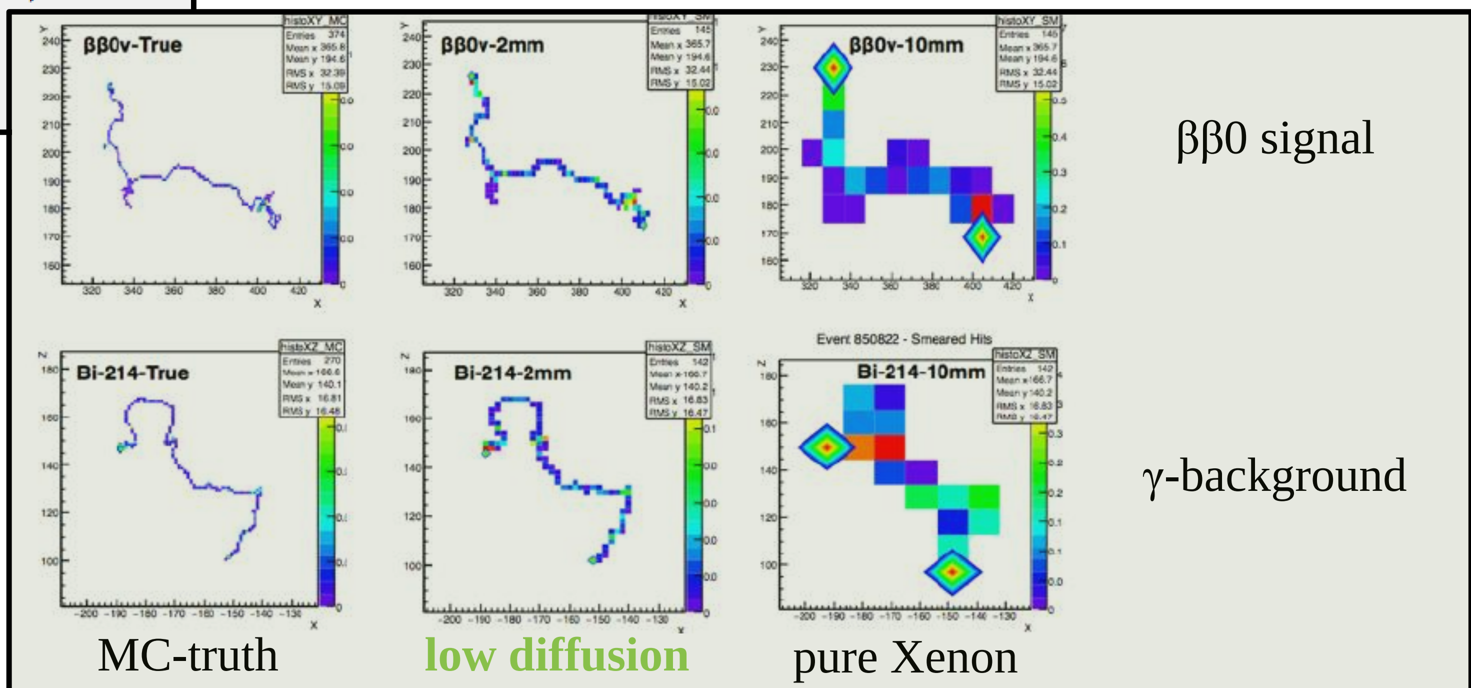
I. The problem

The importance of the ‘topological’ information in NEXT



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





A 'conceptual' magic mixture

From TPC conference 2014!

(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.**

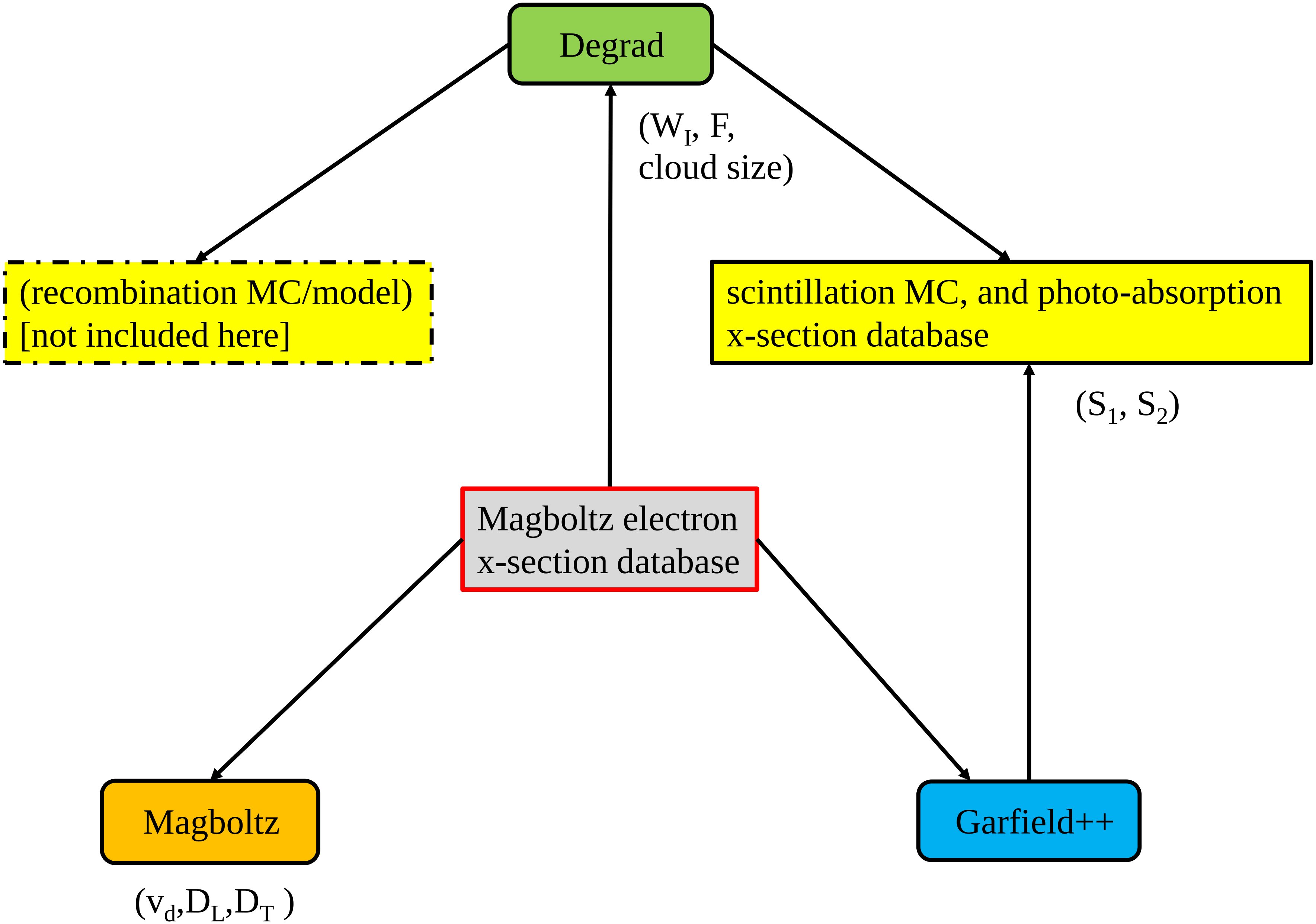
---

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'

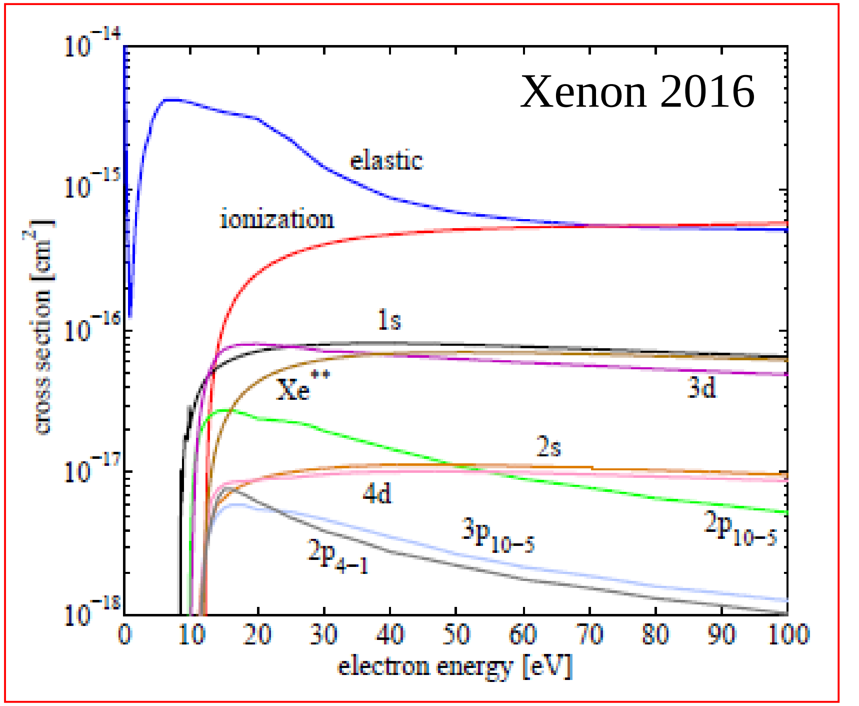
II. The tool

A microscopic software for electron and photon transport in gas



III. Basic considerations

Electron x-sections of relevant gases



I

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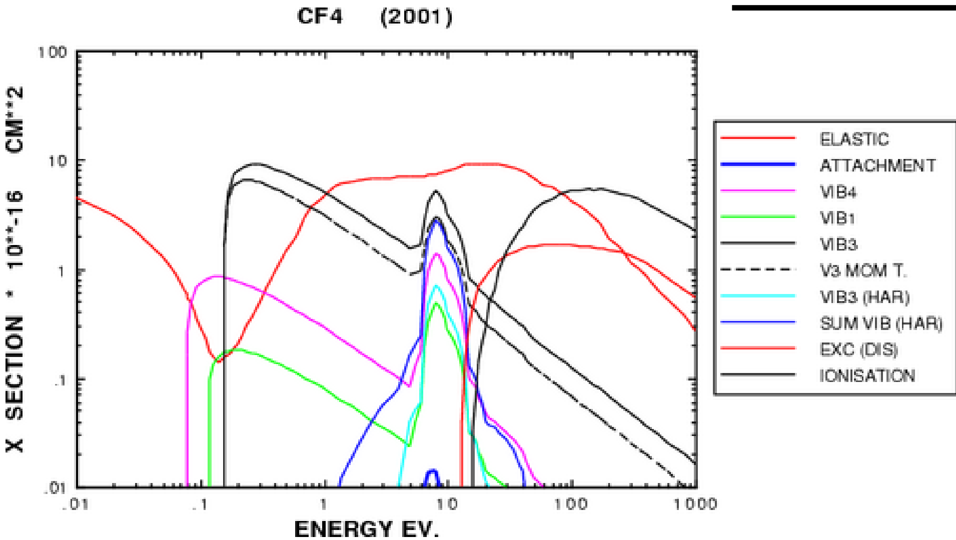
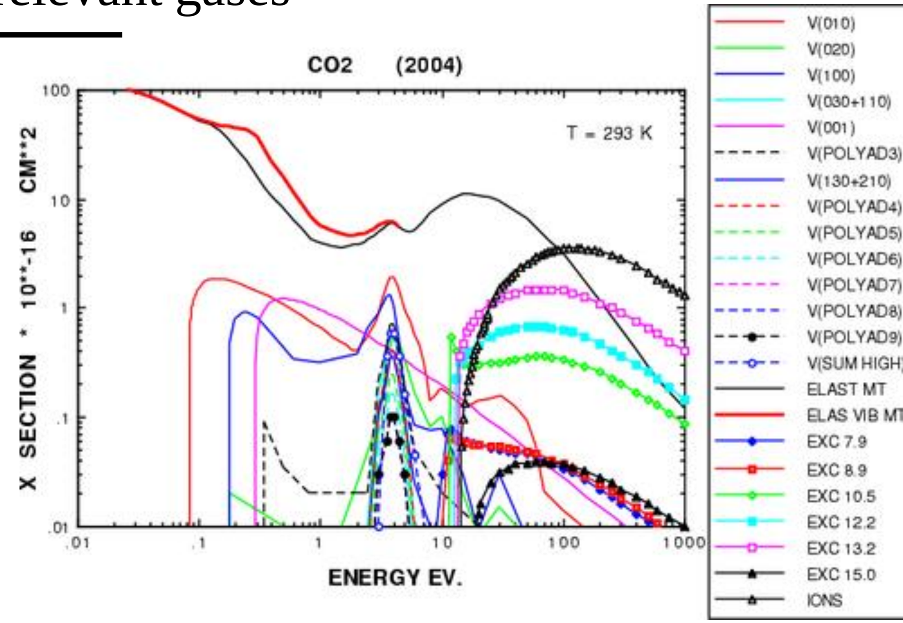
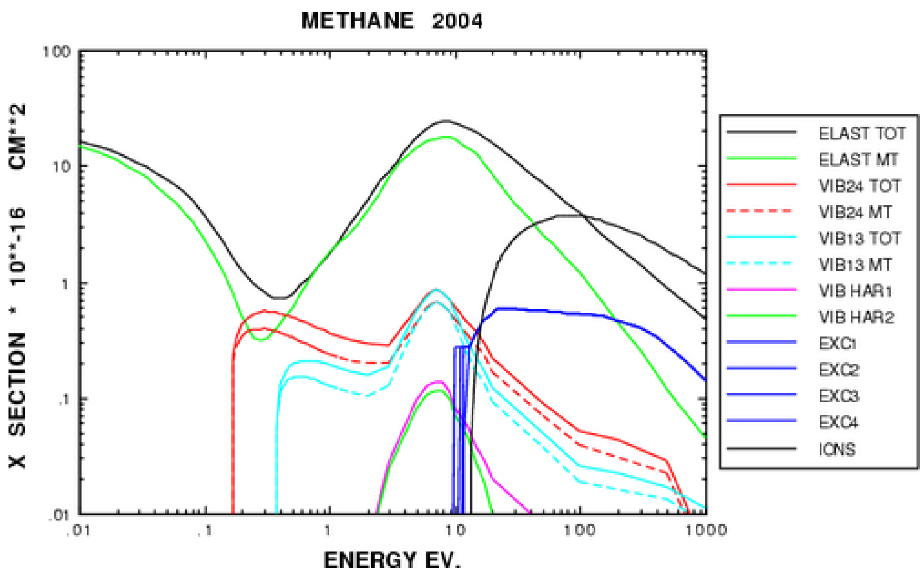
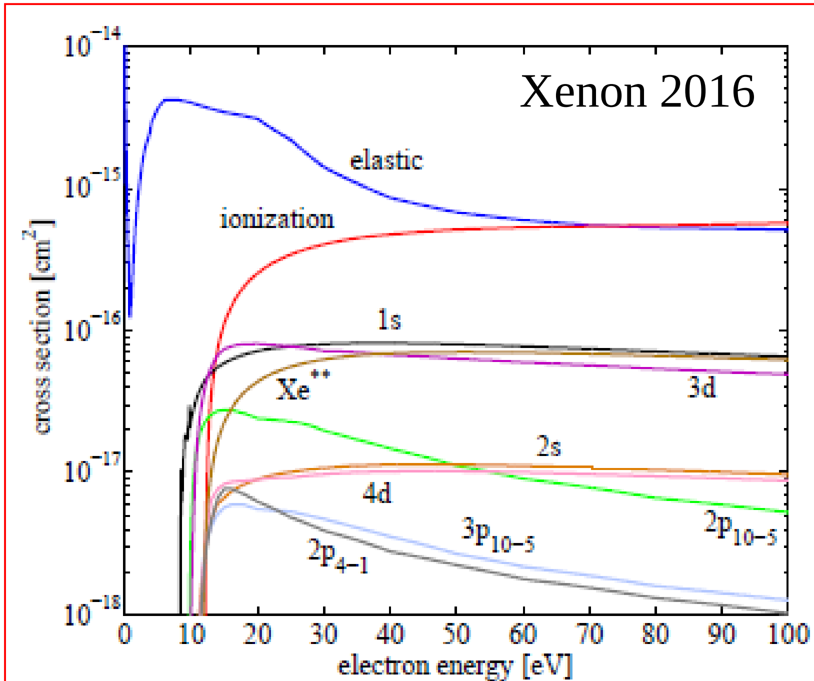








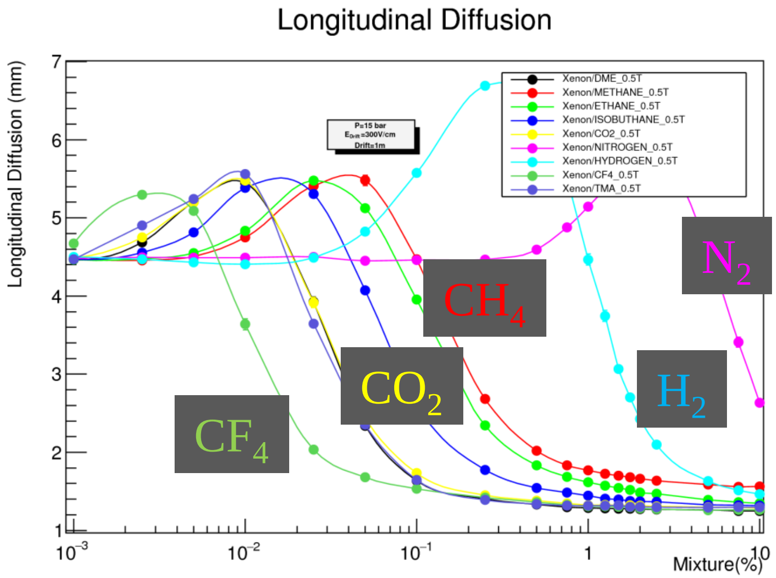
x-sections for molecules that are plot here are actually old ones (just illustrative!)

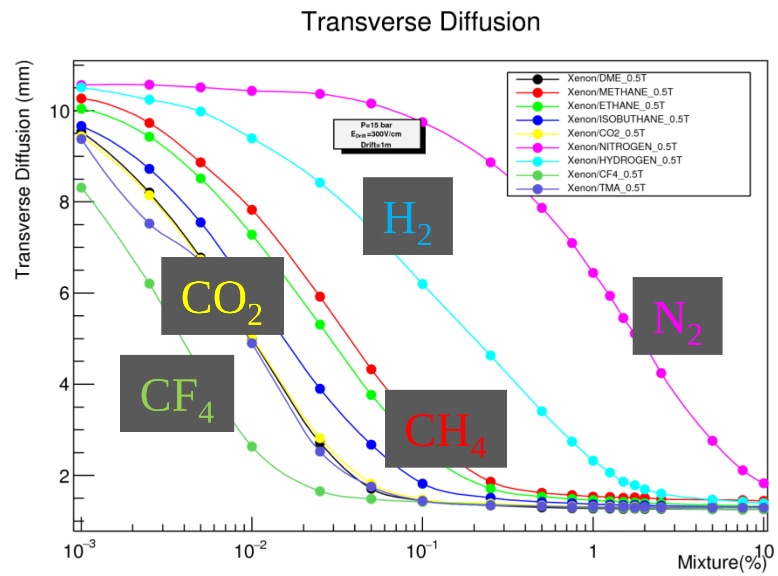
I

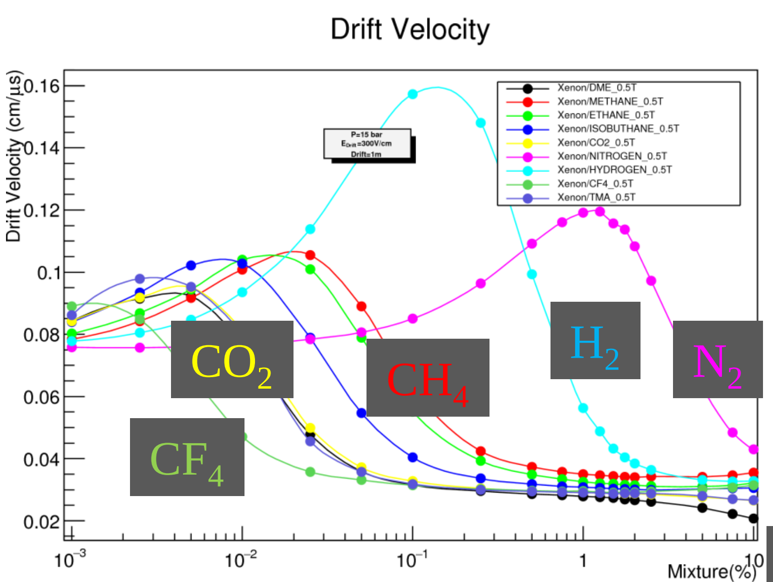
Ionization transport characteristics (v_d, D_L, D_T)

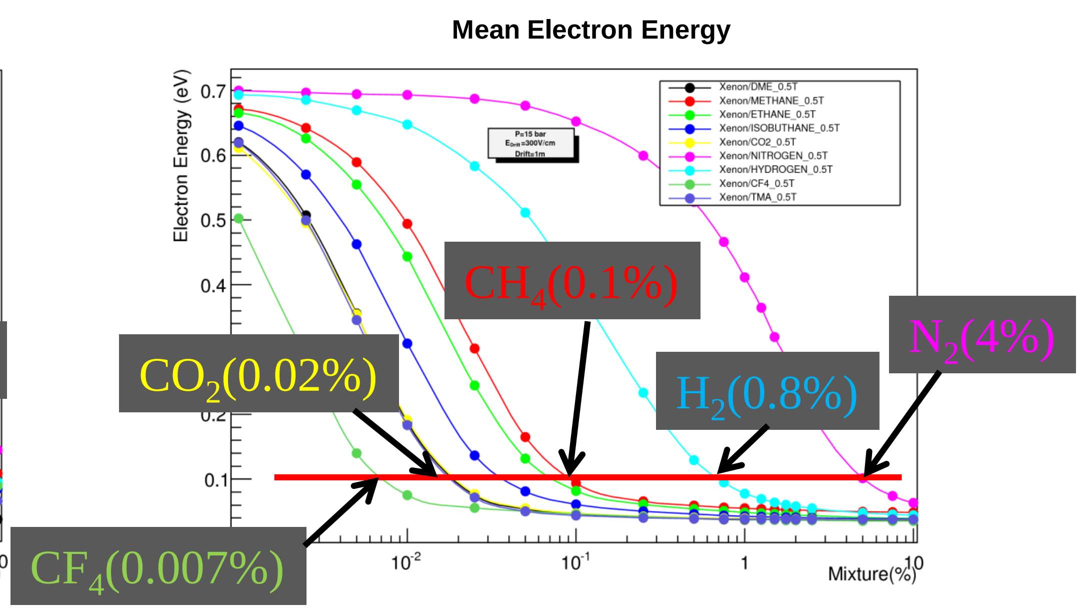
E_d=20 V/cm/bar, P=15bar

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









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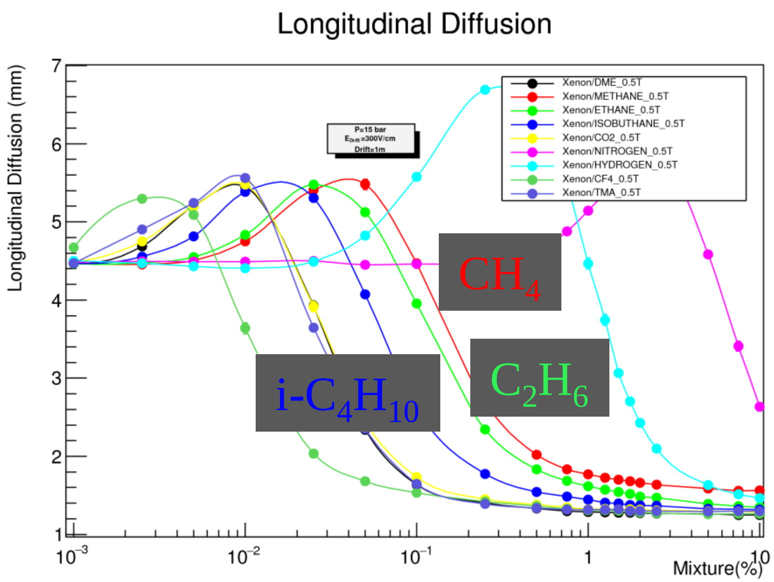
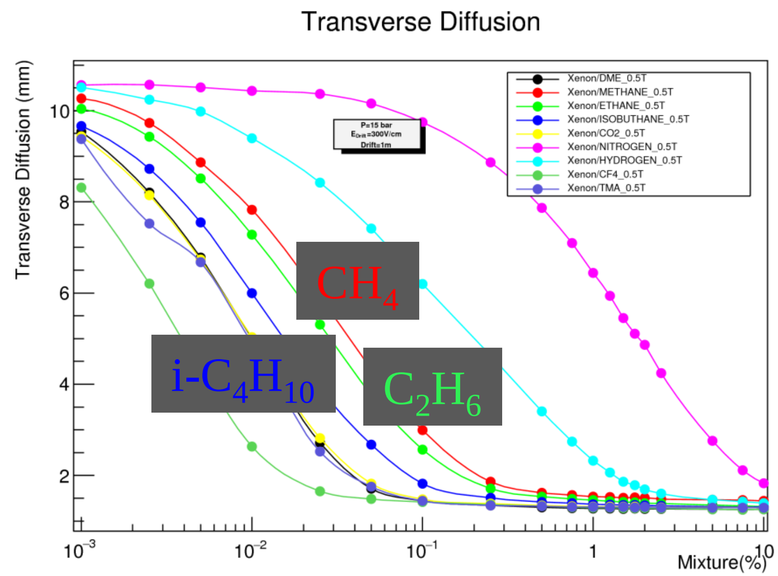
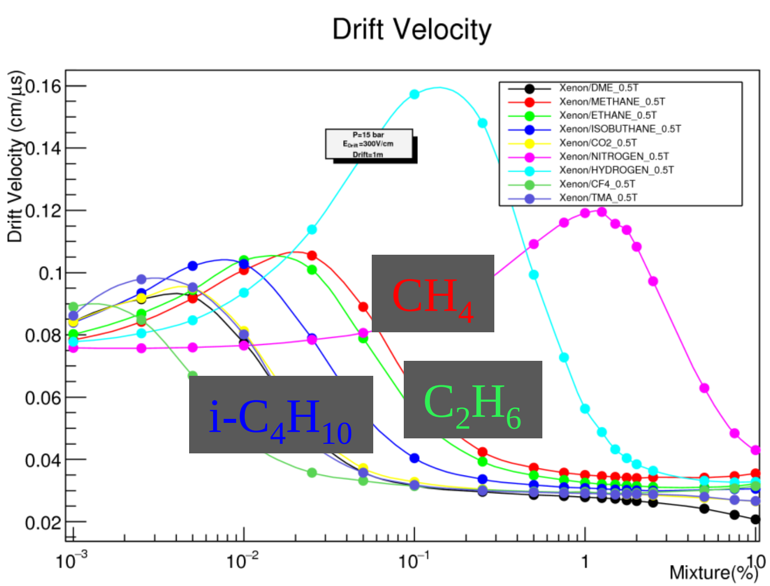
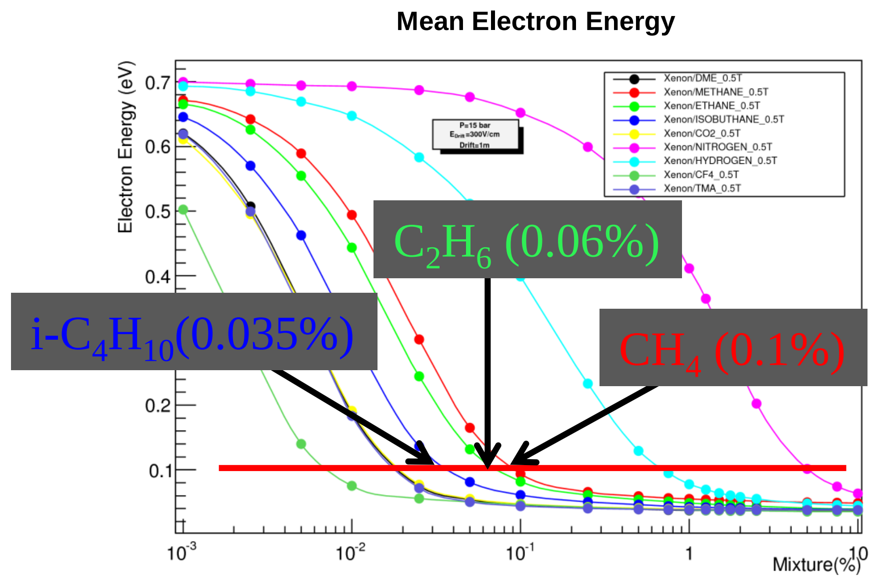








II

Light transparency

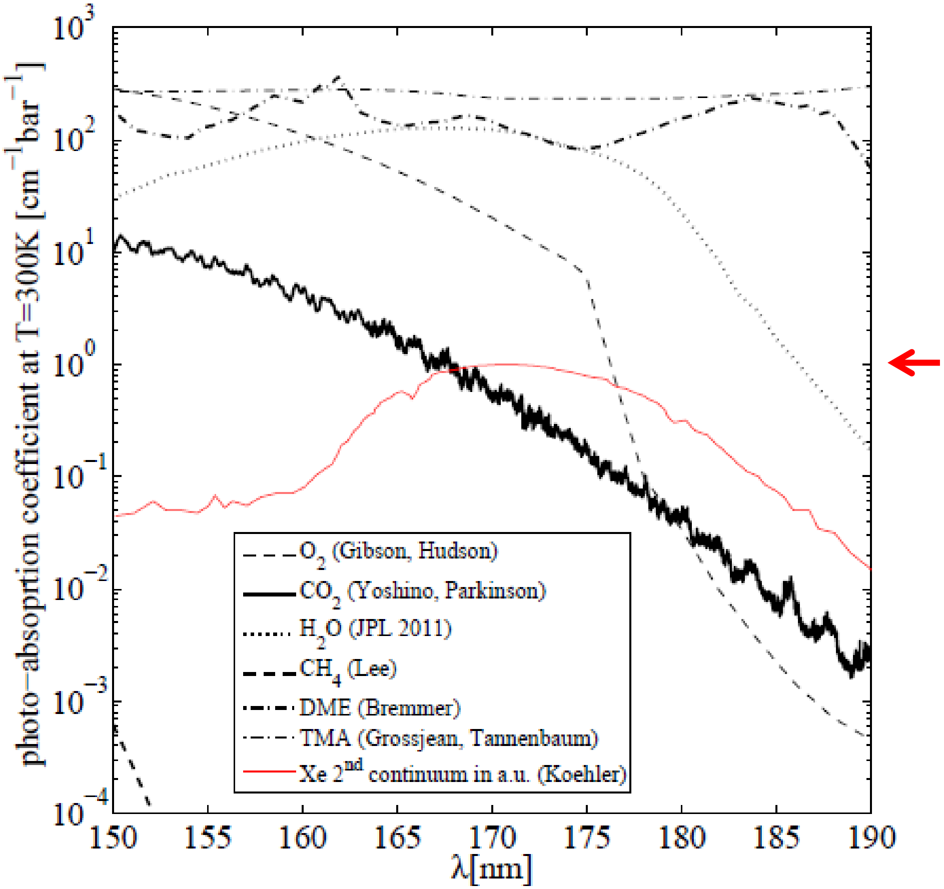


Fig. 1. Compilation of photo-absorption coefficients of some relevant TPC admixtures at around $T = 300$K in the region corresponding to the Xenon 2nd continuum, [9–18]. The reference spectrum from Koehler has been overlaid as a thin continuous line [2]. For H_2, N_2 and CF_4 there is no data in the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

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

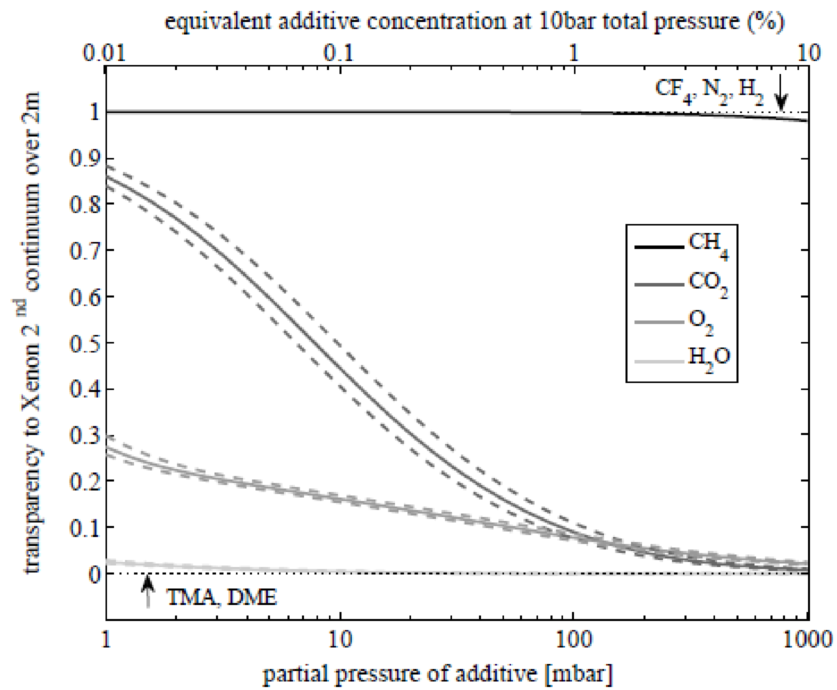
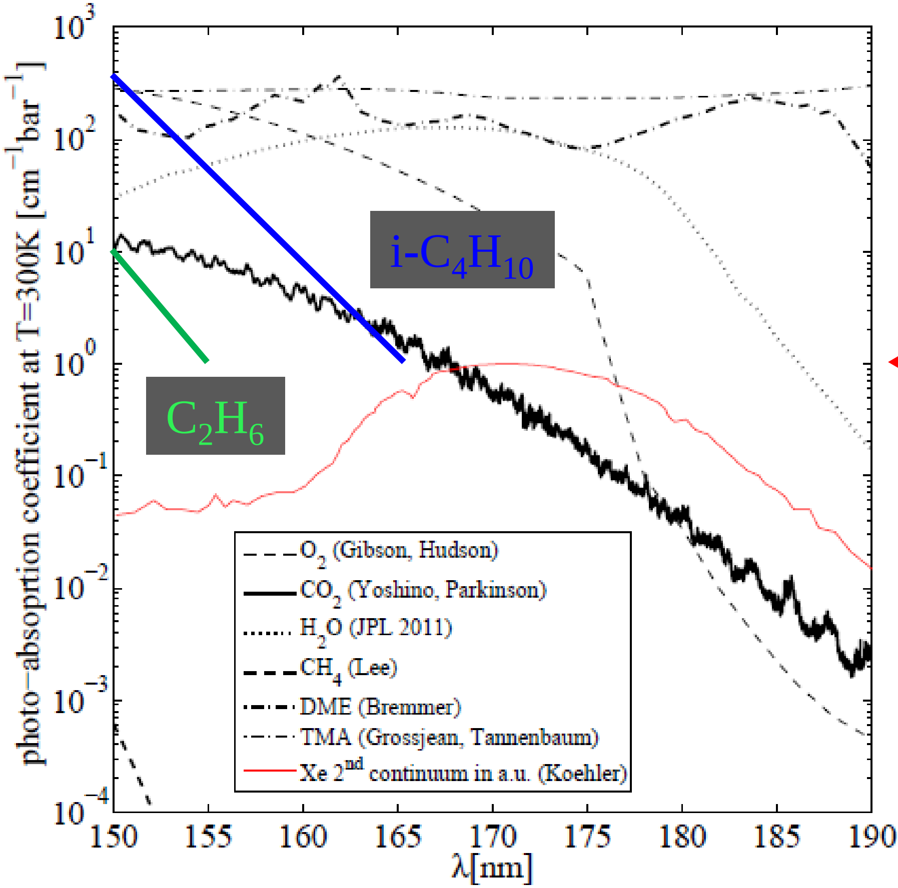


Fig. 2. Estimated transparency to scintillation from Xenon 2nd continuum as a function of partial pressure of the additive, over a 2 meter-long TPC. Dashed lines are obtained assuming 20% errors in the cross-sections.

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

Light transparency



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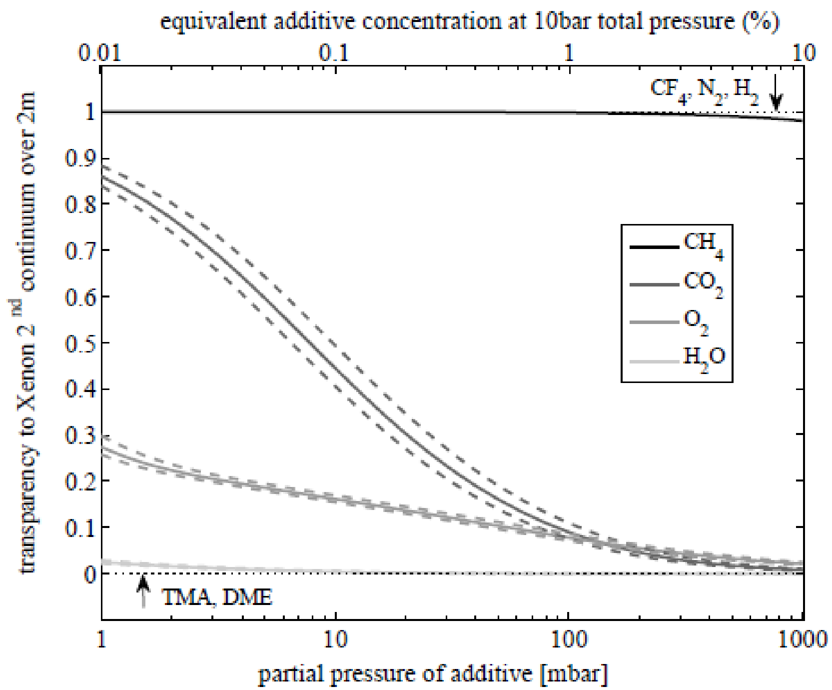

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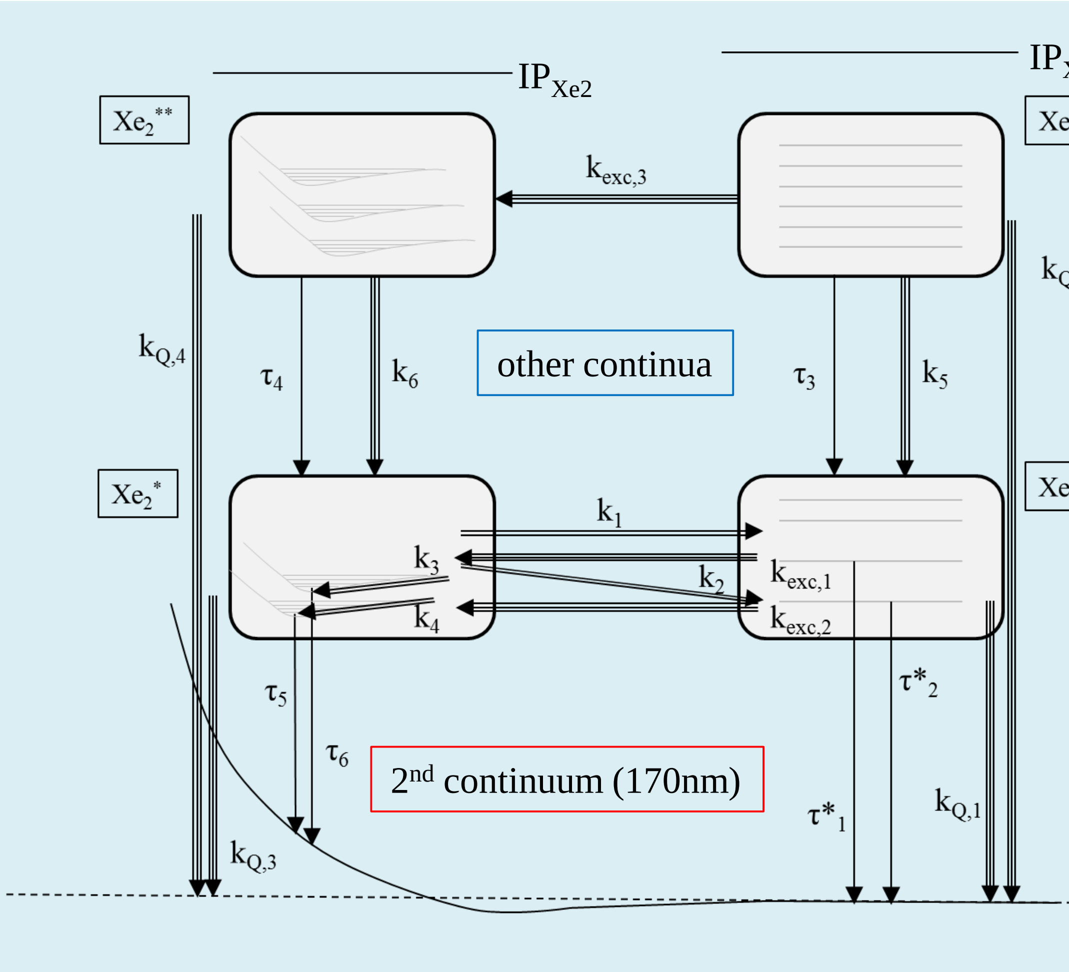
III

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*	81.4^{*3}	81.5[25]	1770^{*5}, 888^{*3}
H_2	0.40[24]	0.40^{*2}	4.21*	4.07^{*3}	4.07^{*3}	85^{*5}, 43^{*3}
N_2	0.48[24]	0.48^{*2}	5.05*	4.88^{*3}	4.88^{*3}	102^{*5}, 51^{*3}
CO_2	11.3[24]	11.2[25]	118.4*	114.0^{*3}	119.0[25]	2400^{*5}, 1200^{*3}
CF_4	0.025[24]	0.025^{*2}	0.26*	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*	76.5^{*1},183.1^{*3}	76.5^{*1},183.1^{*3}	3840^{*5}, 1900^{*3}

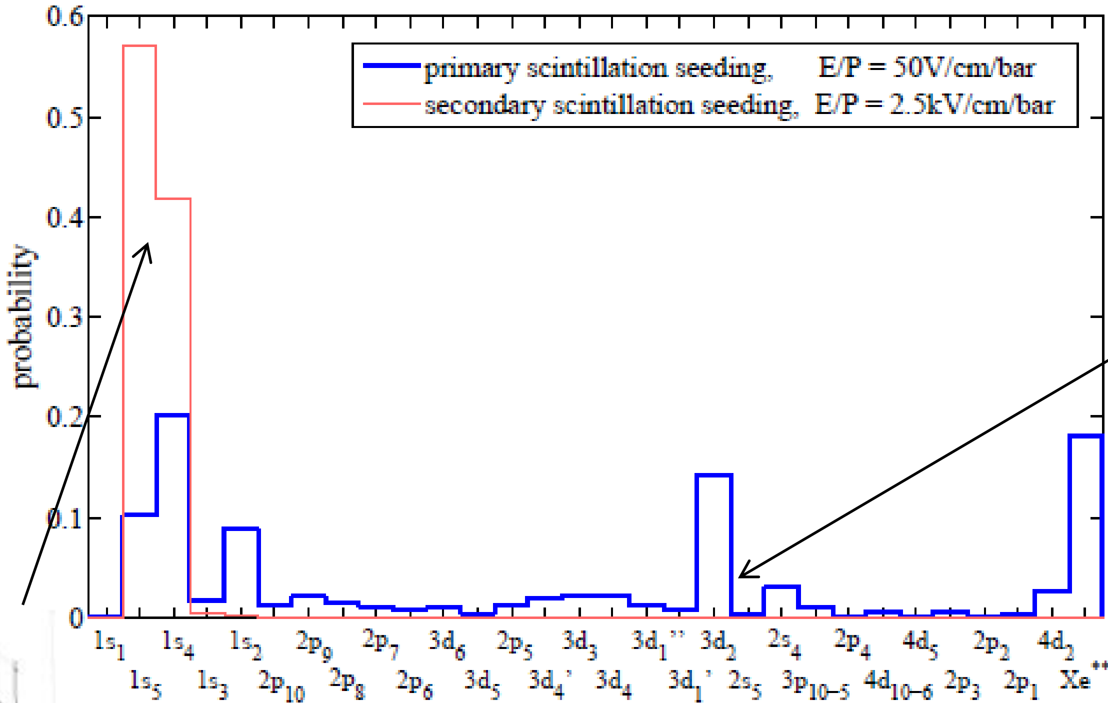
Most serious difficulties related to S_1:
- **Distribution of initial excited states?.**
- **Quenching/decay of Xe^{**}, Xe_2^{**} largely unknown.**

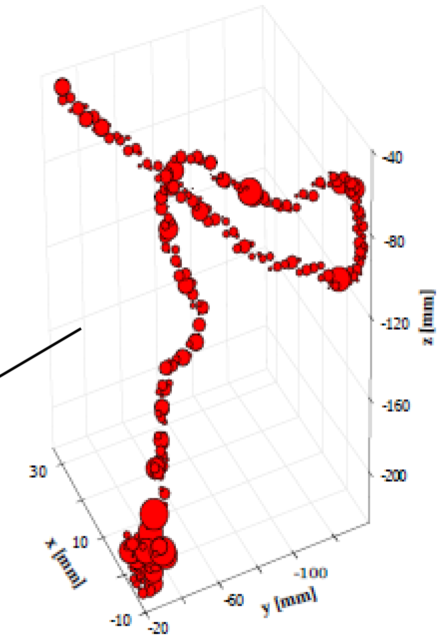
S_2 much more robust (dominated by low-lying states):
- **Measurements exist, and scalings work reasonably.**

IV. Electron transport + scintillation model

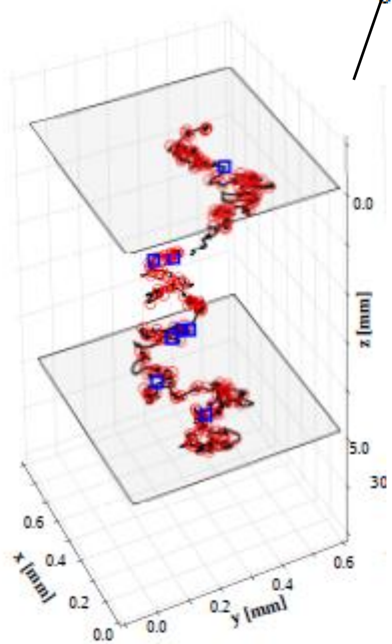
I. Computation of probability distribution of excited states

Degrad





Garfield++



II. Computation of atomic cascade

decay constant

2-body collision rates

3-body collision rates

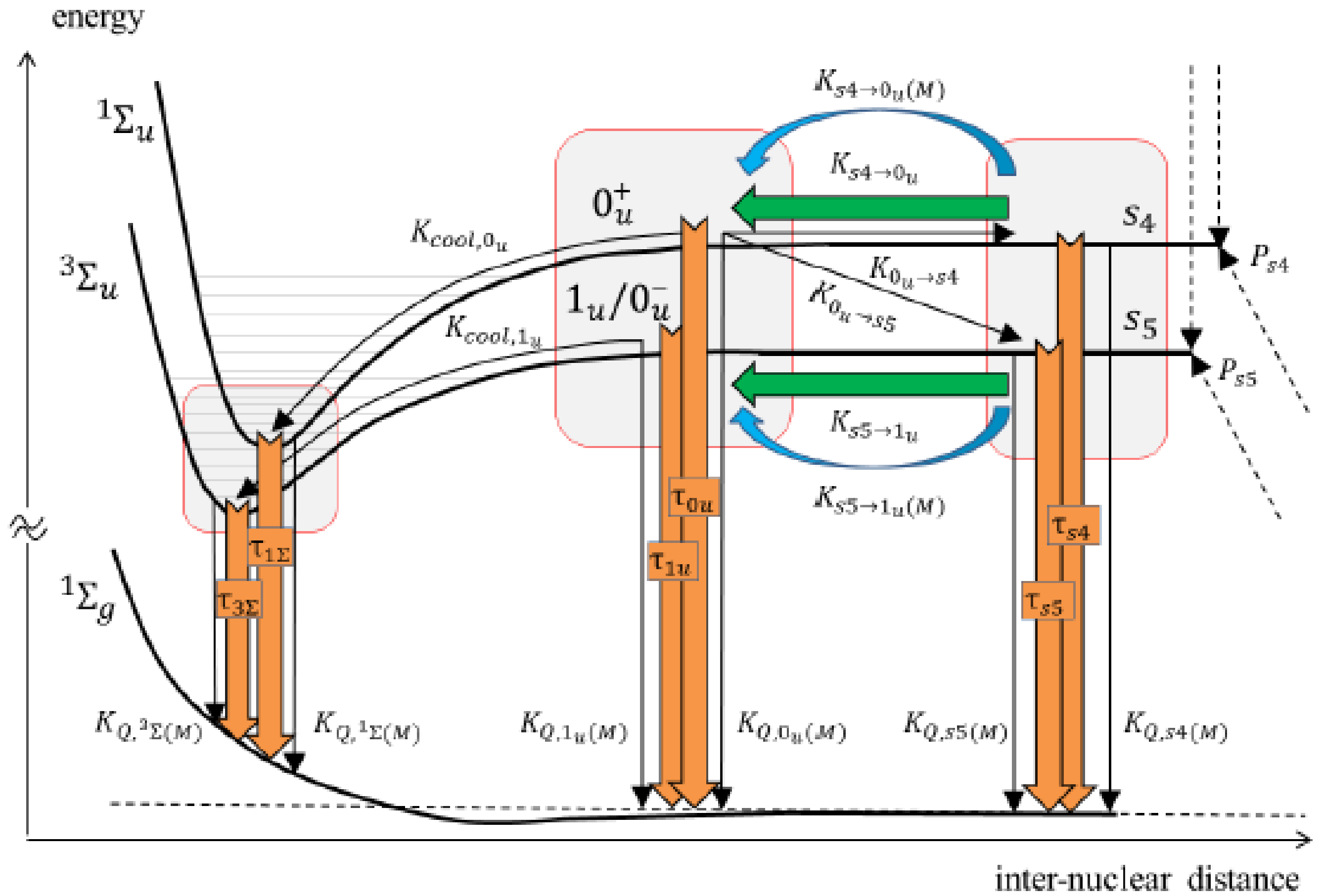
state (Paschen)	state (Racah)	energy [eV]	$\sum_j A_{ij}$ [ns^{-1}]	K_2@1bar [ns^{-1}]	K_3@1bar [ns^{-1}]
$1s_1$	-	0.000	-	-	-
$1s_5$	$6s[3/2]_2$	8.315	2.33×10^{-11}	4.94×10^{-5}	0.1465
$1s_4$	$6s[3/2]_1$	8.437	$0.281/n_H$	-	0.0855
$1s_3$	$6s'[1/2]_0$	9.447	1.28×10^{-8}	0.2224	-
$1s_2$	$6s'[1/2]_1$	9.570	$0.246/n_H$	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	$0.234^{(3)}$	$0.001^{(2)}$	$0.001^{(2)}$	$0.345^{(3)}$	$0.259^{(3)}$	$0.161^{(3)}$	-

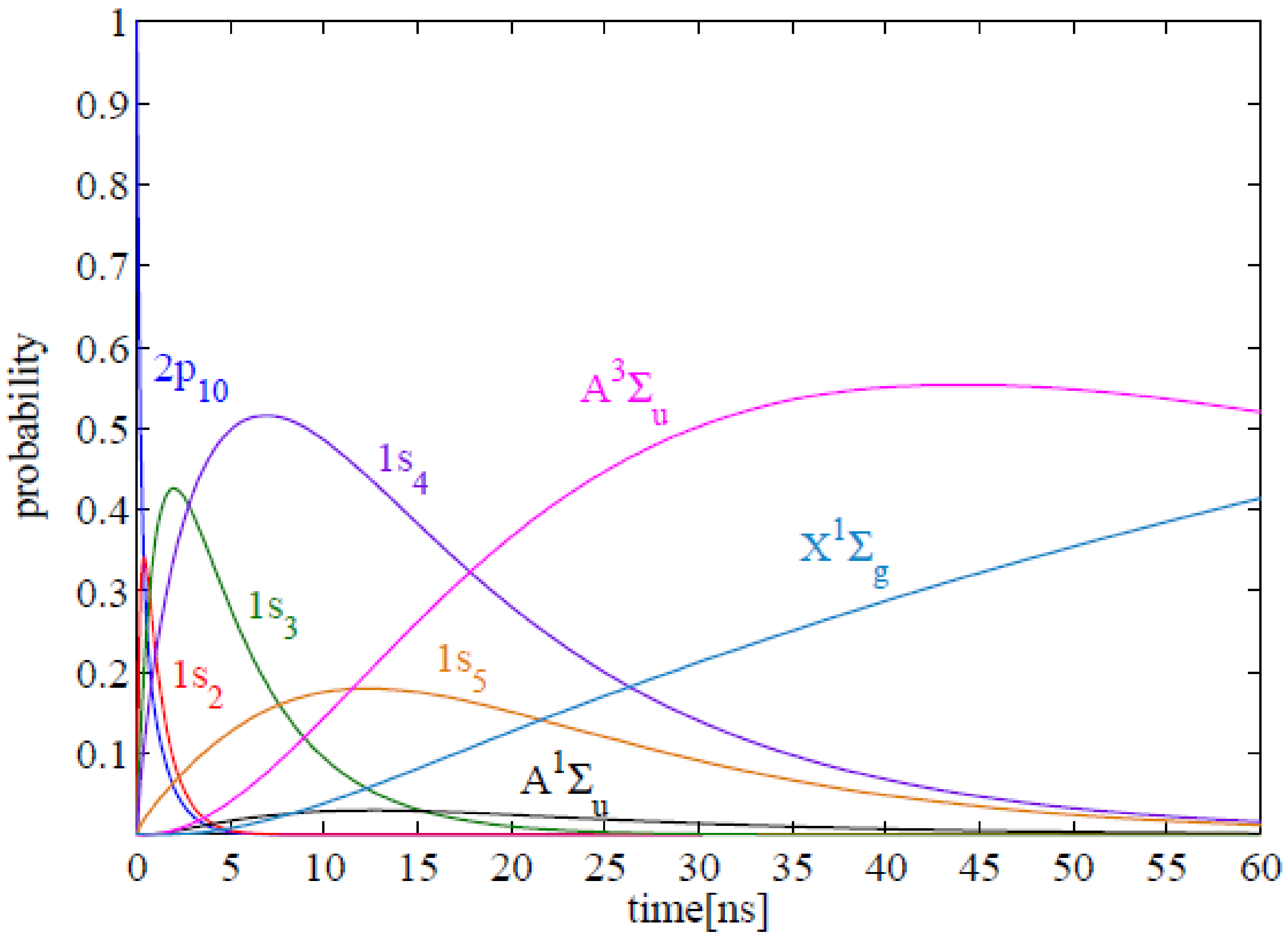
III. Excimer pathways

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



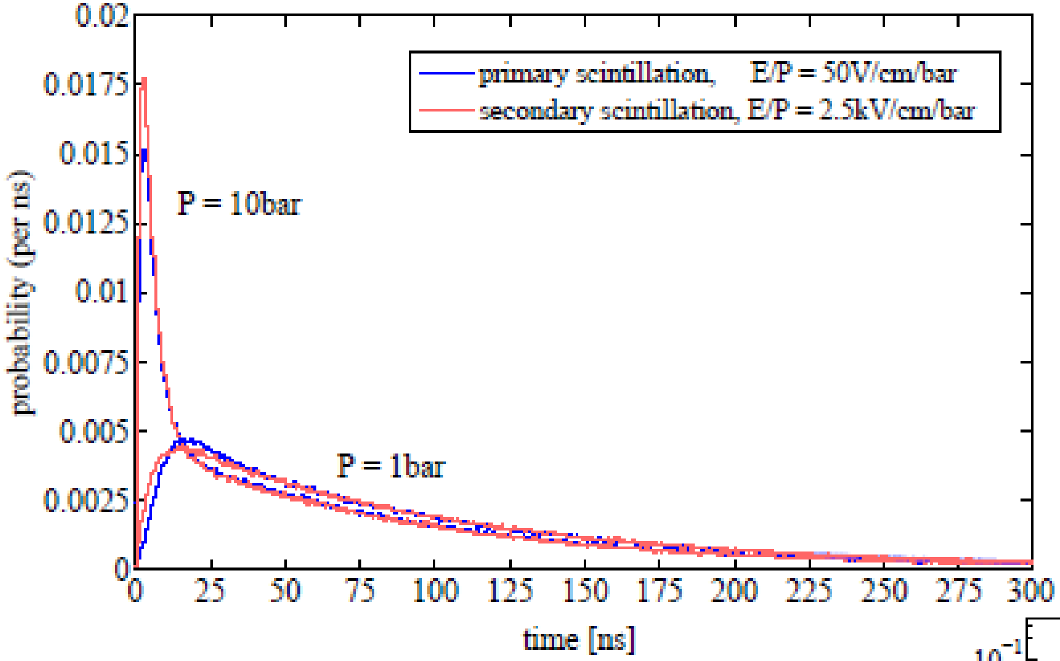
$\tau_{^3\Sigma}$	100 ns[1]	$K_{Q,^3\Sigma(M)}$	$11.12\ ns^{-1}$	$K_{s_5\to 1_u}$	$0.1465\ ns^{-1}$[1]	$K_{s_5\to 1_u(M)}$	$116\ ns^{-1}$
$\tau_{^1\Sigma}$	4.55 ns[1]	$K_{Q,^1\Sigma(M)}$	$12.85\ ns^{-1}$	$K_{s_4\to 0_u}$	$0.0855\ ns^{-1}$[1]	$K_{s_4\to 0_u(M)}$	$116\ ns^{-1}$[6]
τ_{1_u}	40 ns[1]	$K_{Q,1_u(M)}$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

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

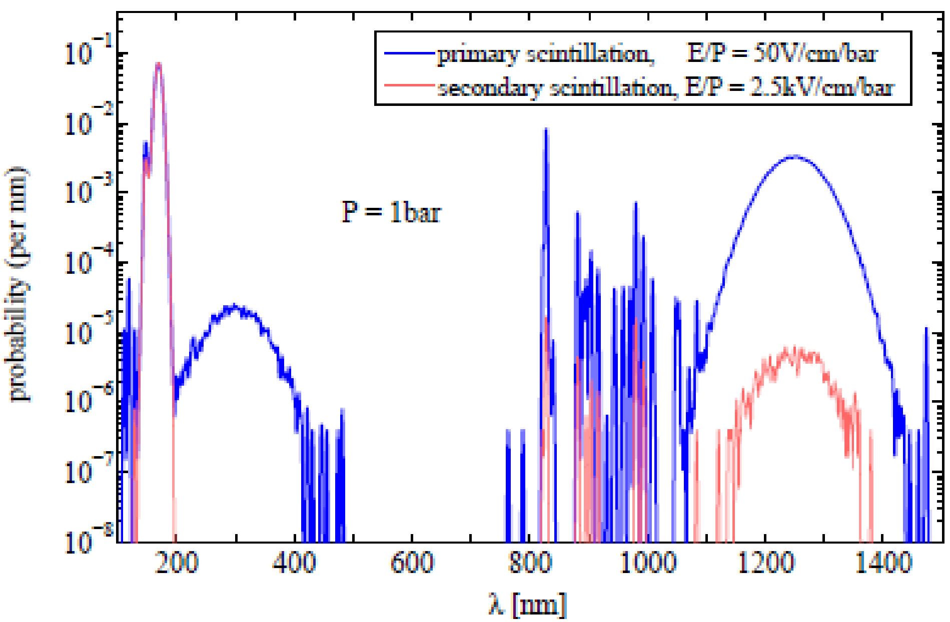


Example of electron transport + light production code

time distributions

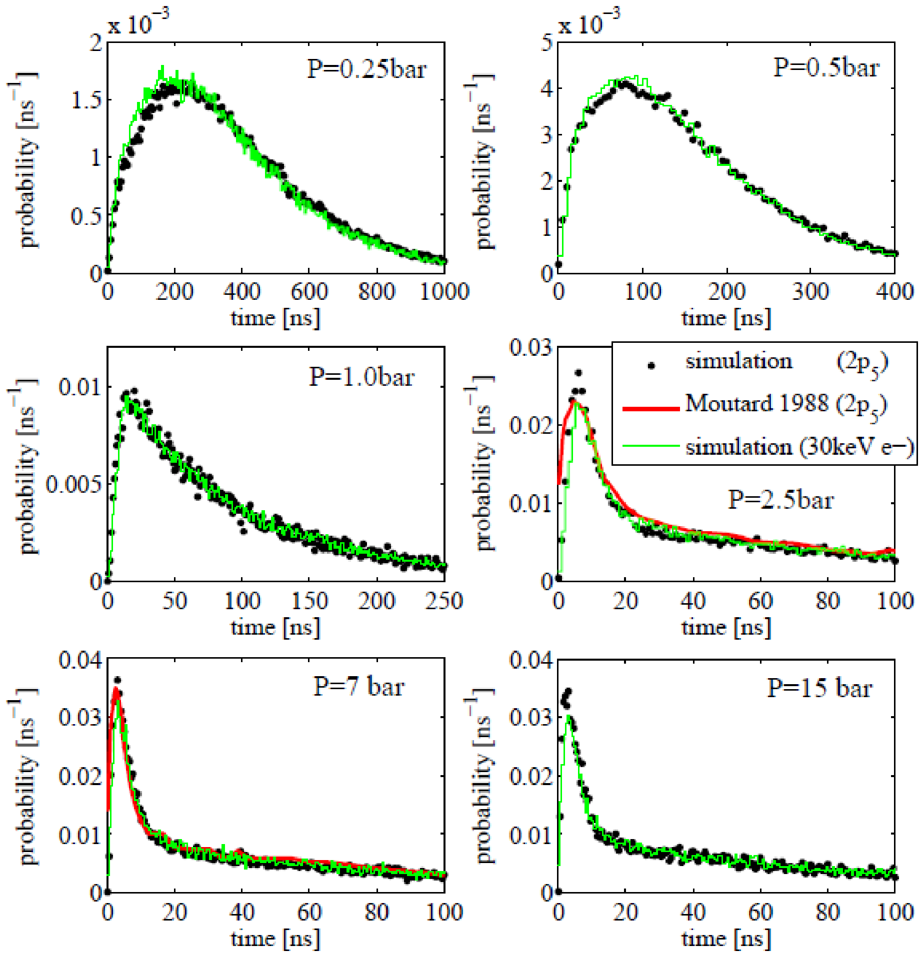


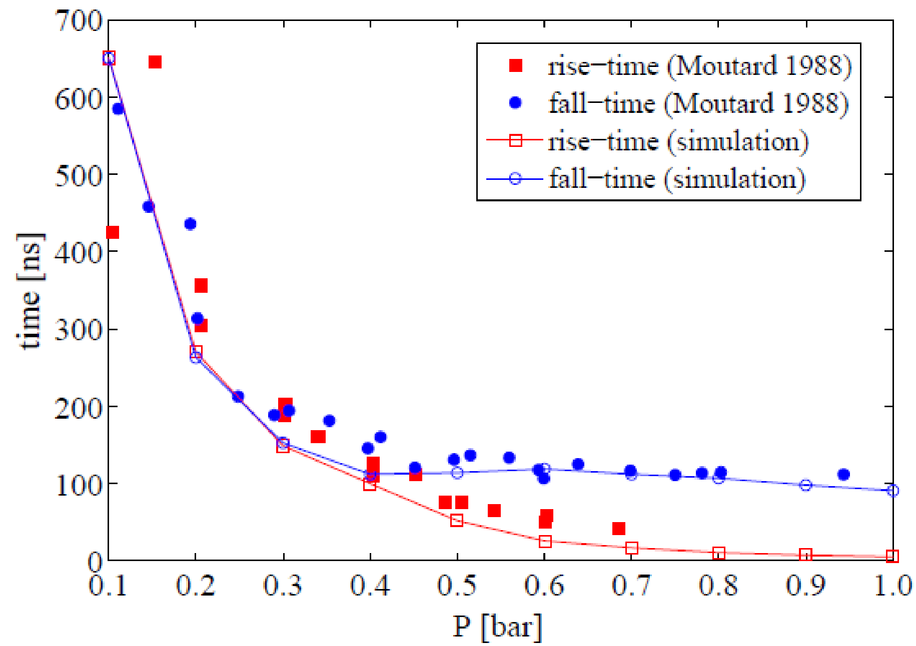
energy spectra



V. Comparison with pure xenon data

Time distributions



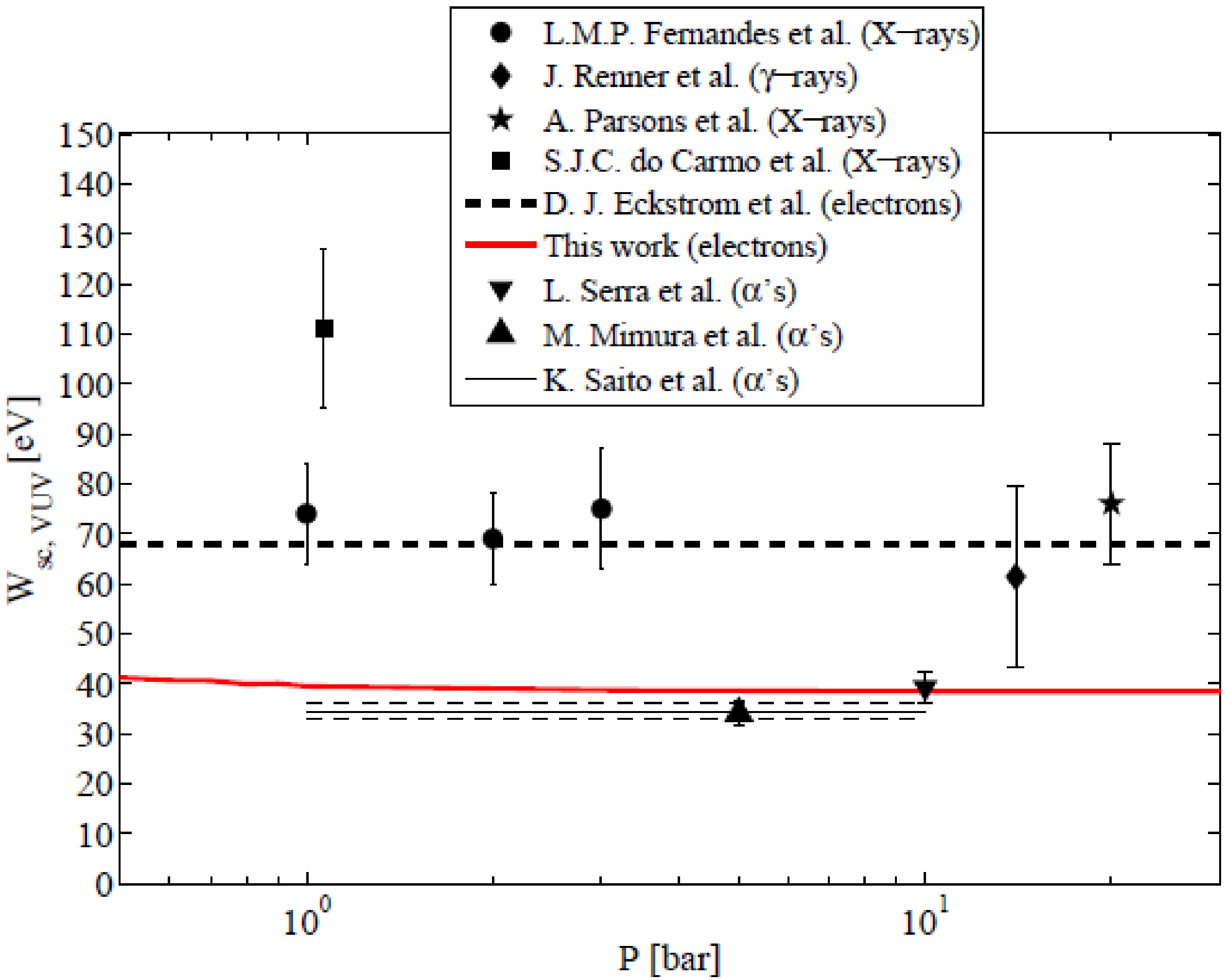


$$\left.\frac{dN_\gamma}{dt}\right|_{2^{\rm nd}} \simeq a e^{-t/t_f} - b e^{-t/t_r}, \qquad (P \lesssim 0.8 \text{ bar})$$

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

Yields

VUV region



IR region

simulated

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

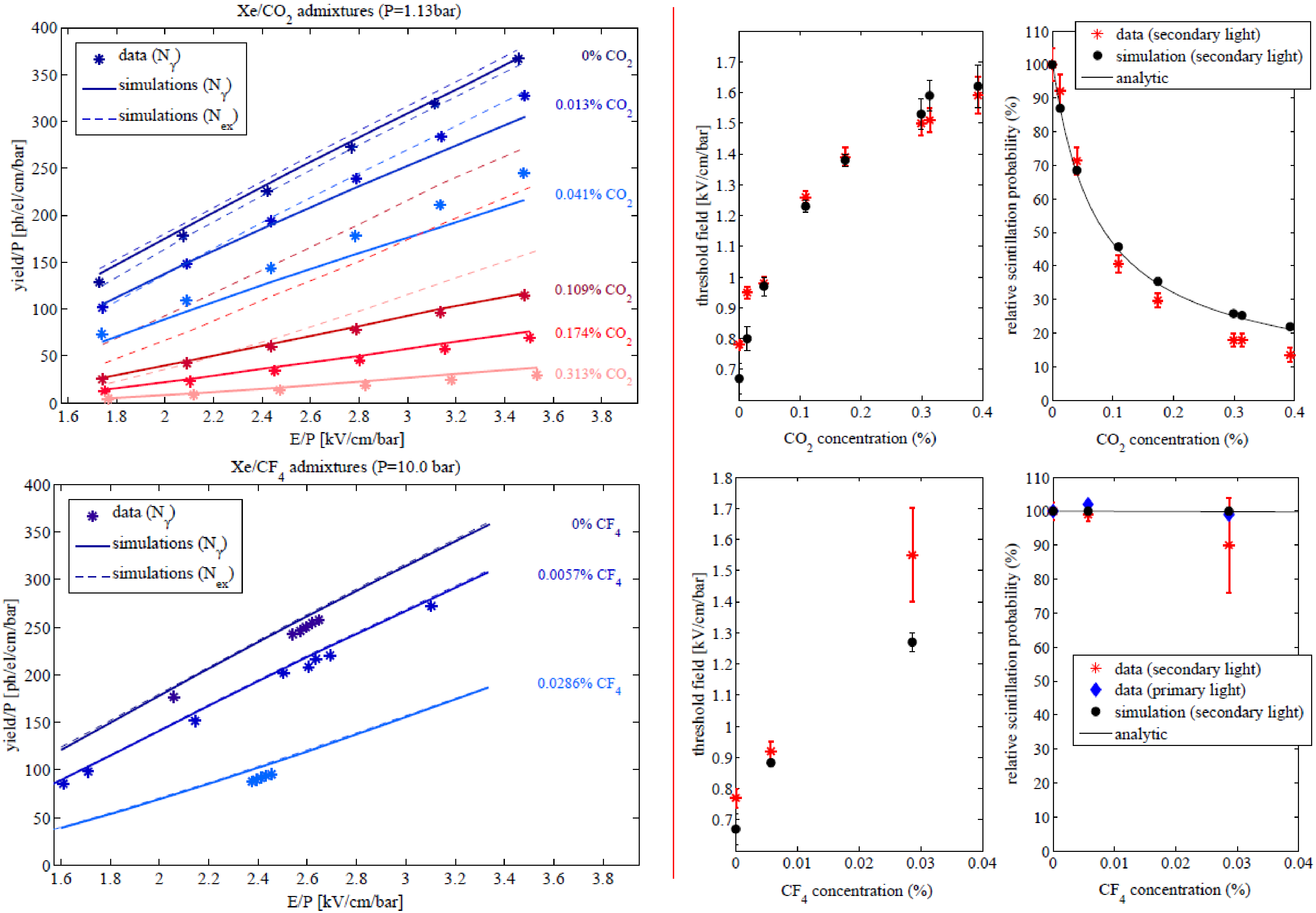
measured (α's)

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

VI. Comparison with xenon + additives

Electroluminescence (yield)

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



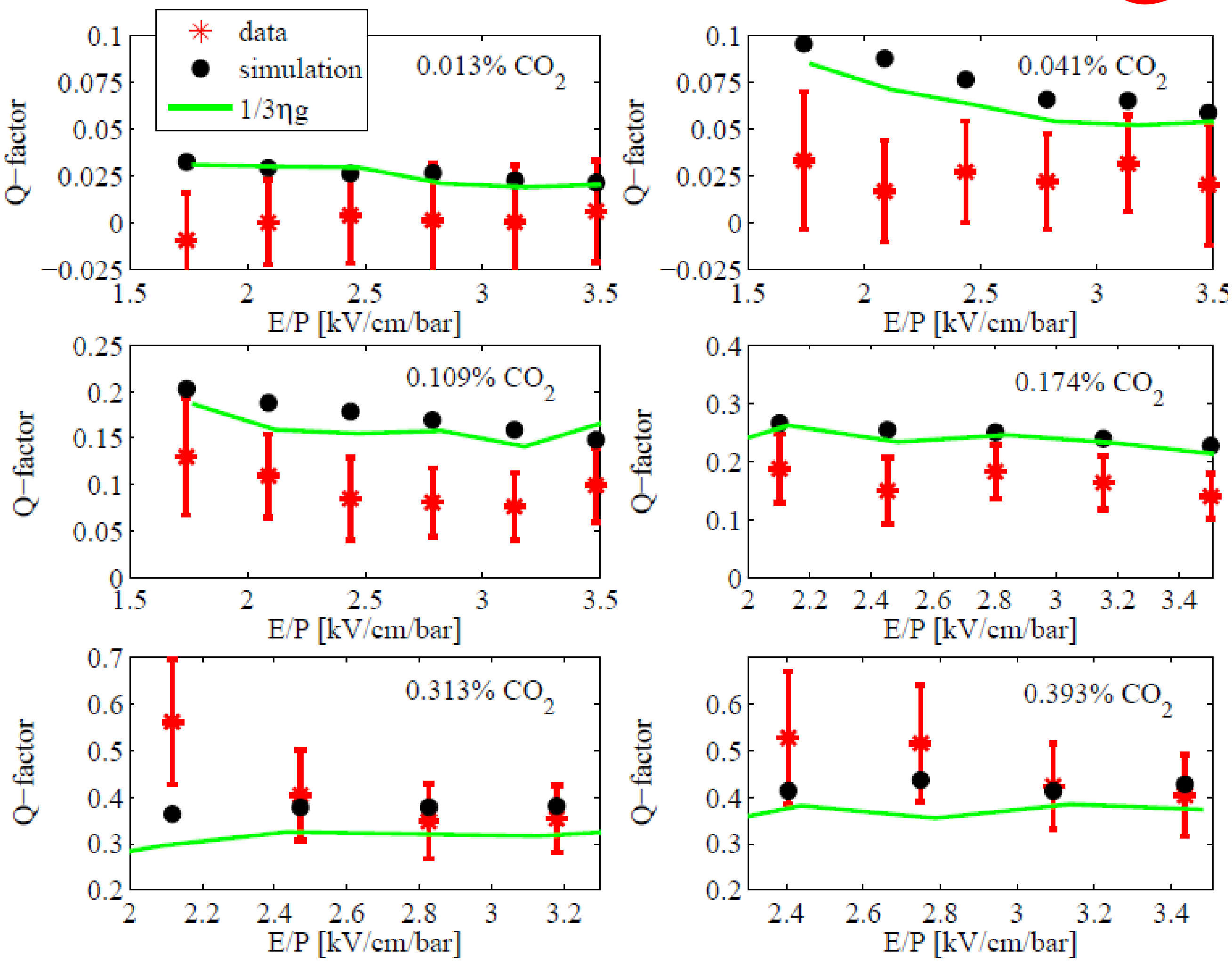
Electroluminescence (light fluctuations, Q)

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

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

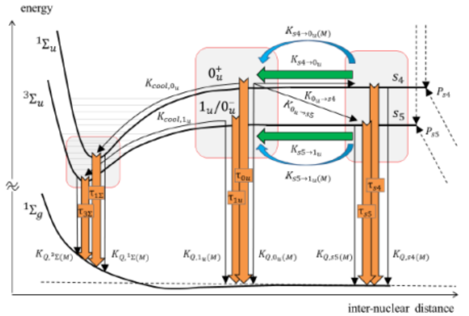
$$Q_{att} \simeq \frac{1}{3}\eta g$$

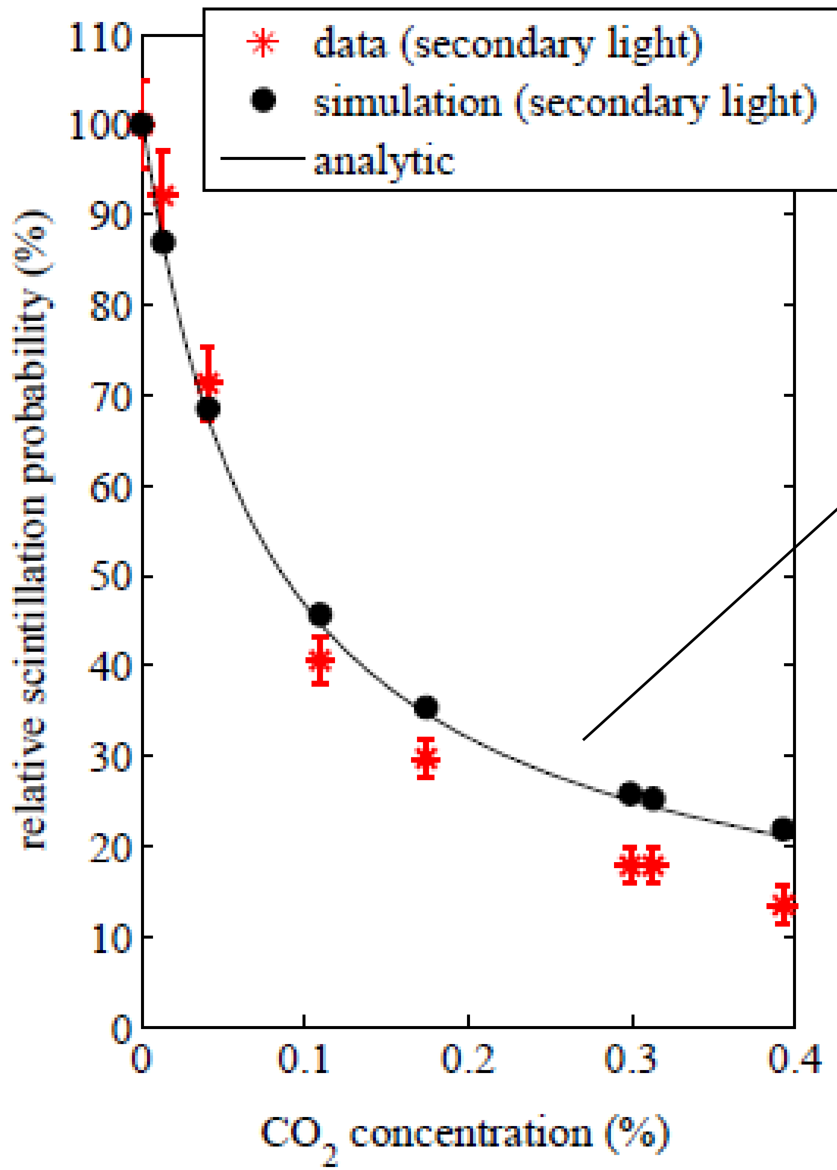
$$Q_{\mathcal{P}_{scin}} = \frac{1}{N_{\gamma}}\mathcal{P}_{scin}(1 - \mathcal{P}_{scin})$$



VII. Fine, but what is happening here?

Xe-CO_2





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

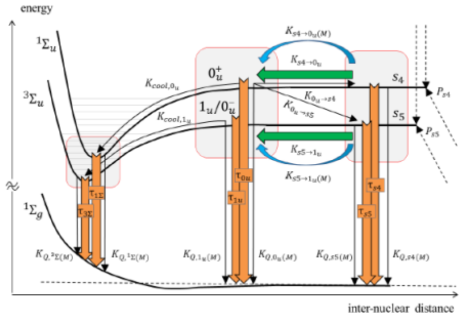
if assuming $\tau = \tau_{3\Sigma}$

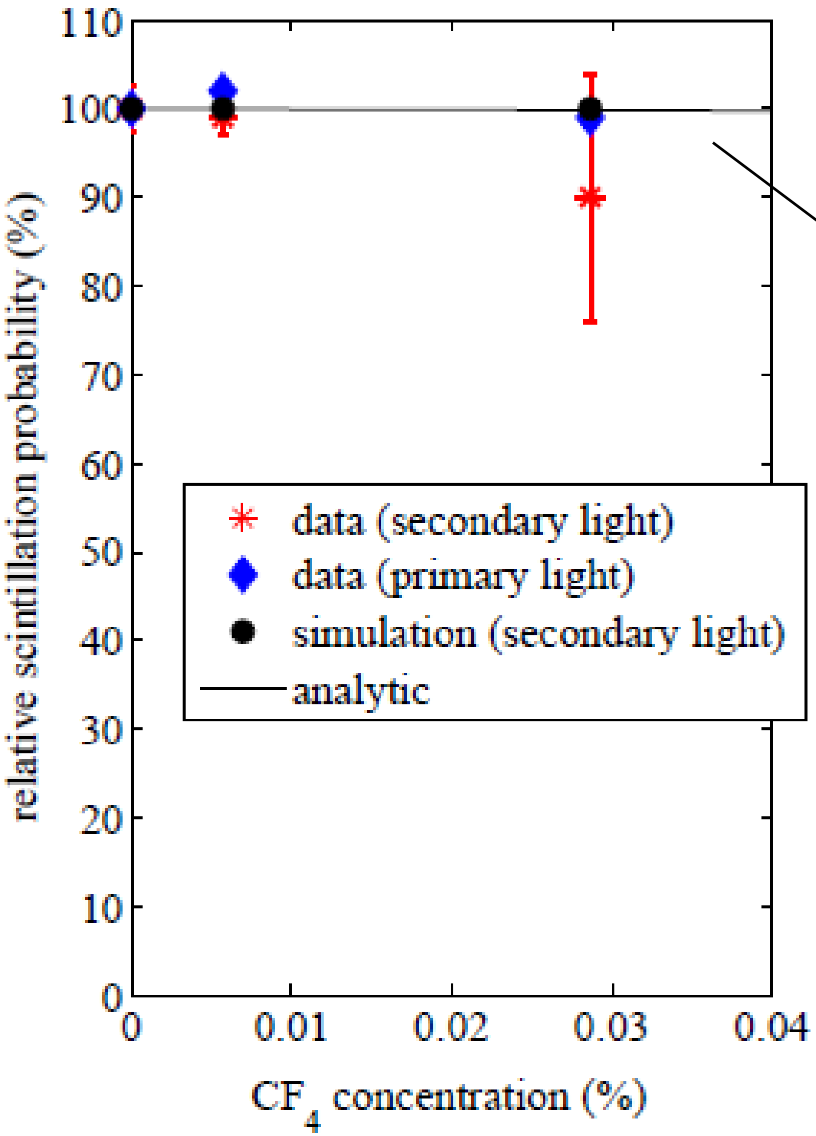
a fit gives: $K_2 = 11.20 \pm 1.0 \text{ ns}^{-1}$

The quenching rate of s_5 state in CO_2 is:

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

Xe-CF_4





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

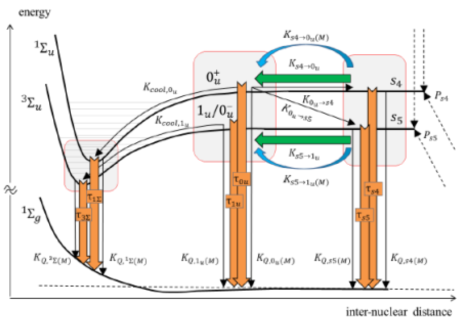
if assuming $\tau = \tau_{3\Sigma}$

and the quenching rate of s_5 state in CF_4:

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

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

An analytic picture… and a simple one (I)

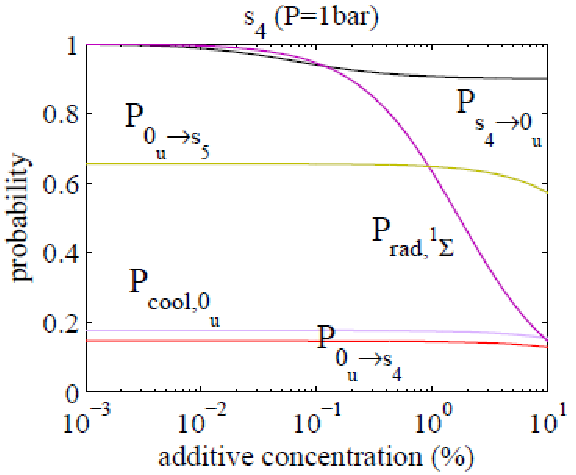


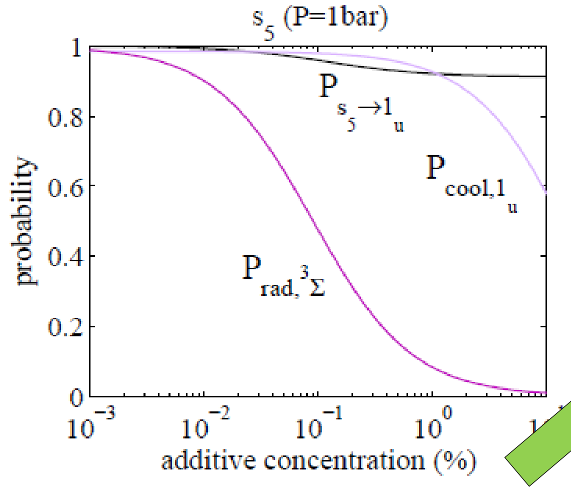
$$\mathcal{P}_{scin,s_4} = \frac{\mathcal{P}_{pop,s_4} \cdot \mathcal{P}_{s_4 \to 0_u}}{1 - \mathcal{P}_{s_4 \to 0_u} \cdot \mathcal{P}_{0_u \to s_4}} \times$$

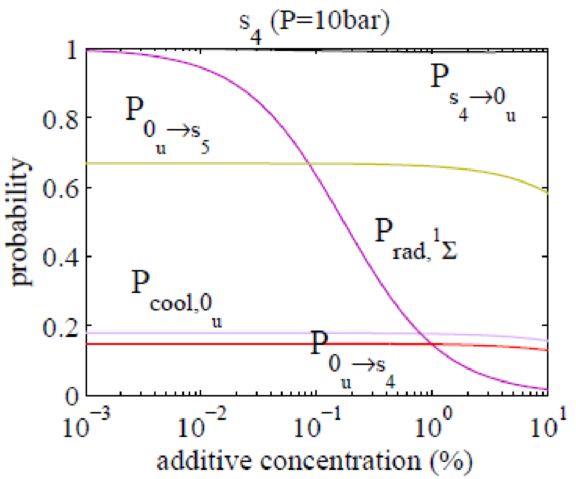
$$\left(\mathcal{P}_{cool,0_u} \cdot \mathcal{P}_{rad,^1\Sigma} + \mathcal{P}_{0_u \to s_5} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,^3\Sigma}\right)$$

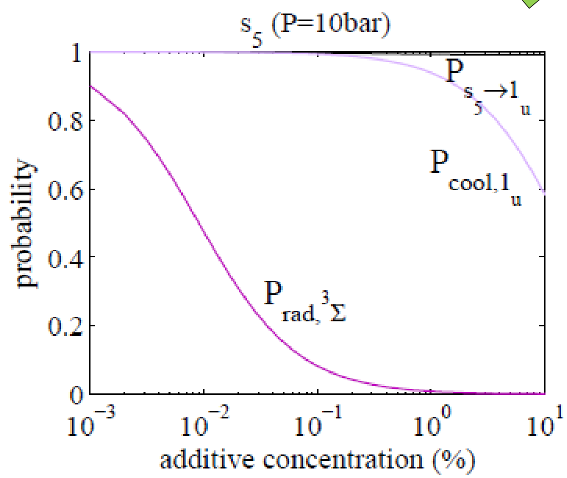
$$\mathcal{P}_{scin,s_5} = \mathcal{P}_{pop,s_5} \cdot \mathcal{P}_{s_5 \to 1_u} \cdot \mathcal{P}_{cool,1_u} \cdot \mathcal{P}_{rad,^3\Sigma}$$

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









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

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

$n = P/P_o$

Indeed: dominance of triplet state scintillation above 1bar!

An analytic picture… and a simple one (II)

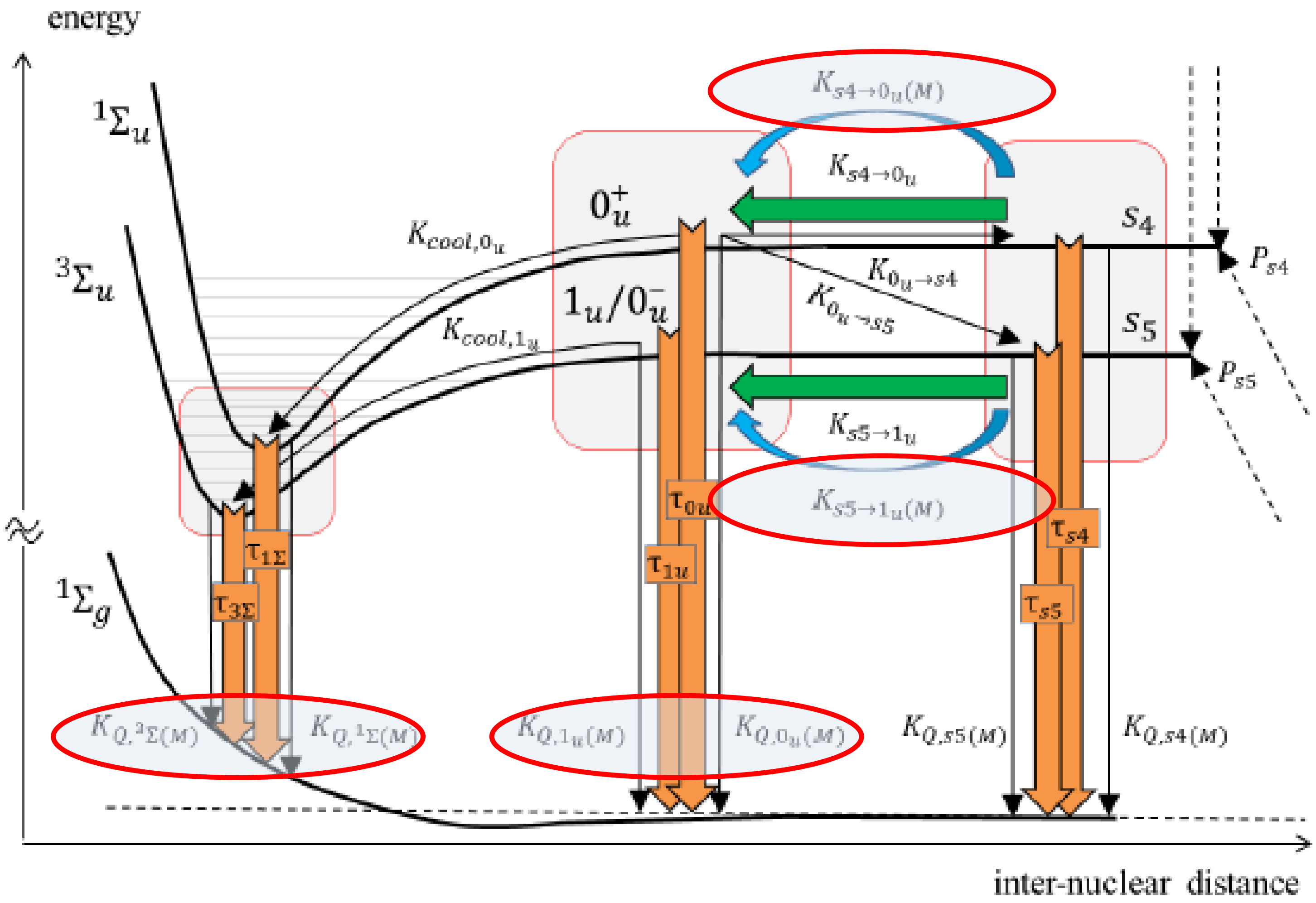
- This simple picture (triplet dominance) describes the quenching effect in earlier data by Suzuki for Ar-CO_2 and Ar-CH_4 (1983) and Conde and Policarpo for Xe-N_2 (1968),

  …quantitatively!

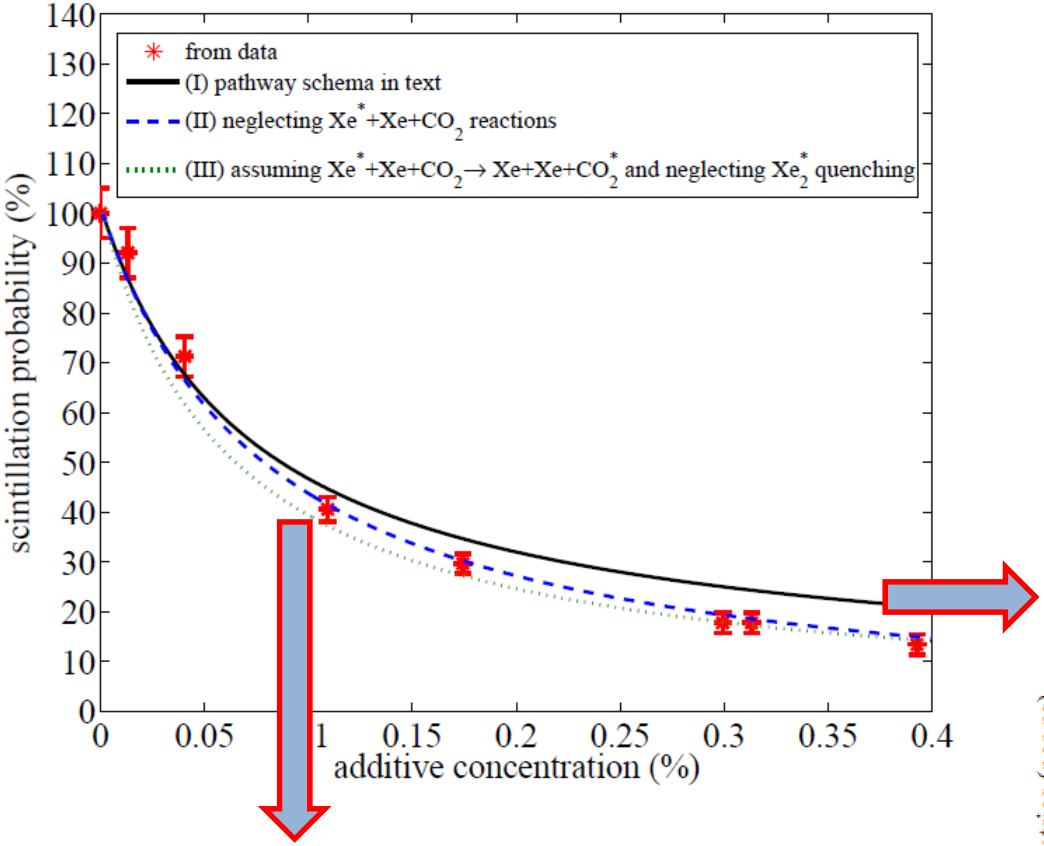
- It does describe the data for Xe-CH_4 from GIAN group (Carlos Henriques), but with a quenching rate for the excimer that is about x4-x8 less than that of the atom (!). This seems to enable CH_4 for high pressure operation in NEXT, and its figure of merit perhaps even surpasses the one from CO_2, contrary to the initial expectations…

still a lot to learn from good measurements!

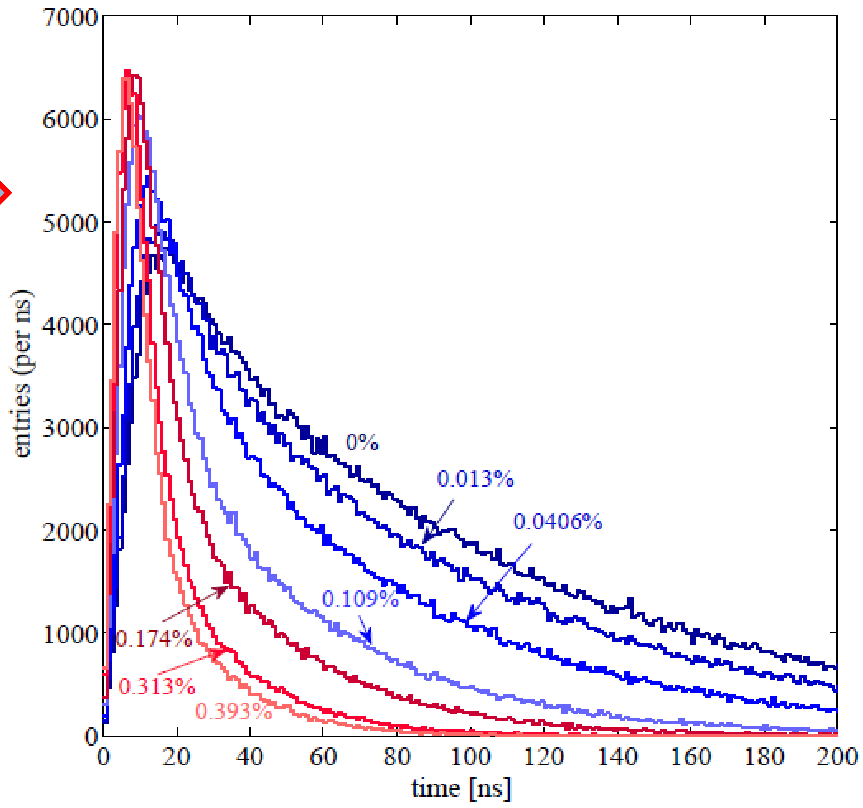
Ambiguities in the scintillation model (I)



Ambiguities in the scintillation model (II)

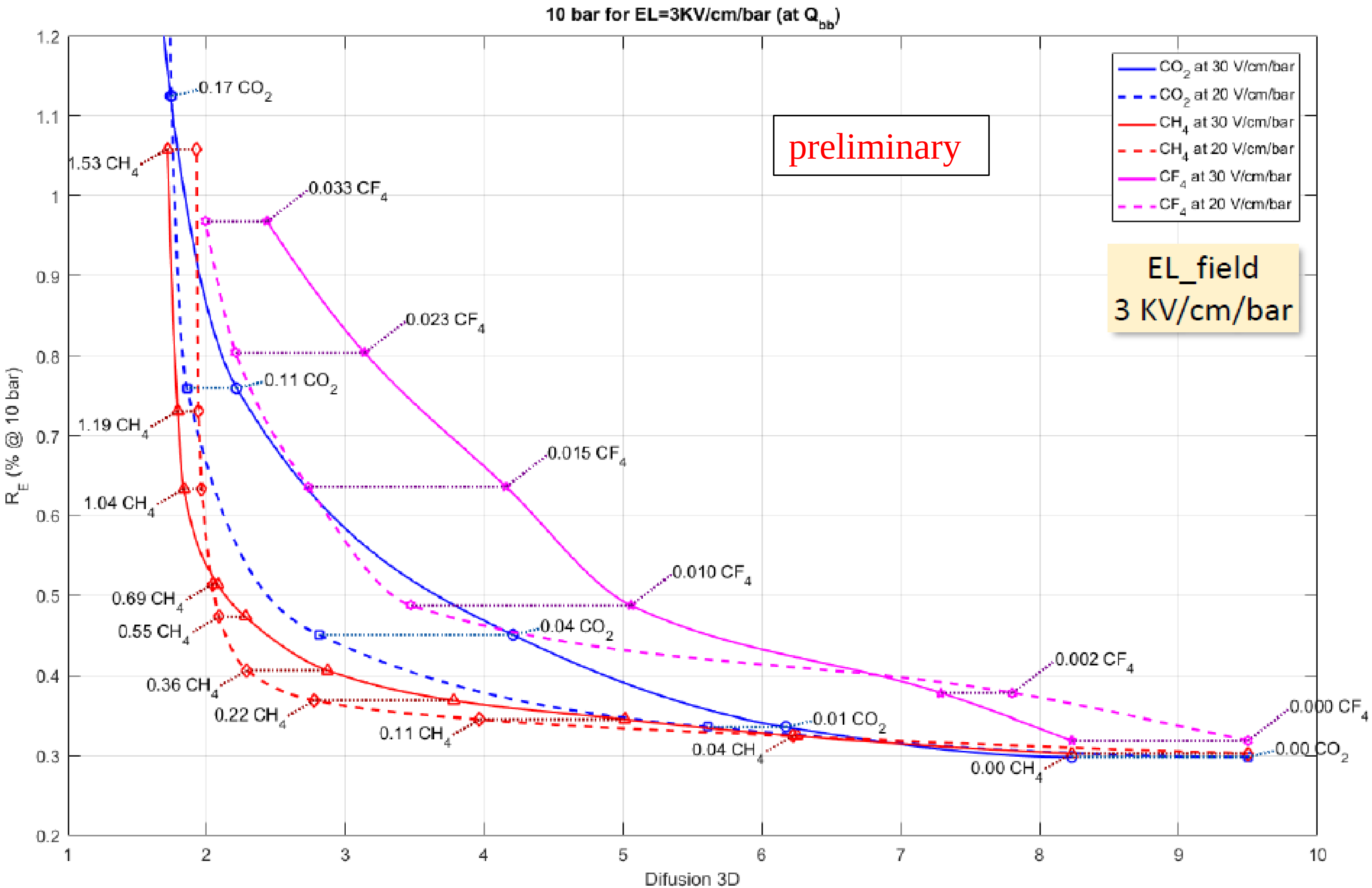


default model used in simulations



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

conclusions I (projections for NEXT)



conclusions II (Ozkan/Rob's feedback parameter β)

Secondary avalanches in gas mixtures

Özkan Şahin [a,*], İlhan Tapan [a], Rob Veenhof [b]

[a] Department of Physics, Uludağ University, 16059 Bursa, Turkey
[b] RD51 Collaboration, CERN, Genève, Switzerland

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

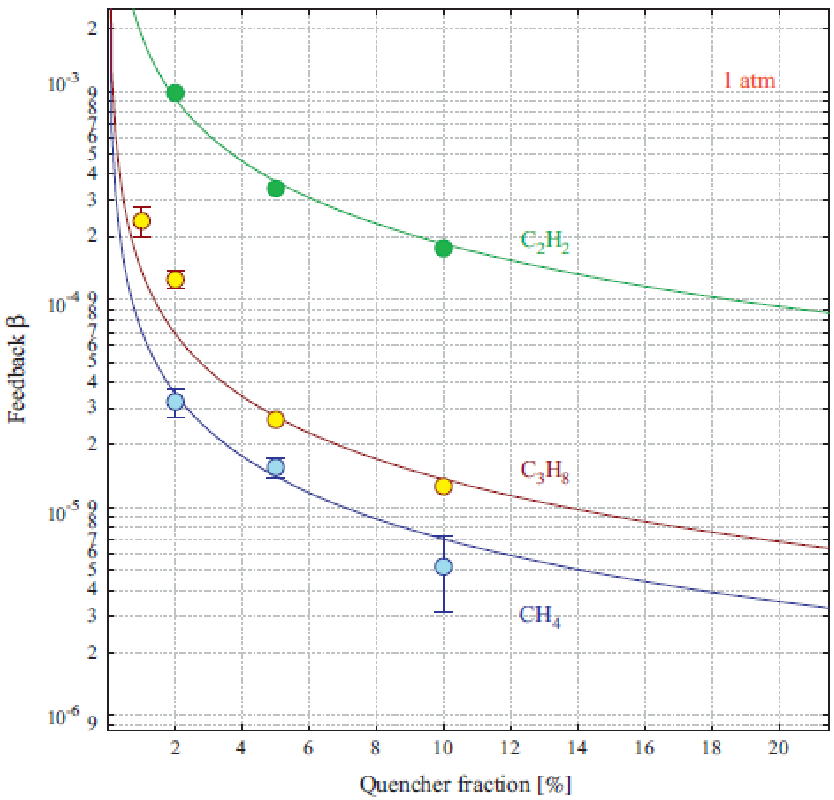


Fig. 2. Photon feedback β versus quencher fraction. The circles are fits using Eq. (1) and the solid lines are proportional to $1/f_q$

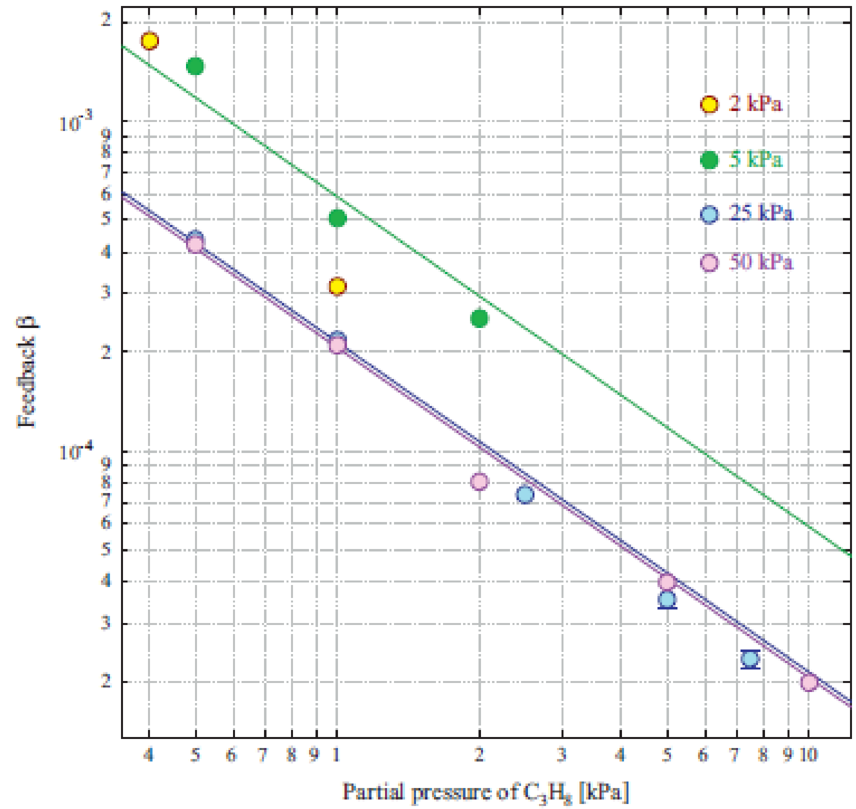
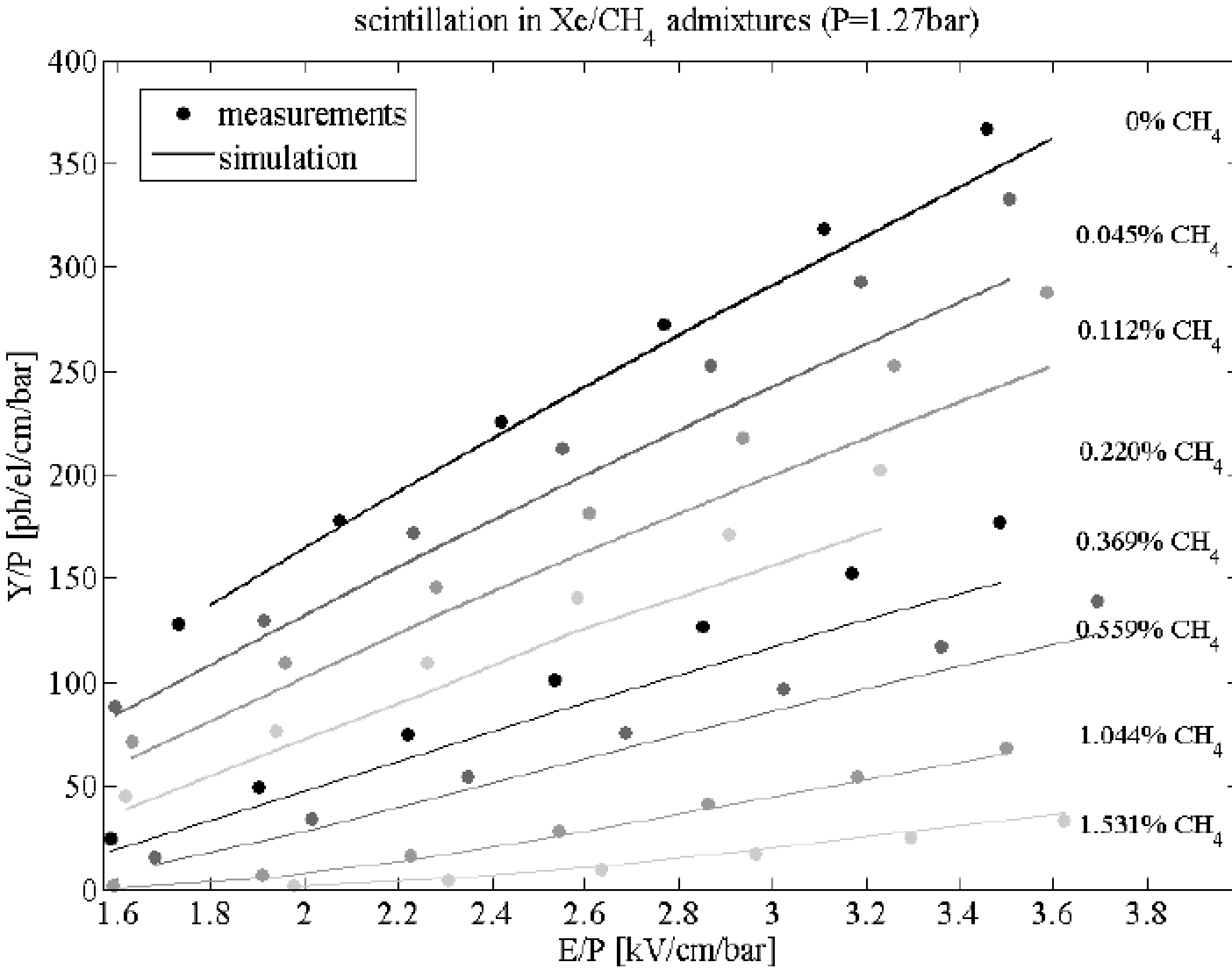


Fig. 3. Photon feedback β versus partial pressure of C_3H_8. The circles are fitted feedback parameters and the solid lines are the fits with $1/(f_q p_{gas})$.

VI. Appendix



scintillation in Xe/CH_4 admixtures (P=1.27bar)
measurements
simulation
0% CH_4
0.045% CH_4
0.112% CH_4
0.220% CH_4
0.369% CH_4
0.559% CH_4
1.044% CH_4
1.531% CH_4
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 $CO_2/CH_4/CF_4$