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Negative ion drift operation below the thermal limit





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NID observation





He:CF₄ 60:40 1 kV/cm (ED) He:CF₄:SF₆ 59:39.4:1.6 0.4 kV/cm (NID)

O(us) rise for ED O(ms) rise for NID

O(0.1 us) time extent for ED O(10 ms) time extent for NID

0.90 atm (LNGS atmospheric pressure)

Recap of measurements & observation



Drift velocity and diffusion measurements with He:CF4SF6

- Demonstration of NID operation at LNGS atmospheric pressure (900 mbar)
- Measured drift velocity and mobility consistent with literature

Diffusion measurements with He:CF₄ / He:CF₄SF₆ / CF₄SF₆

- He:CF₄ consistent with literature and Garfield++ simulation
- He:CF4:SF6 factor 3.6 below the thermal limit
- CF4:SF6 nearly at the thermal limit (slightly below, but uncertainty on the actual temperature of the gas during measurement)
- Results point towards Helium as the component inducing the lower than thermal diffusion
- Diffusion measurements He:CF4SF6 result so innovative and such beyond current expectation that we would like to aim at a very high impact journal (Nature/Science)
 - For this reason, extensive review focused on diffusion measurement only for the moment

G S Diffusion constant & coefficient vs drift field



Drift field below 300 V/cm introduce additional smearing from effects not depending on diffusion (i.e. disuniformities in the drift field): to not be considered for the final publication





sCMOS images analysis



- Alphas selection:
 - tracks reconstructed with iterative DBSCAN algorithm [10]
 - track length > 1.47 cm
 - track slimness < 0.3
 - # of peaks in the transverse profile == 1 (select single tracks)
 - Chi2/nDOF of transverse fit profile < 5 (remove additional multiple tracks)



[10] E. Baracchini et al, JINST 15 (2020) 12 T12003



Sigma of track profile and track integral fitted with Gaussian to estimate diffusion and light yield





Variables checked for track passing selection and used for the diffusion estimation

Integral, slimness, variance of diffusion RMS, tgausssigma, tgaussampl, lenght, width, alphas rate: all nicely Gaussian and following expected behaviour as a function of distance/drift field

Verified that tgausssigma * tgaussampl = integral

Repeated the analysis using tgaussigma as estimate of diffusion

All results (ED, NID1 and NID2) consistent with standard analysis

Checked the pedestal integral, RMS and mean for ED, NID1 and NID2

ED and NID1 consistent, NID2 slightly lower values

Check effect of DBSCAN reconstruction on final results

We are re-running a set of ED and NID1 data with larger and smaller sigma noise parameters of DBSCAN, stay tuned





Is the light yield affecting the diffusion measurements? No, will show in multiple ways and also repeat measurements

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Light yield vs distance vs drift field





Light yield is within a factor 2 between ED and NID1 NID1 has larger light yield than NID2, but show significantly smaller diffusion

S G **ED** measured diffusion independent of light yield



Diffusion measurement gain



Same diffusion coefficient measured for ED within nearly one order of magnitude light yield variation

Check track image "by eye"



(...big systematics from myopia... :D)

even though large systematic associated, track dimension by eye seems consistent with analysis results





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To convince without any possible doubt everybody we will:

1) repeat all the measurement again in a more consistent way and with 2 different light yield also for NID1(and NID2?)

2) perform diffusion measurement with varying concentration of Helium





Big uncertainty in the estimate of the constant σ₀ term: can you improve it it? YES

Fitting as a function of L/E



Note: all the data plotted together, i.e. 300 V/cm, 350 V/cm, 400 V/cm, 600 V/cm for 2, 3, 4, 6, 9 and 12 cm, i.e. 24 points per plot



<u>Consistency of all data when plotted</u> <u>together further strenghten our</u> <u>measurement and improves the</u> <u>estimate of all paramters</u>

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 $\label{eq:He:CF4} $$ He:CF_4 kT_{eff}/e = 0.0525 + - 0.0007 V $$ CF_4:SF_6 kT_{eff}/e = 0.0207 + - 0.0003 V $$ He:CF_4:SF_6 kT_{eff}/e = 0.00824 + - 0.0001 V $$ \end{tabular}$





- Many experimental and analysis aspects verified
- All of them results consistent with expectations and further strenghten the robustness of the measurements
- Final crosschecks under way
- New measurements foreseen in next 2 weeks to
 - show reproducibility
 - demonstrate once and for all diffusion measurement independence on light yield
 - improve consistency among different data taking point
 - test the performances with varying Helium concentration





Do we all agree in pushing for a very high impact journal and writing that our measurements are poses challenges to the current knowledge of ions transport properties in gases or do we want to aim at JINST and just publish the numbers?





Backup slides

Electrons diffusion during drift



$$\sigma^2 = 2Dt = \frac{2DL}{v_d} = \frac{2L}{E} \frac{D}{\mu}$$
$$v_d = \mu E$$

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Macroscopic quantities σ r.m.s. normal distance at time t D diffusion coefficient V_d constant drift velocity <<< c μ mobility

L = v_dt distance travelled after time t

- **Microscopic quantities**
- c instantaneous velocity between collisions
- lo mean free path of the drifting particle
- **τ** average time between collisions
- **N** number density

t o_{int} interaction cross section

$$\sigma^{2} = 2Dt = \int \left(\sum_{1}^{n} l_{i} \cos \theta_{i}\right)^{2} \prod_{1}^{n} g(l_{k}) dl_{k} \frac{d \cos \theta_{k}}{2} = n \frac{2}{3} l_{0}^{2} = \frac{2}{3} \frac{l_{0}^{2}}{\tau} t.$$

$$D = \frac{l_{0}^{2}}{3\tau} = \frac{c^{2} \tau}{3}$$





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lons diffusion during drift



$\sigma^2 = 2Dt = \frac{2DL}{v_d} = \frac{2L}{E}\frac{D}{\mu}$ $v_d = \mu E$

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Macroscopic quantities σ r.m.s. normal distance at time t **D** diffusion coefficient v_d constant drift velocity <<< c **u** mobility

 $L = v_d t$ distance travelled after time t

- **Microscopic quantities**
- c instantaneous velocity between collisions
- lo mean free path of the drifting particle
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- **N** number density
- σ_{int} interaction cross section

$$\sigma^{2} = 2Dt = \int \left(\sum_{1}^{n} l_{i} \cos \theta_{i}\right)^{2} \prod_{1}^{n} g(l_{k}) dl_{k} \frac{d \cos \theta_{k}}{2} = n \frac{2}{3} l_{0}^{2} = \frac{2}{3} \frac{l_{0}^{2}}{\tau} t.$$

$$D = \frac{l_{0}^{2}}{3\tau} = \frac{c_{rel}^{2} \tau}{3}$$



*Detector operated at LNGS (1100 m): atm pressure is 900 mbar

Experimental setup: the MANGO detector

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A MANGO "in the keg"



Longer drift distance is necessary to measure diffusion: MANGO was installed in a vacuum vessel that could host a longer field cage



Because of geometry constraints, the camera is now at 26.6 cm distance (w.r.t. 20.5 cm of the previous setup): the light yield reaching the camera sensor is reduced of 2/3 with respect to previous configuration

For this reason and in order to be able to measure the diffusion at ~15 cm drift length and low ~150 V/cm drift fields, we reduced the pressure to 650 mbar in the diffusion measurements

NOTE: diffusion is expected to be independent of pressure



fatto con tgaussigma





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 $\label{eq:heicF4} $$ He:CF_4 kT_{eff}/e = 0.0441 + - 0.0006 V $$ CF_4:SF_6 kT_{eff}/e = 0.0223 + - 0.0003 V $$ He:CF_4:SF_6 kT_{eff}/e = 0.0079 + - 0.0002 V $$$

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$$\sigma_{meas}(E,L) = \sqrt{\sigma_0^2(E) + \frac{2kT_{eff}L}{eE}} = \sqrt{\sigma_0^2(E) + \xi^2(E)L} = \sqrt{\sigma_0^2(E) + 2\delta(E)L}$$





Pedestal study CF4:SF6 data





He:CF4 &

He:CF4:SF6

data

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- NID1 2 cm 400 vcm 5803-5812
- NID1 12 cm 400 vcm 5941-5955
- NID1 6 cm 400 vcm 6273-6288
- ED 12 cm 400 vcm 6585-6594
- ED 2 cm 400 vcm 6921-6930
- ED 6 cm 400 vcm 7535-7544

dalla tesi di rita dipendenza Drift field





Figure 4.1: Drift field optimisation for CF_4 , He-40% CF_4 , and P-10: the normalised charge gain (left), scintillation yield (right), and corresponding energy resolution (bottom) are presented as a function of drift field. The curves are normalised to the first measurement, taken at the lowest drift field. Although these are experimental results, solid lines and coloured areas (3- σ confidence interval) are used to improve the plot legibility.

dalla tesi di rita dipendenza da Vgem





Figure 4.4: **GEM-induced scintillation yield in He-CF₄ mixtures:** the total emission (left) and visible component of the scintillation (right) are presented as a function of GEM bias. The measurements are depicted by the open triangles, whereas the solid lines illustrate the exponential trendlines fitted to each He-CF₄ mixture.

	He-30%CF ₄	$He-40\% CF_4$	$He-50\% CF_4$	$He-60\% CF_4$	$\mathbf{CF_4}$
Avalanche electrons					
β	0.0209(10)	0.0217(8)	0.0219(5)	0.0220(5)	0.0230(5)
$\eta_{e^-}^{ m max}$ (×10 ⁶)	1.26(6)	1.27(6)	2.04(10)	2.50(12)	1.93(10)
FWHM ^{min} [%]	13.47(16)	13.48(19)	14.50(14)	15.83(23)	21.79(23)
Total scintillation					
β	0.0207(13)	0.0216(11)	0.0216(8)	0.0216(7)	0.0229(7)
Y^{\max} (×10 ⁴)	2.13(14)	2.37(17)	4.10(30)	5.2(4)	5.5(4)
FWHM ^{min} [%]	20.5(5)	20.1(4)	19.55(27)	20.8(4)	26.81(29)
Visible scintillation					
β	0.0207(10)	0.0228(11)	0.0224(8)	0.0226(5)	0.0229(5)
$Y^{\max}(\times 10^4)$	1.47(21)	1.50(15)	2.14(21)	3.36(31)	4.1(4)
FWHM ^{min} [%]	20.10(32)	20.09(31)	20.20(27)	20.82(30)	26.17(26)



Molecular structures







Octahedral

6

sp³d²

26

S **SF₆ Molecular orbital structures** G



Molecular Orbitals in SF₆

The Lewis structure of SF6 describes six pairs of electrons as bond pairs, despite the availability of only four valence orbitals on sulphur. The valence bond description of this hypervalent complex must therefore invoke d-orbitals. However, high-level theoretical calculations suggest that the electronic structure involves not d-orbitals and six bonds, but instead only four bonds. each delocalized over all seven atoms.

O _h	Е	8C3	6C ₂	6C4	$3C_2$	í	6S₄	$8S_6$	$3\sigma_h$	$6\sigma_d$	
A _{1g}	1	1	1	1	1	1	1	1	1	1	$x^{2} + y^{2} + z^{2}$
A _{2g}	1	1	-1	-1	1	1	-1	1	1	-1	
E _g	2	-1	0	0	2	2	0	-1	2	0	$(z^2, x^2 - y^2)$
T ₁₉	3	0	-1	1	-1	-1	1	0	-1	-1	
T _{2g}	3	0	1	-1	-1	-1	-1	0	-1	1	(xy,xz,yz)
A _{1u}	1	1	1	1	1	1	-1	1	-1	-1	
A _{2u}	1	1	-1	-1	1	1	1	1	-1	1	
Eu	2	-1	0	0	2	2	0	-1	-2	0	
T _{1u}	3	0	-1	1	-1	-1	-1	0	1	1	(x,y,z)
T _{2u}	3	0	1	-1	-1	-1	1	0	1	-1	

Four S AOs:



The six F 2s orbitals give linear combinations that transform as a1g eg and t1u, but they are very low in energy and remain effectively non-bonding. The eighteen F 2p orbitals give linear combinations transforming as $a_{1g} e_g t_{1g} t_{2g} 2 \times t_{1u}$ and t_{2u} . Most of these remain non-bonding, but four combinations, and one of the t₁₀ sets, can overlap with the S AOs to give four bonding and four anti-bonding MOs. Shown below are all four bonding MOs and one of each symmetry of the F 2p non-bonding MOs.

Selected MOs of SF





The resulting MO diagram contains:

- 6 non-bonding MOs derived from F 2s AOs
- 4 bonding and 4 anti-bonding MOs of a_{1g} and t_{1g} symmetry, derived from F 2p AOs
- 14 non-bonding MOs, also derived from F 2p AOs

The 48 valence electrons of SF₆ fill the first 24 available MOs: 20 non-bonding and 4 bonding MOs. This leads to an interpretation that is different than that of the Lewis structure: not 18 LPs and 6 BPs, but 20 F-based lone pairs and only 4 bond pairs! The total bond order equals 4, or an "average" of only 2/3 bond per S-F interaction. In MOT, hypervalency manifests as electron-deficient bonding, with fewer than 2 bonding electrons per formal bonding interaction. Weird. Eerie.

CF4 Molecular orbital structures



