SIMULATED ATTACHMENT

A closer look at PyBoltz Attachment

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OVERVIEW

- Introduction and background
- Pure O_2
- CF_4
- C_2H_4, H_2O, and O_2
- Argon PyBoltz vs MagBoltz
- P-10
- Argon oxygen mixtures

INTRODUCTION

- I spoke at the Monday MPD meeting June 15th (https://indico.fnal.gov/event/43887/)
- Using PyBoltz to simulate and understand electron drift properties.
- Showed PyBoltz attachment to oxygen under several conditions. Cross checking PyBoltz reported attachments.
- Comparing PyBoltz attachment output to several papers on oxygen attachment.
- Also checking MagBoltz (Andrew Cudd)

PURE OXYGEN

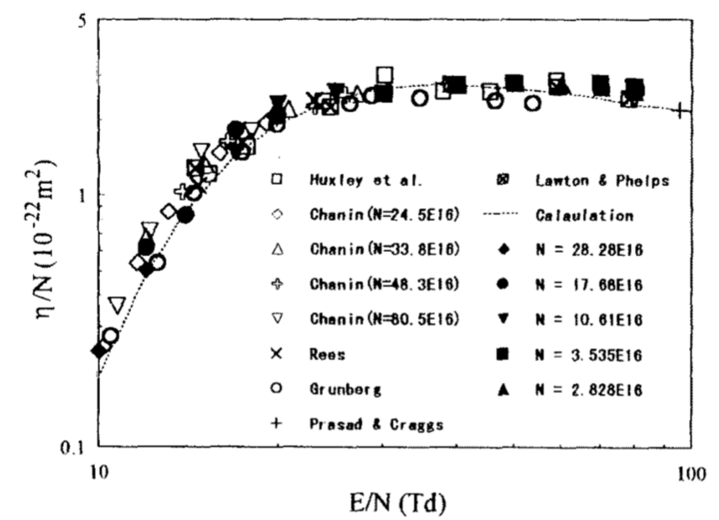


Figure 3. The density normalized electron attachment coefficients, η /N, as a function of E/N being two-body attachment processes in pure oxygen.

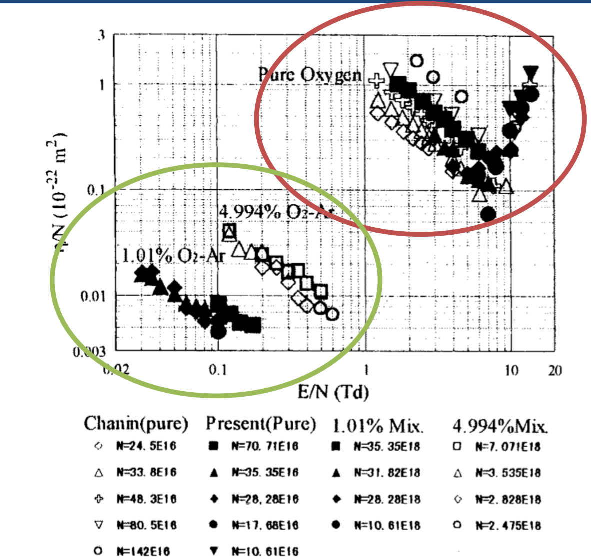


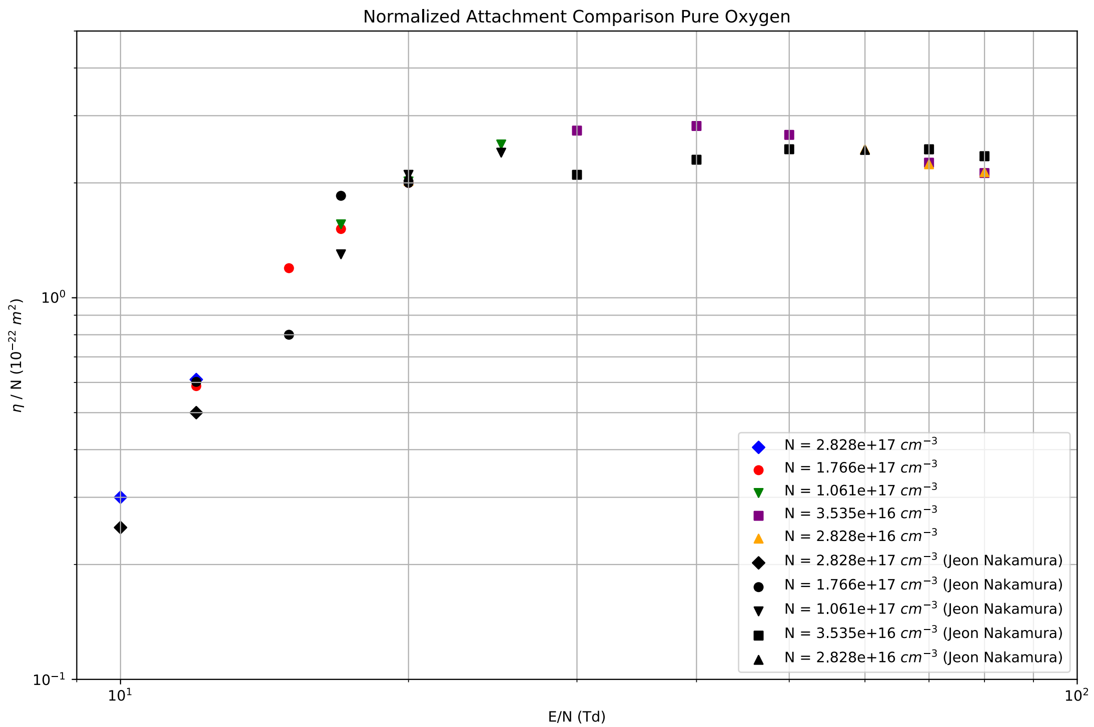
Figure 6. The density normalized electron attachment coefficients, η /N, as a function of E/N being three-body attachment processes in pure oxygen and in oxygen-argon mixtures.

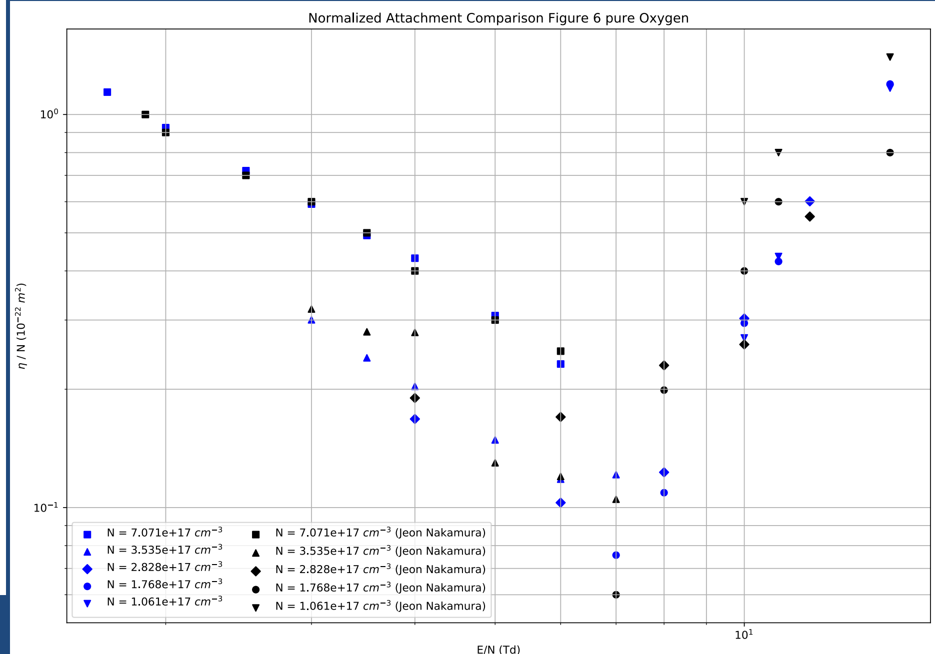
Jeon, B. H., & Nakamura, Y. (1998). Measurement of Electron Attachment Coefficient in Oxygen and Oxygen-Argon Mixtures. *IEEJ Transactions on Fundamentals and Materials*, *118*(7-8), 874-879.

- Looking at normalized attachment $\frac{\eta}{N}$ for Jeon Nakamura figures 3 and 6.
- N the gas number density determines the settings to run PyBoltz.
  - $N = \frac{n}{V} = \frac{P}{RT}$
- Start by looking at pure oxygen
- Look at 4.994% and 1.01% at the end.

PURE OXYGEN

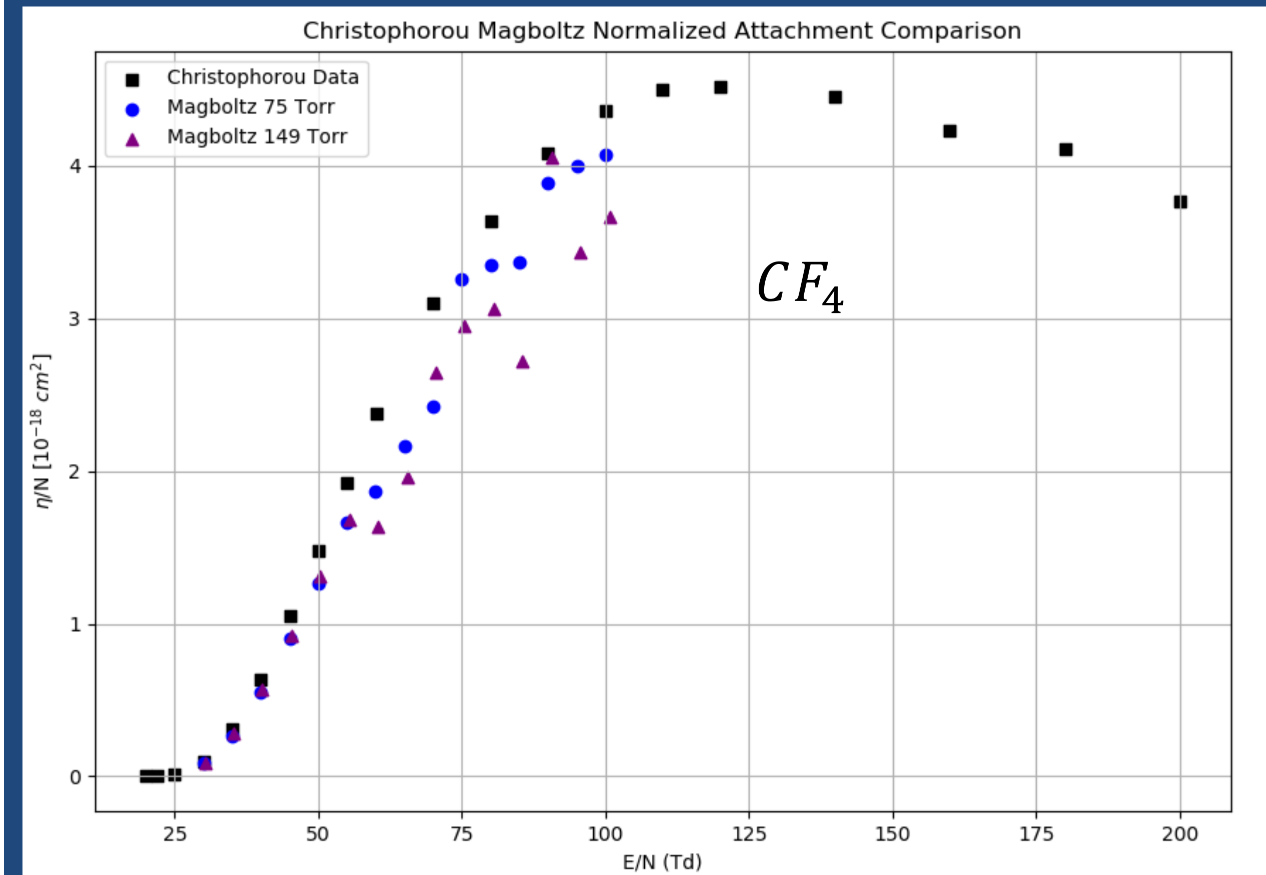
- Simulations match data





Color points PyBoltz simulation
Black points are data

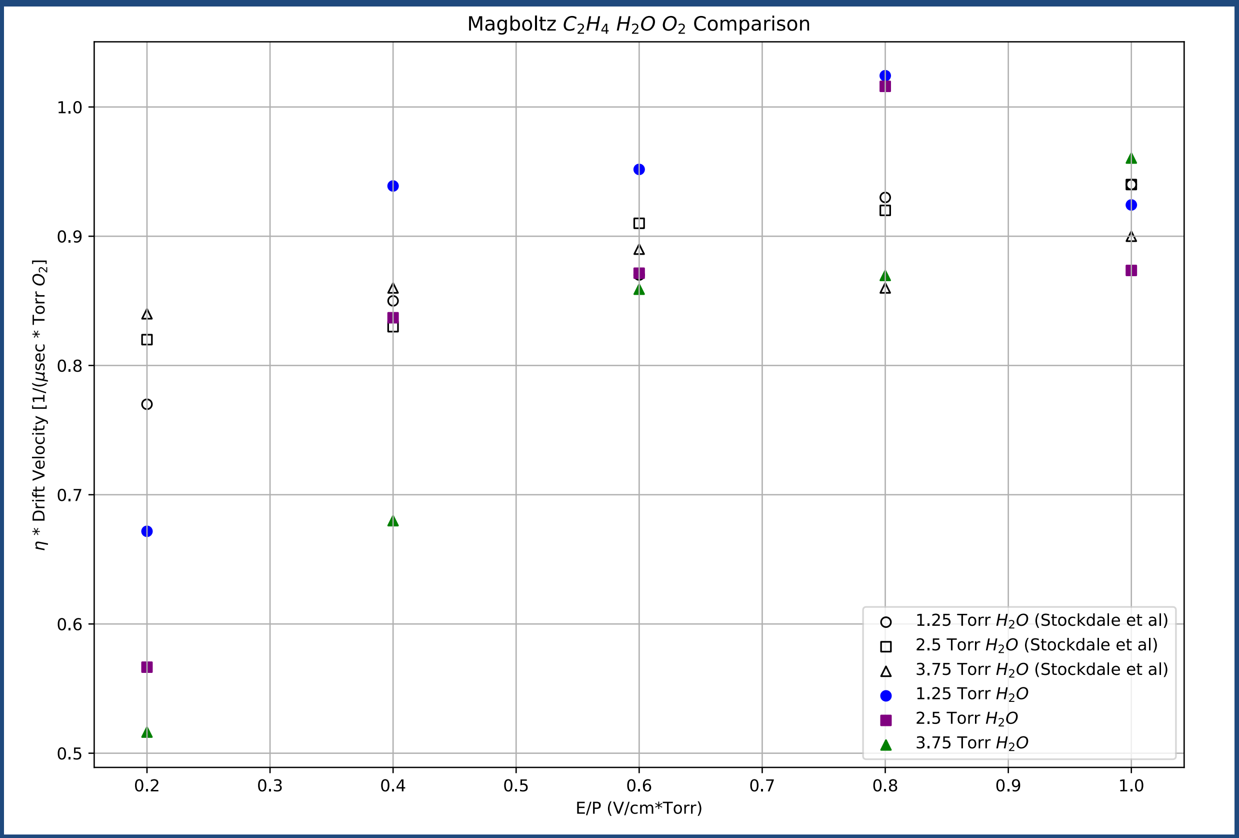
CF_4



J. Chem. Phys. **86**, 693 (1987); https://doi.org/10.1063/1.452272
S. R. Hunter, J. G. Carter, *and* L. G. Christophorou

- MagBoltz attachment matches CF_4 data.

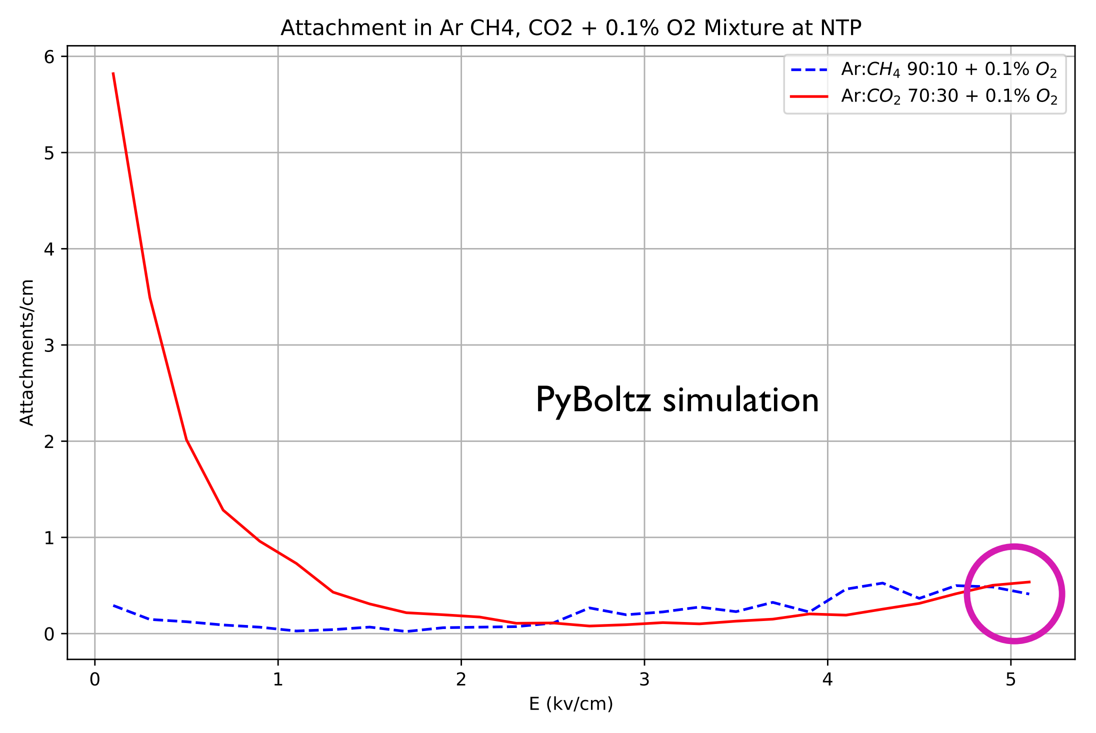
ETHYLENE : WATER : OXYGEN



J. Chem. Phys. **47**, 3267 (1967); https://doi.org/10.1063/1.1712388
J.A. Stockdale, L. G. Christophorou, *and* G. S. Hurst

- Data and simulation agree within 0.35 $\eta * D_V$ (not so well at low E/P)
- The discrepancy between this data and simulation is not multiple orders of magnitude off…

ARGON-METHANE, ARGON CARBON DIOXIDE (PYBOLTZ VS MAGBOLTZ)



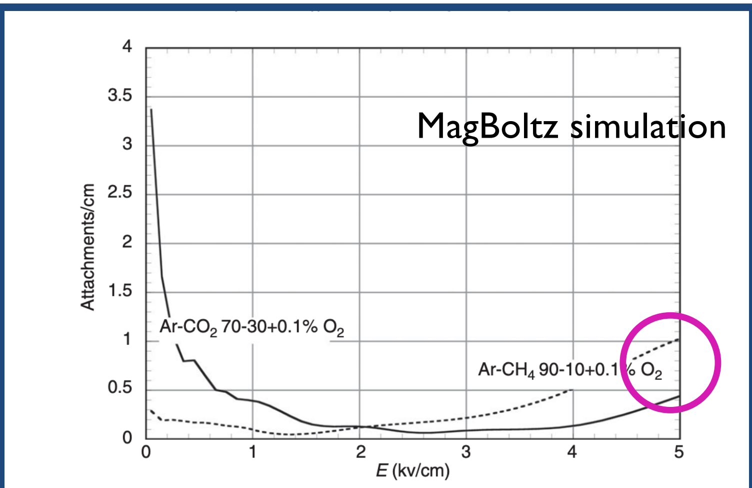


Figure 4.69 Electron attachments/cm as a function of field for equal addition of oxygen to argon–carbon dioxide and argon–methane mixtures.

Sauli, F. (2014). *Gaseous radiation detectors : Fundamentals and applications*. Retrieved from https://ebookcentral.proquest.com

- Similar results
- MagBoltz version from 2014 or earlier.

P-10 AND OXYGEN

Table 4
Attachment to O_2 as a function of the argon/methane ratio. Gas: argon/methane = 90/10, 80/20; with 200 ppm oxygen. Pressure: 4 bar.

argon / methane	E/P [V/cm bar]	v [cm/μs]	A [μs^{-1}]	$C_{O_2,M}$ [μs^{-1} bar^{-2}]
90/10	100	5.36	0.048 ± 0.003	15.1 ± 1.5
	138	5.45	0.034 ± 0.003	10.5 ± 1.4
	163	5.32	0.029 ± 0.003	9.2 ± 1.4
	200	5.07	0.024 ± 0.003	7.4 ± 1.3
	250	4.70	0.019 ± 0.003	5.9 ± 1.1
80/20	100	5.54	0.102 ± 0.006	32.0 ± 3.0
	138	6.61	0.098 ± 0.007	30.6 ± 3.3
	163	6.91	0.089 ± 0.007	27.7 ± 3.2
	200	7.08	0.074 ± 0.007	23.1 ± 3.1
	250	7.10	0.069 ± 0.007	21.5 ± 3.0

Nuclear Instruments and Methods in Physics Research A267 (1988). Electron Attachment to Oxygen, Water, and Methanol, In Various Drift Chamber Gas Mixtures. M. Huk, P. Igo-Kemenes, and A. Wagner

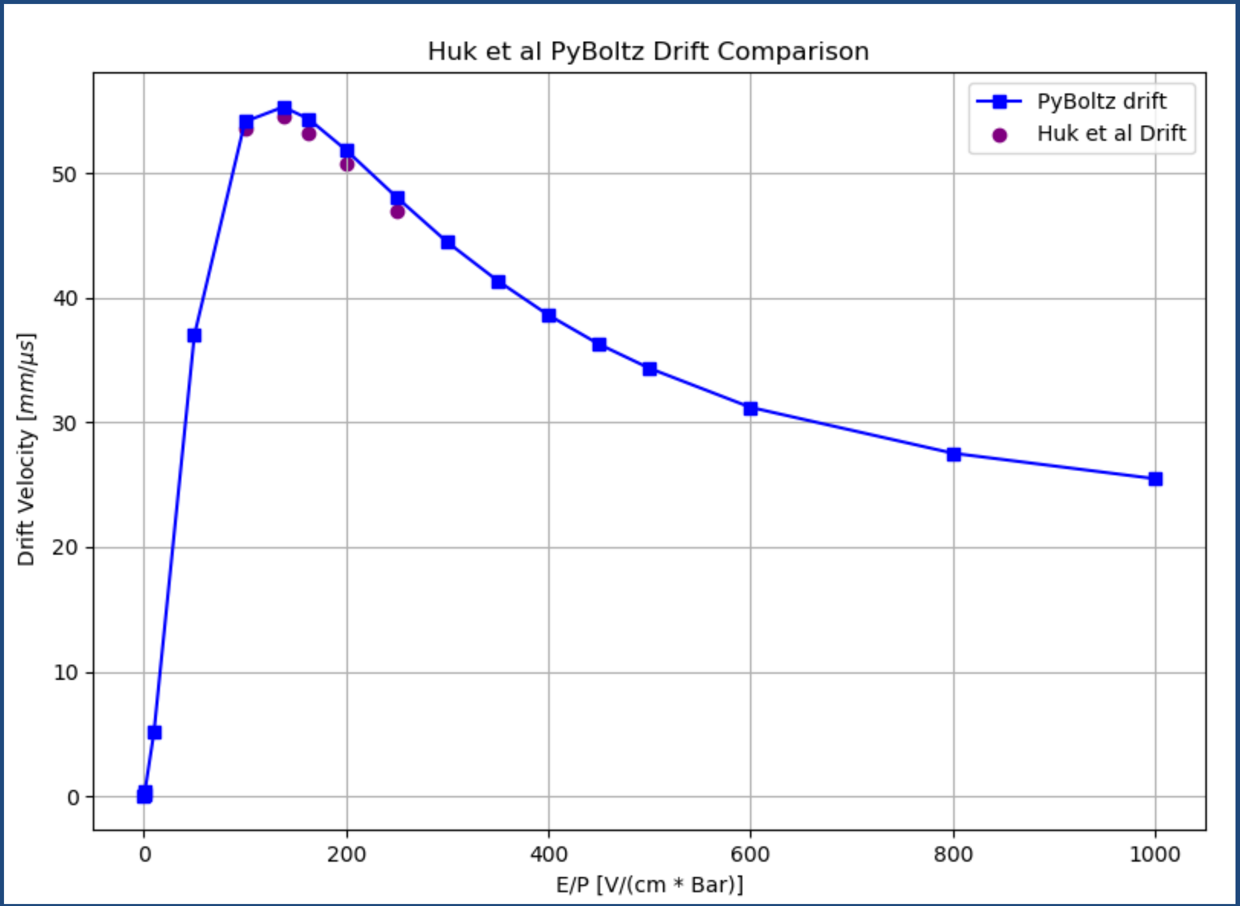
Pg 113 Electron attachment in drift chamber gas mixture

- Huk calls:
  - $C_{O_2,M}$: the Attachment coefficient
  - A: the attachment rate (found by partial pressures and attachment coefficient)
    - $N(t) = N(0)e^{-At}$
    - $N(s) = N(0)e^{\frac{-s}{\lambda}} \Longrightarrow A = \frac{v}{\lambda}$
    - however this does not appear to be the case: off by a factor of 100

$\frac{Argon}{Methane}$	E/P $[\frac{V}{cm*Bar}]$	v $[\frac{cm}{\mu s}]$	Attachment rate $[\mu s^{-1}]$
$\frac{90}{10}$	100	5.41	$(4.999) \pm (1.55 * 10^{-3})$
	138	5.53	$(3.788) \pm (1.03 * 10^{-3})$
	163	5.43	$(3.155) \pm (8.25 * 10^{-4})$
	200	5.18	$(3.004) \pm (8.75 * 10^{-4})$
	250	4.81	$(2.261) \pm (6.97 * 10^{-4})$

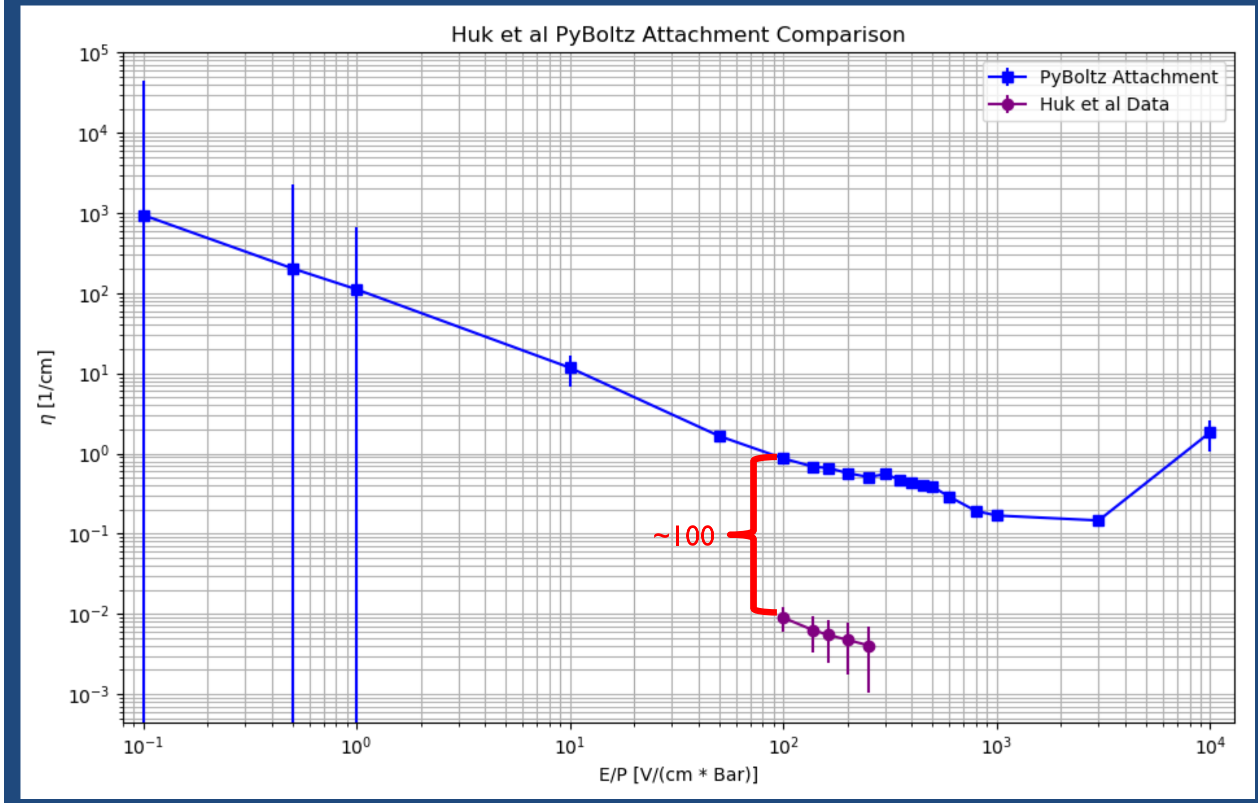
PyBoltz simulation data

P-10 DRIFT



- Drift velocity lines up well
- Discrepancy in attachment does not lie with drift velocity difference.

P-10 AND OXYGEN ATTACHMENT



- 1/λ not reported in paper.
  - Convert A to 1/λ,: $1/\lambda_{Huk} = \frac{A}{v}$
- Even though the drift matches attachment is ~2 orders of magnitude off.

ARGON : METHANE : ISOBUTANE (88:10:2)

About a factor of 100 to 200 off.

Table 2 [a)]
Attachment to O_2 as a function of the O_2 concentration. Gas: argon/methane/isobutane = 88/10/2. Pressure: 4 bar.

E/P [V/cm bar]	$[O_2]$ [ppm]	v [cm/μs]	A [μs^{-1}]	$C_{O_2,M}$ [μs^{-1} bar^{-2}]
100	50	4.67	0.062 ± 0.005	77.7 ± 10.5
	100	4.67	0.111 ± 0.005	69.5 ± 6.7
	200	4.67	0.215 ± 0.007	67.1 ± 4.9
	300	4.67	0.353 ± 0.011	73.7 ± 5.1
	440	4.67	0.566 ± 0.019	80.4 ± 5.6
200	50	5.43	0.037 ± 0.005	46.1 ± 9.4
	100	5.43	0.066 ± 0.005	41.3 ± 5.3
	100	5.43	0.130 ± 0.006	40.6 ± 3.6
	300	5.43	0.199 ± 0.008	41.5 ± 3.1
	440	5.43	0.287 ± 0.009	40.8 ± 2.8

Nuclear Instruments and Methods in Physics Research A267 (1988). Electron Attachment to Oxygen, Water, and Methanol, In Various Drift Chamber Gas Mixtures. M. Huk, P. Igo-Kemenes, and A. Wagner.

Pg 112 table 2.

E/P $[\frac{V}{cm*Bar}]$	$O_2[ppm]$	v $[\frac{cm}{\mu s}]$	Attachment rate $[\mu s^{-1}]$
	50	4.53	$(1.459) \pm (3.29 * 10^{-4})$
	100	4.53	$(2.858) \pm (9.01 * 10^{-4})$
100	200	4.52	$(6.143) \pm (2.87 * 10^{-3})$
	300	4.52	$(8.606) \pm (4.75 * 10^{-3})$
	440	4.51	$(13.12) \pm (8.93 * 10^{-3})$
	50	5.42	$(0.997) \pm (1.62 * 10^{-4})$
	100	5.43	$(2.058) \pm (4.77 * 10^{-4})$
200	200	5.42	$(3.978) \pm (1.29 * 10^{-3})$
	300	5.42	$(6.157) \pm (2.48 * 10^{-3})$
	440	5.42	$(8.726) \pm (4.18 * 10^{-3})$

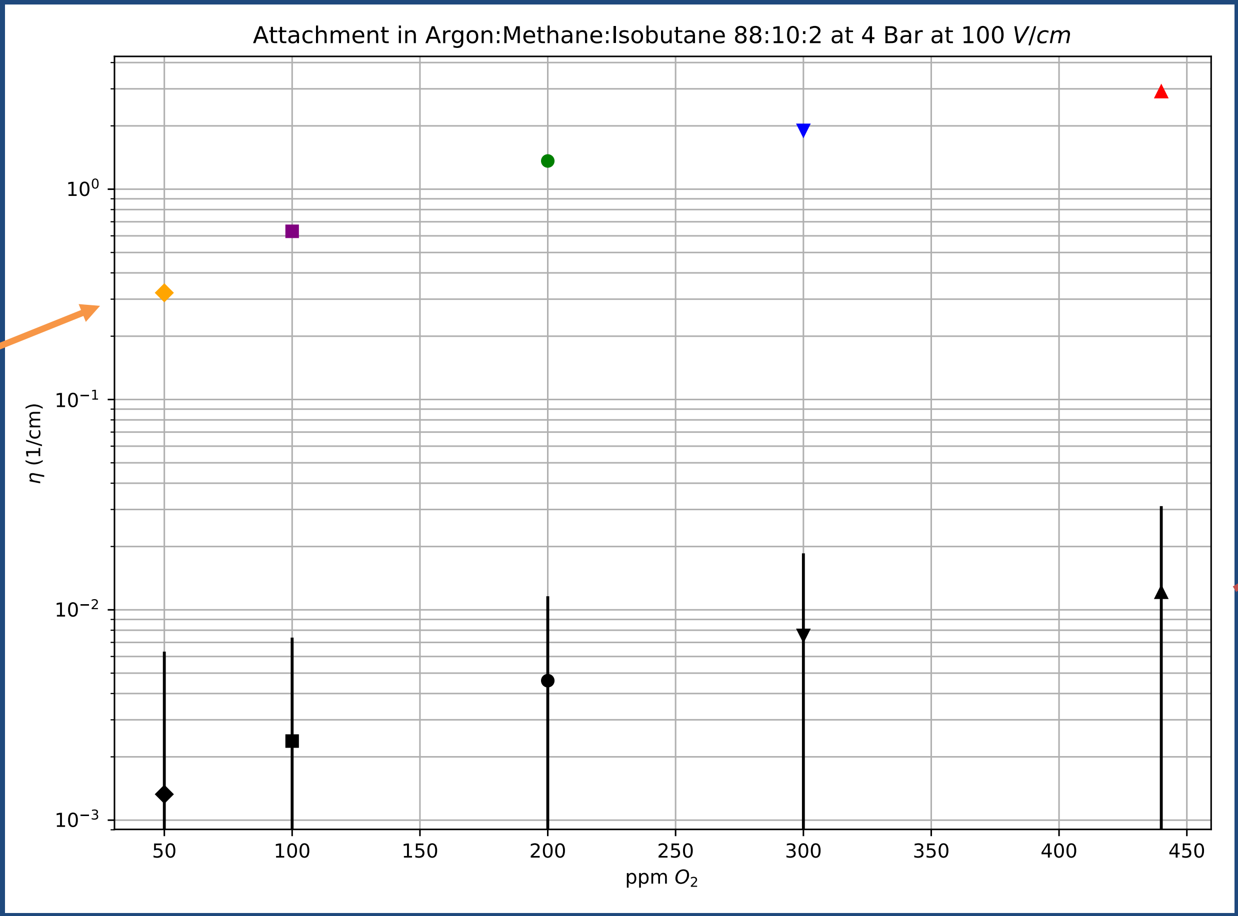
Table 1: PyBoltz Output for comparison of Huk et al table 2. 88:10:2 Argon:Methane:Isobutane + Oxygen mixture at 4 Bar (I assume temp of 23 C)

PyBoltz simulation data

ARGON : METHANE : ISOBUTANE (88:10:2)

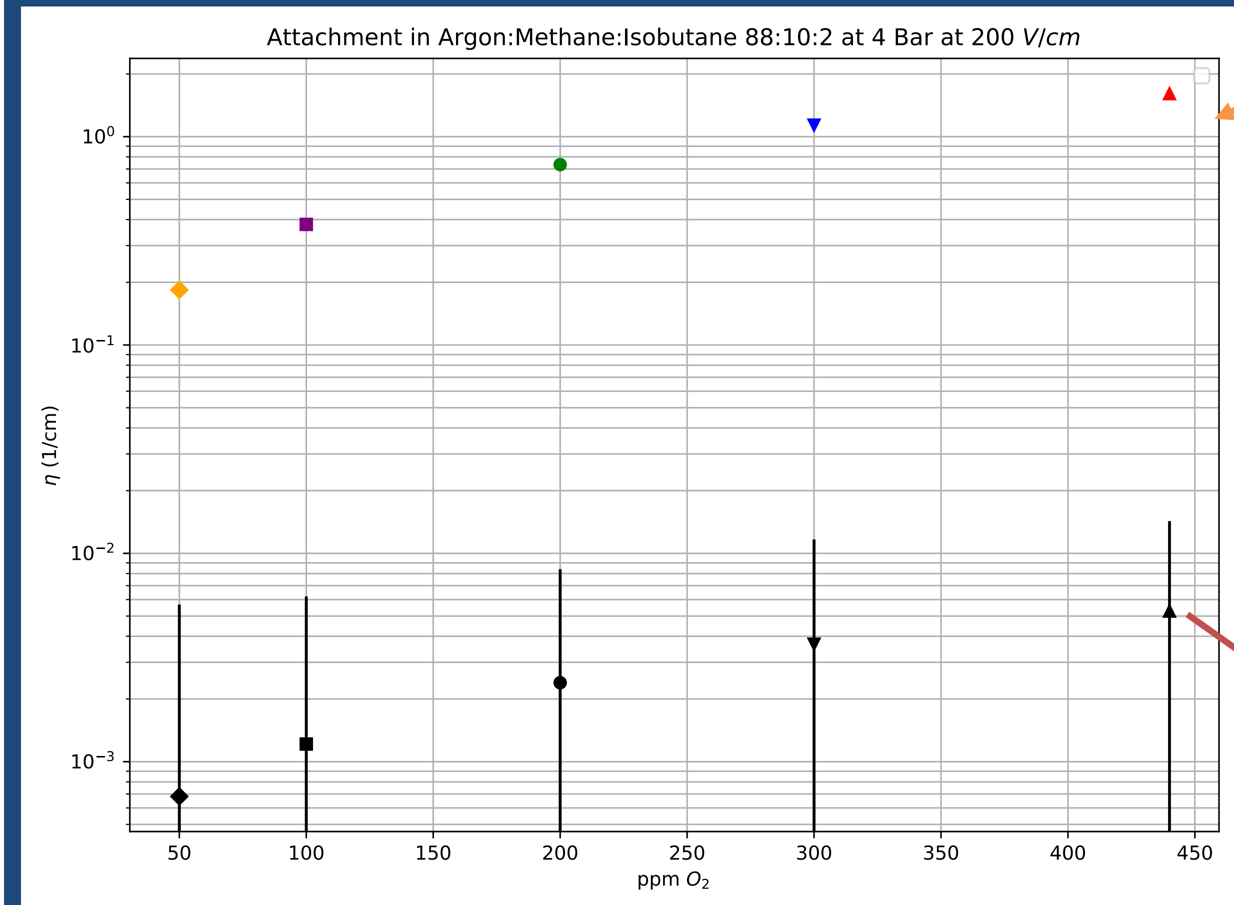
Huk data and PyBoltz ~2 orders of magnitude apart for any given ppm O_2.

PyBoltz sim data



Huk data

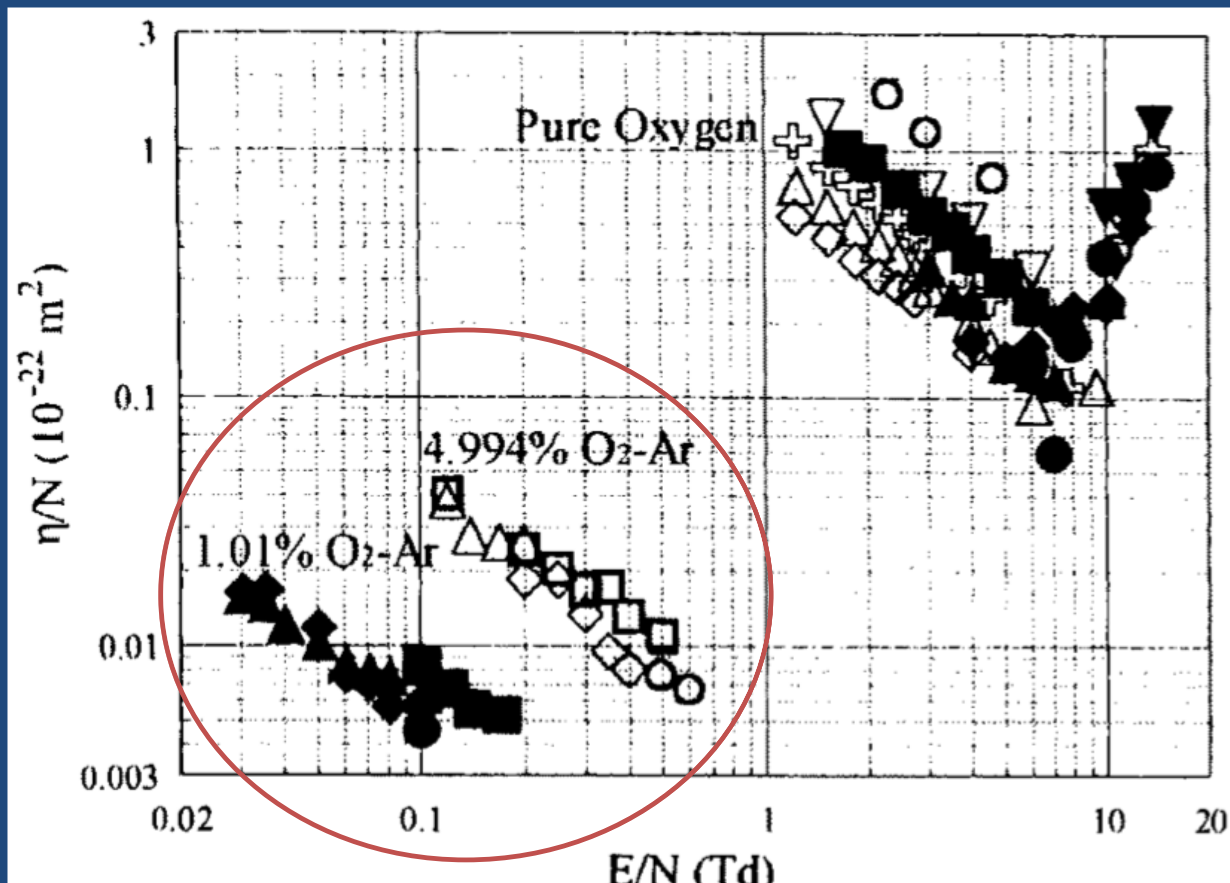
ARGON : METHANE : ISOBUTANE (88:10:2)



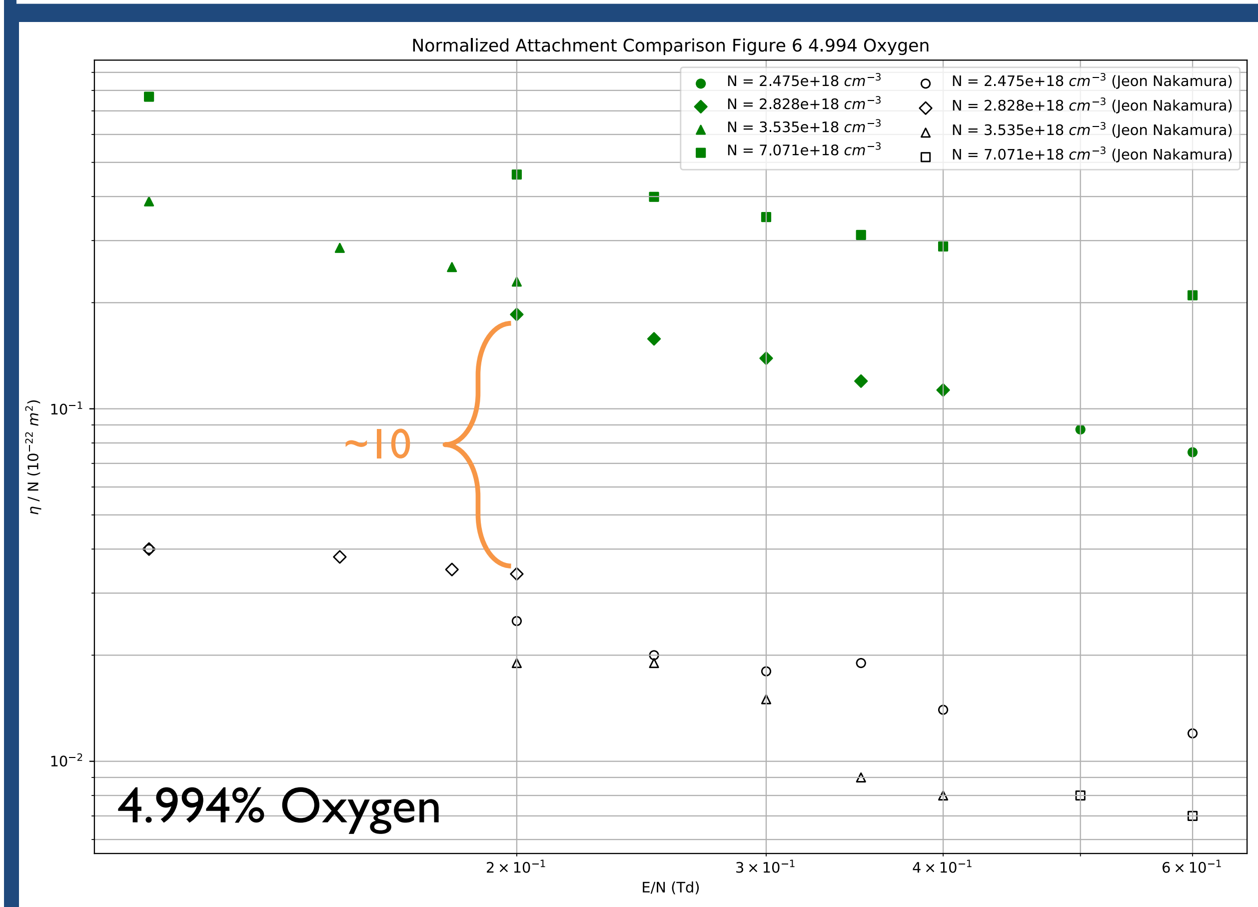
PyBoltz sim data

Huk data

ARGON : OXYGEN

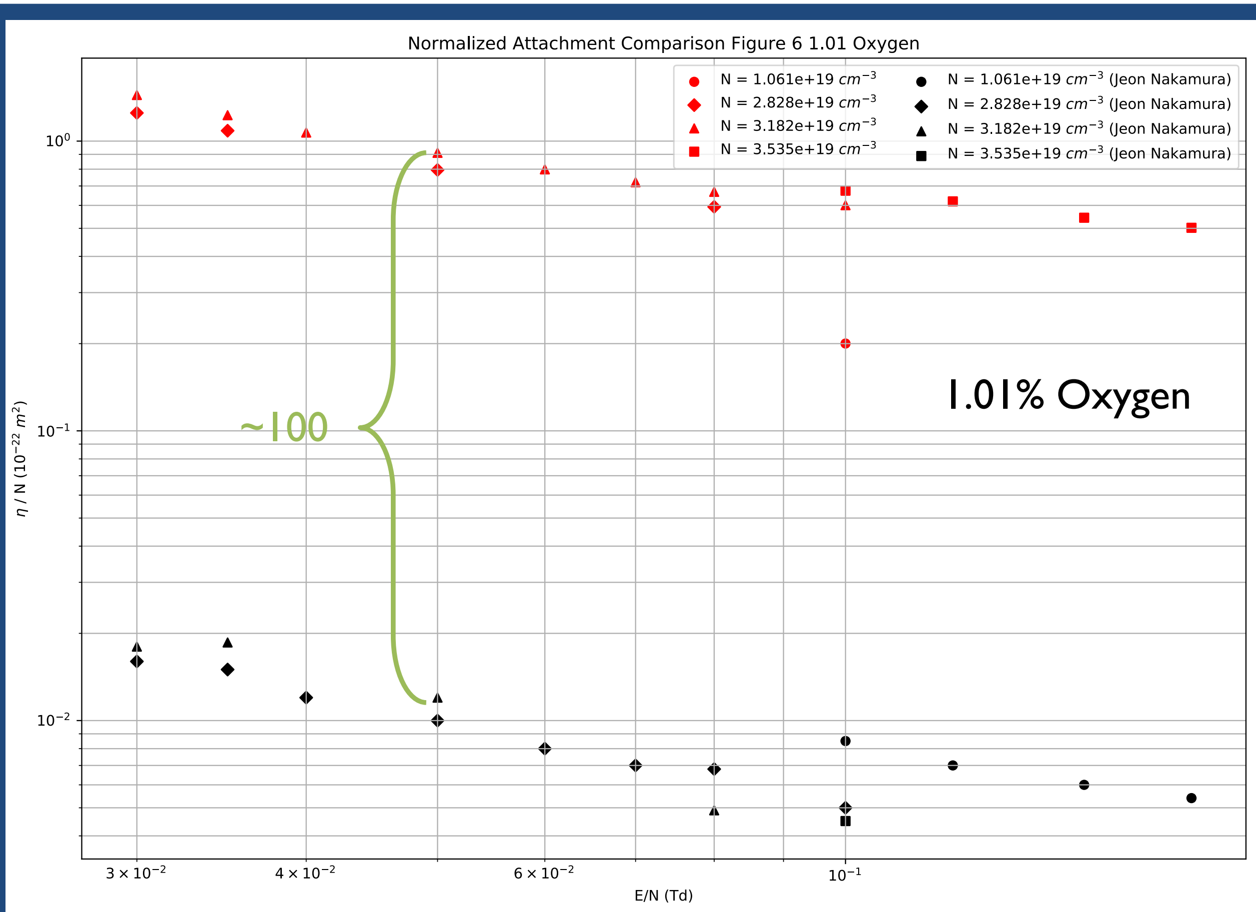


ARGON : OXYGEN (95.006:4.994)



- Again a difference of difference of ~10 for ~5% O_2

ARGON : OXYGEN (98.99:1.01)



Again a difference of ~100 for ~1% O_2

SUMMARY

- PyBoltz and MagBoltz attachment line up closely but not perfectly (Expected).
- MagBoltz (and PyBoltz) can match attachment rates for CF_4 and pure O_2. Starts to vary when more than one gas is simulated.
- MagBoltz attachment comparison in C_2H_4, H_2O, and O_2 might suggest that the issue lies with Argon.
- We're seeing a difference of 2 orders of magnitude for ~1% and 0.02% (200 ppm) O_2 in Argon, methane mixture and 0.005% - 0.044% (50 – 440 ppm) O_2 in an ~88:10:2 $\mathrm{Ar}:CH_4:C_4H_{10}$ mixture
- A difference of ~1 order of magnitude for ~5% O_2 (~95% Argon).
- Data is reported in the 3-body attachment region. Noticing incorrect attachment for Argon in the 3-body regime in simulations.