# Ion mobility in Ne-$CO_2$-$N_2$ mixtures

Pedro Encarnação
Laboratório de Instrumentação e Física Experimental de Partículas (LIP-Coimbra)
Physics Department
University of Coimbra
Coimbra, Portugal
E-mail: pedro.crispim.encarnacao@gmail.com

1 Basic Concepts

2 Experimental Setup and Working Principle

3 Ion Identification Process

4 Experimental results in:

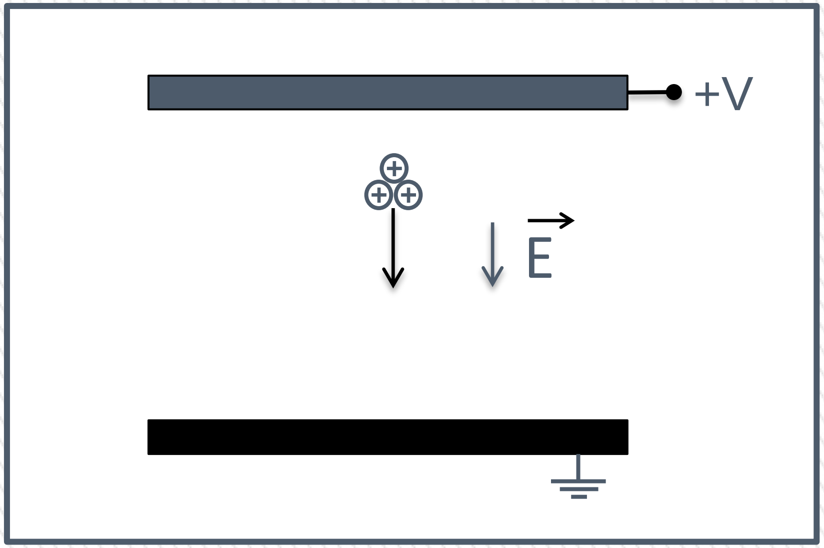
- a Ne, $CO_2$, $N_2$
- b Ne-$CO_2$, Ne-$CO_2$-$N_2$

5 Ion Mobility resume:

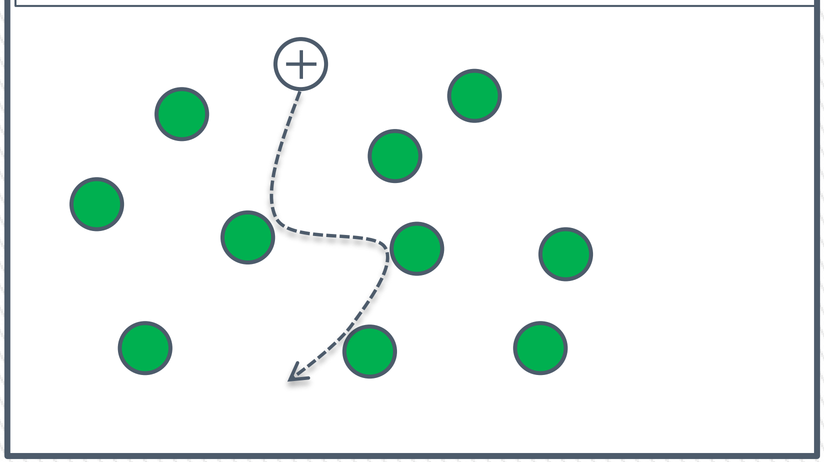
- a Ar-$CO_2$, Xe-$N_2$, Ar-$CH_4$, Ar-$C_2H_6$, Ne-$CO_2$, Xe-TMA

# Basics

Let us consider a group of ions moving in a gaseous medium under the influence of a uniform electric field…




**Microscopically …**



### Drift velocity

$$v_d = KE$$

E- Electric Field

K-Ion Mobility

### Reduced Mobility

$$K_0 = KN/N_0$$

N – Gas number density

$N_0$–Loschmidt Number

### Langevin Limit

$$K_0 = 13.88\left(\frac{1}{\alpha\mu}\right)^{\frac{1}{2}}$$

μ – reduced mass

α – neutral polarizability

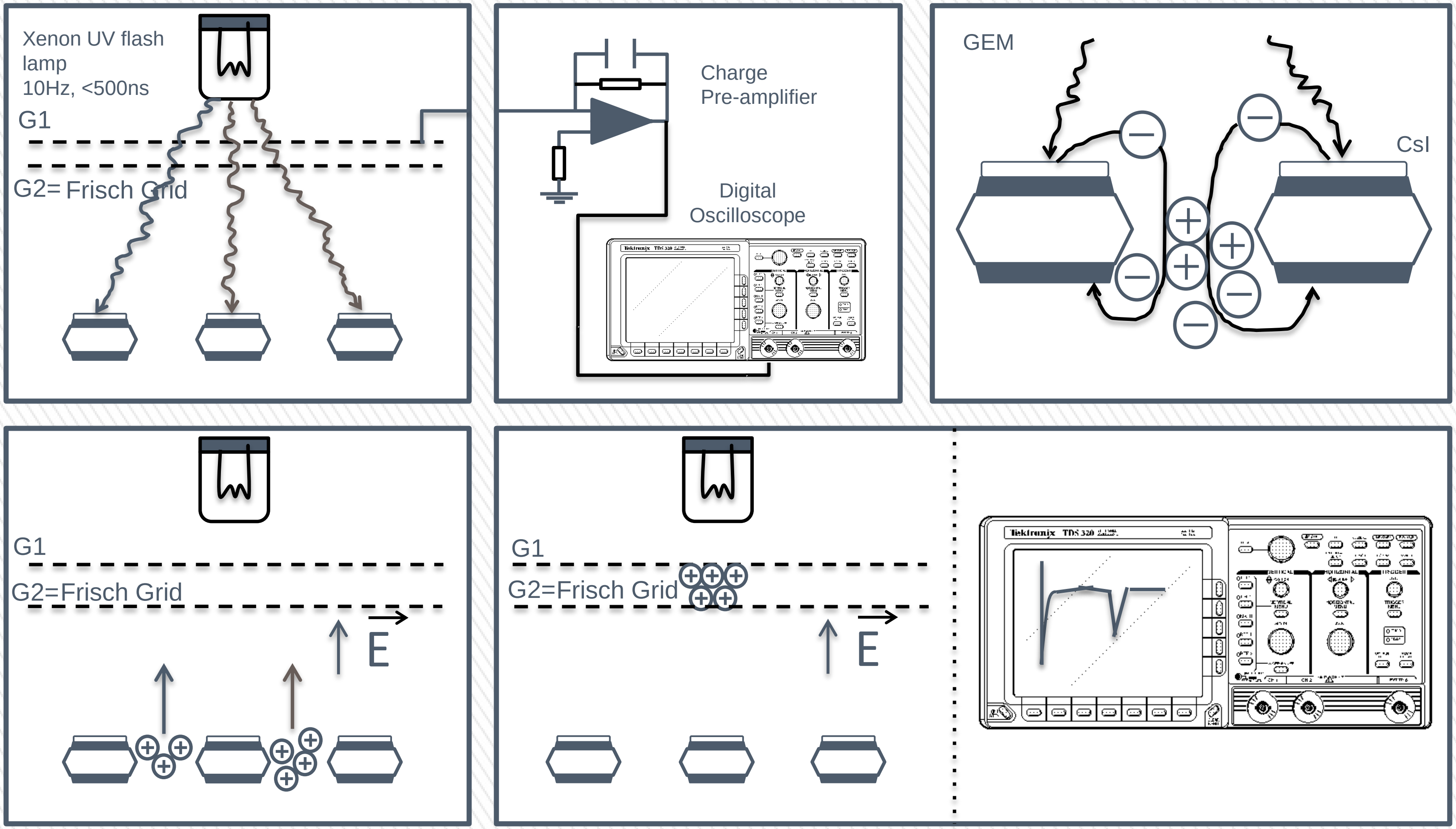
### Blanc's Law

$$\frac{1}{K_{0mix}} = \frac{f_1}{K_{0g1}} + \frac{f_2}{K_{0g2}}$$

$f_1$,$f_2$– molar fraction of gas 1, 2

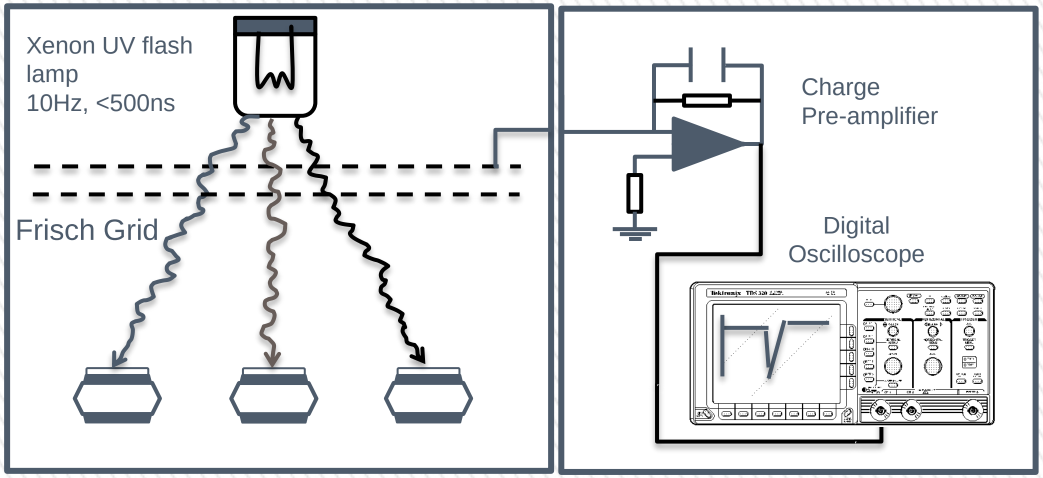
$K_{0g1}$, $K_{0g2}$ – ion mobility in the gas 1 and 2

# Experimental Setup and Working Principle




(Neves, Conde and Távora, 2007)

# Experimental Setup and Working Principle



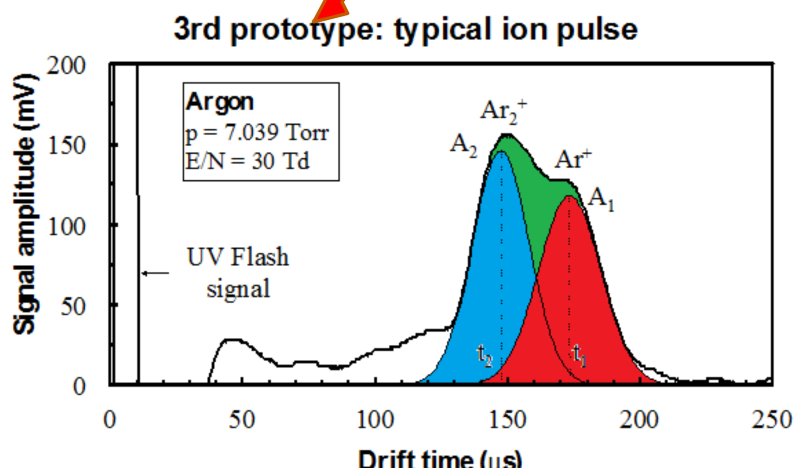

- Subtract the background to the signal
- Identify possible peaks
- Fit Gaussian curves to the peaks obtained

**Peaks centroids**

↓

average drift time of the ion's distribution ($t_{\mathrm{drift}}$)

$$v_{\mathrm{d}} = \frac{x_{drift}}{t_{drift}} \rightarrow K = \frac{v_{\mathrm{d}}}{E}$$




$K_{01}$ = 1.57 $cm^2V^{-1}s^{-1}$ ($Ar^+$)
$K_{02}$ = 1.92 $cm^2V^{-1}s^{-1}$ ($Ar_2^+$)

# Ion Identification Process

**Identification of candidate ions**

- GEM Voltage
- Possible Reactions
  - Cross Section
  - Reaction Rates

**Selection of Candidate ions**

+

**Calculation of expected mobility**

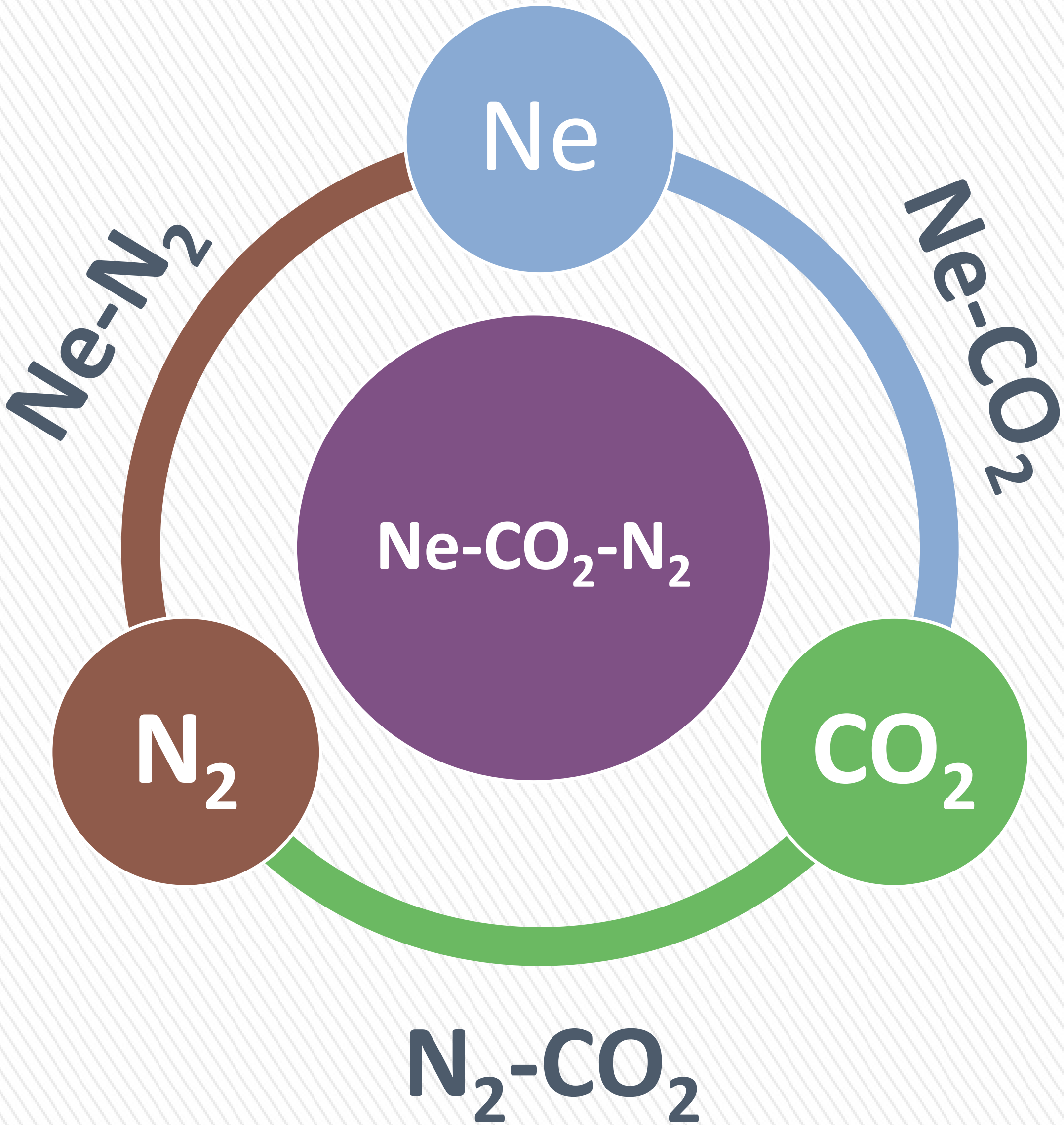
- Langevin Limit (formula)
- Blanc's law (mixtures)

**Comparison with experimental results**

Theoretical Values = Experimental Values

**Match?**

# Experimental Results



# Experimental Results: Ne

**Ionization**

$Ne + e^{-} \rightarrow Ne^{+} + 2e^{-}$

**Above 21.56 eV**

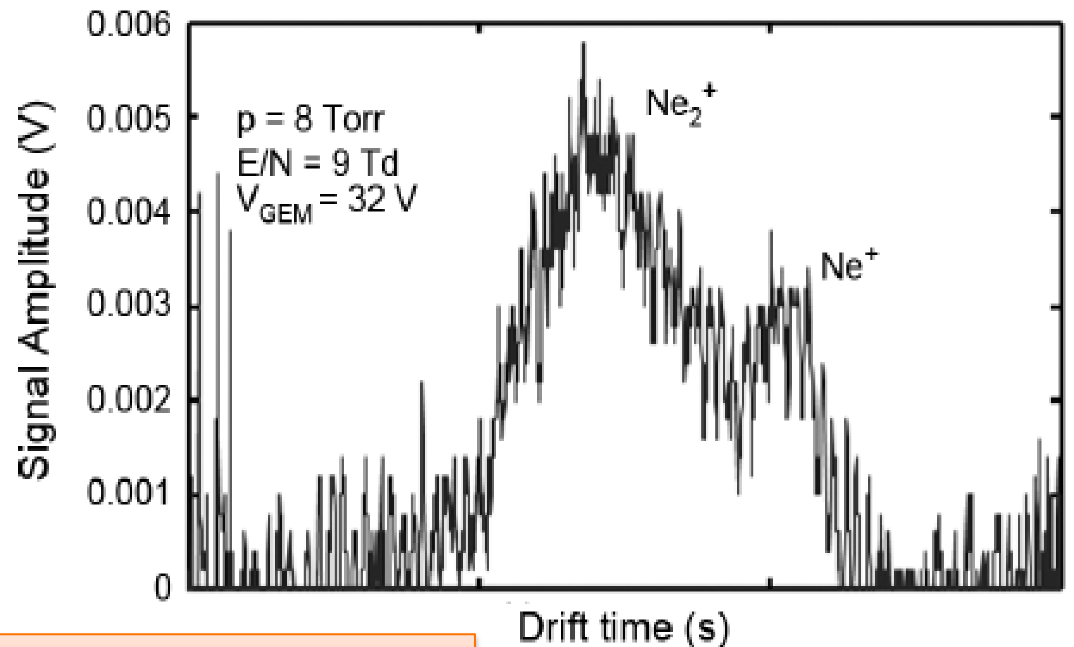
**Appearance Energies**

$Ne^{+}$ 21.56 eV

**Secondary Reactions**

$Ne^{+} + 2Ne \rightarrow Ne_2^{+} + Ne$

$Ne^{+} + Ne \rightarrow Ne + Ne^{+}$




$K_{01} = 4{,}4\ cm^2V^{-1}s^{-1}$ ($Ne^{+}$)
$K_{02} = 6{,}2\ cm^2V^{-1}s^{-1}$ ($Ne_2^{+}$)

P.N.B.Neves, 2011, IEEE

# Experimental Results: $CO_2$

**Ionization**

$CO_2 + e^- \rightarrow CO_2^+ + 2e^-$

**Above 13.8 eV**

**above 19.5 eV**

$CO_2 + e \rightarrow CO_2^+ + 2e^-$

$\rightarrow CO^+ + \frac{1}{2}O_2 + 2e^-$

$\rightarrow O^+ + CO + 2e^-$

**Secondary Reactions**

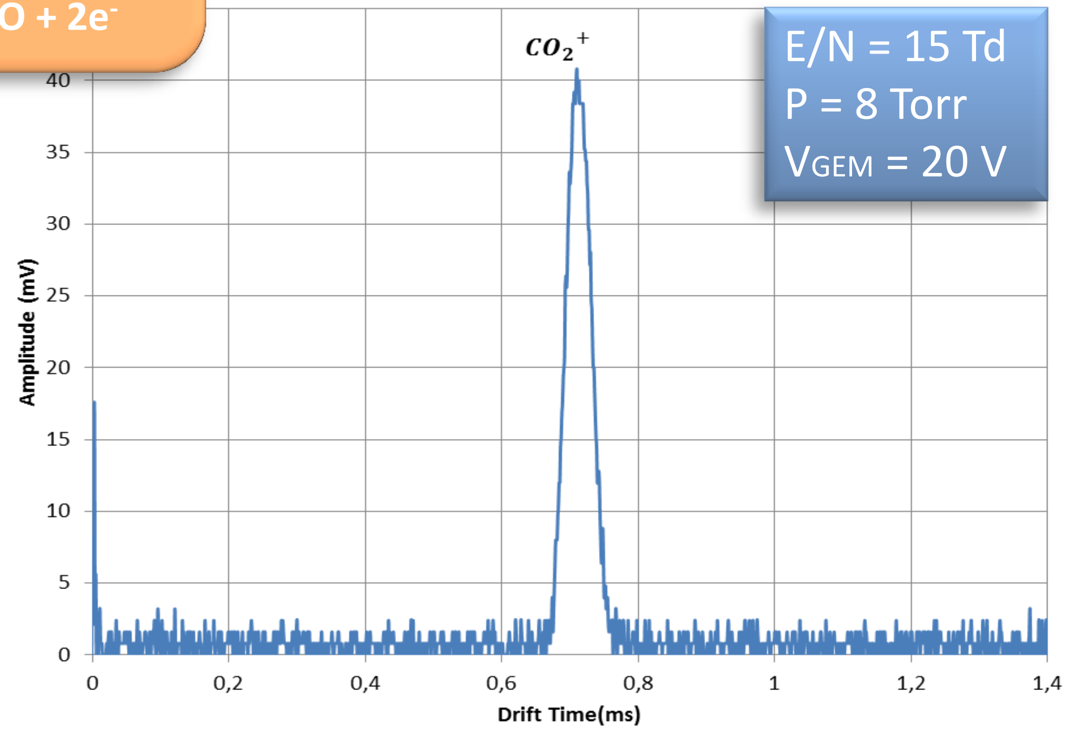
$CO_2^+ + CO_2 \rightarrow CO_2 + CO_2^+$

$CO^+ + CO_2 \rightarrow CO_2^+ + CO$

$O^+ + CO_2 \rightarrow O_2^+ + CO$

## Appearance Energies

| | |
|---|---|
| $CO_2^+$ | **13.8 eV** |
| $CO^+$ | **19.5 eV** |
| $O^+$ | **19.1 eV** |




P.M.C.C. Encarnação, 2015, JINST

# Experimental Results: $CO_2$

$K_{01} \sim 1.17\ cm^2V^{-1}s^{-1}$ **$CO_2^+$**

Good agreement with earlier reported works:

1. **W. T. Huntress et al. :** $1.23\ cm^2V^{-1}s^{-1}$
2. **G. Schultz et al. :** $1.09\ cm^2V^{-1}s^{-1}$

**Langevin Formula**

$1.82\ cm^2V^{-1}s^{-1}$

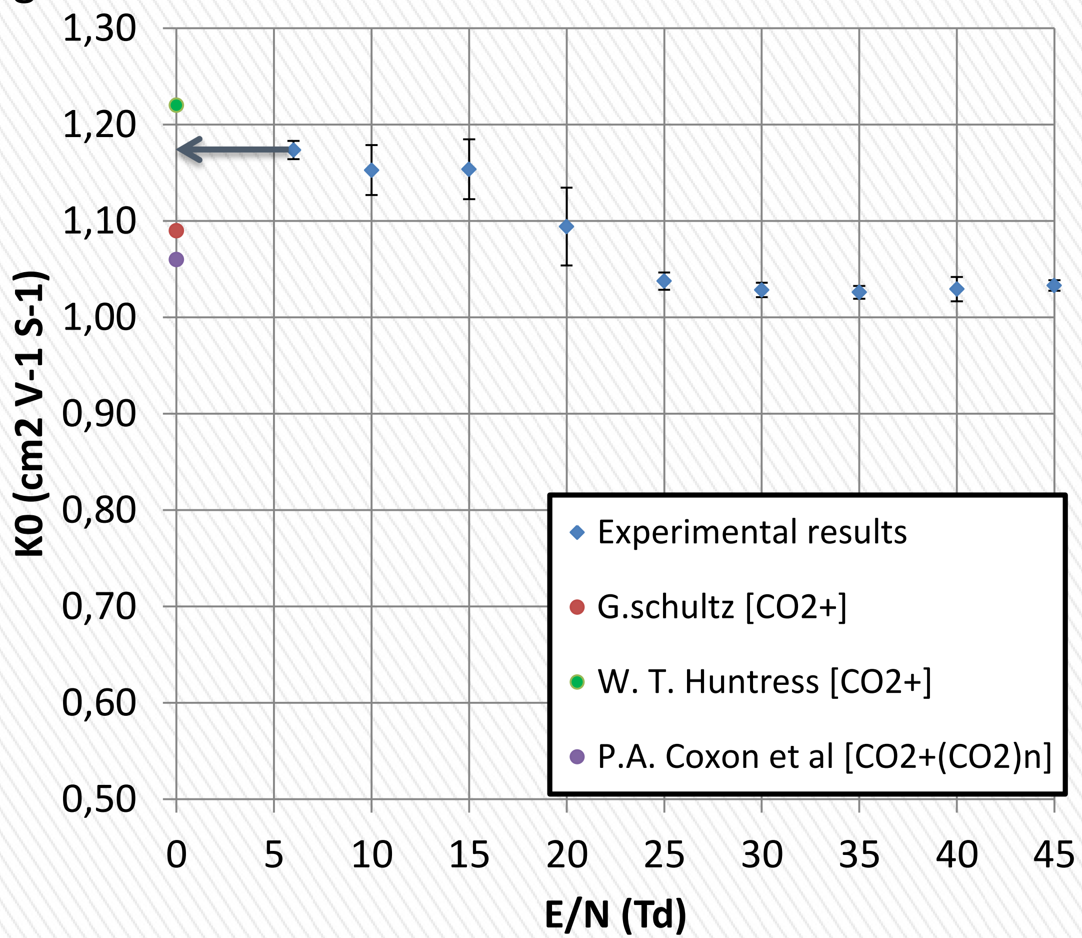
$\neq$

**Extrapolated Value (E/N→0)**

$1.17\ cm^2V^{-1}s^{-1}$

**Charge Transfer Process**

$CO_2^+ + CO_2 \rightarrow CO_2 + CO_2^+$



# Experimental Results: $N_2$

**Ionization**

$N_2 + e \rightarrow N_2^{+} + e$

**Above threshold 15,6 eV**

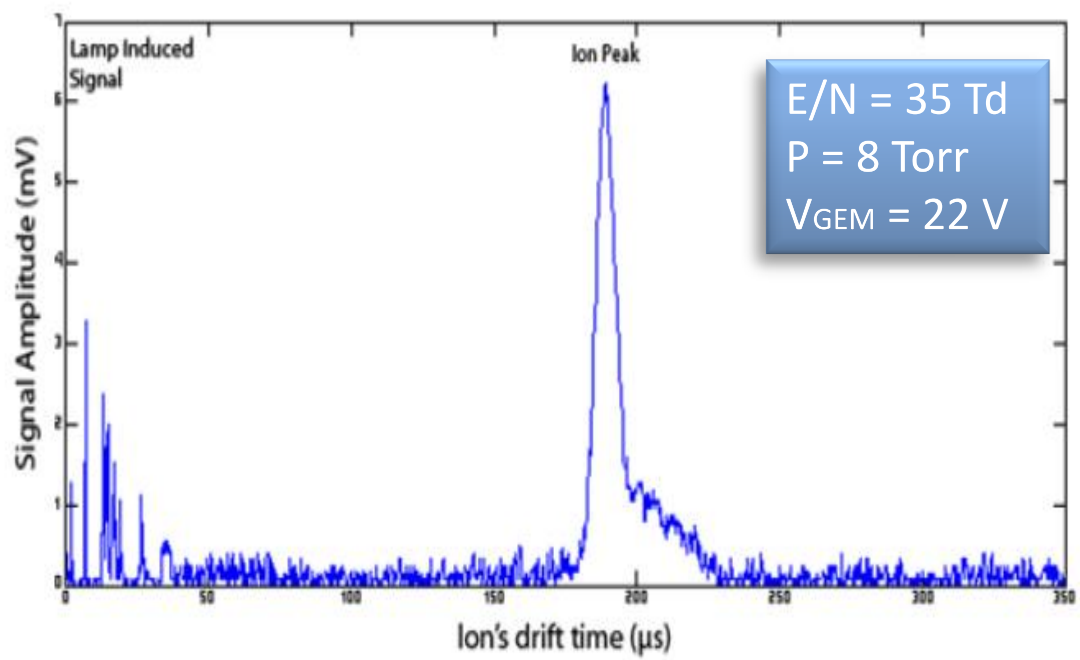
**Appearance Energies**

| | |
|---|---|
| $N_2^{+}$ | 15,6 eV |
| $N_3^{+}$ | 21,1 eV |
| $N^{+}$ | 24,2 eV |

**Secondary Reactions**

$N_2^{+} + 2N_2 \rightarrow N_4^{+} + N_2 + 0{,}87$ eV

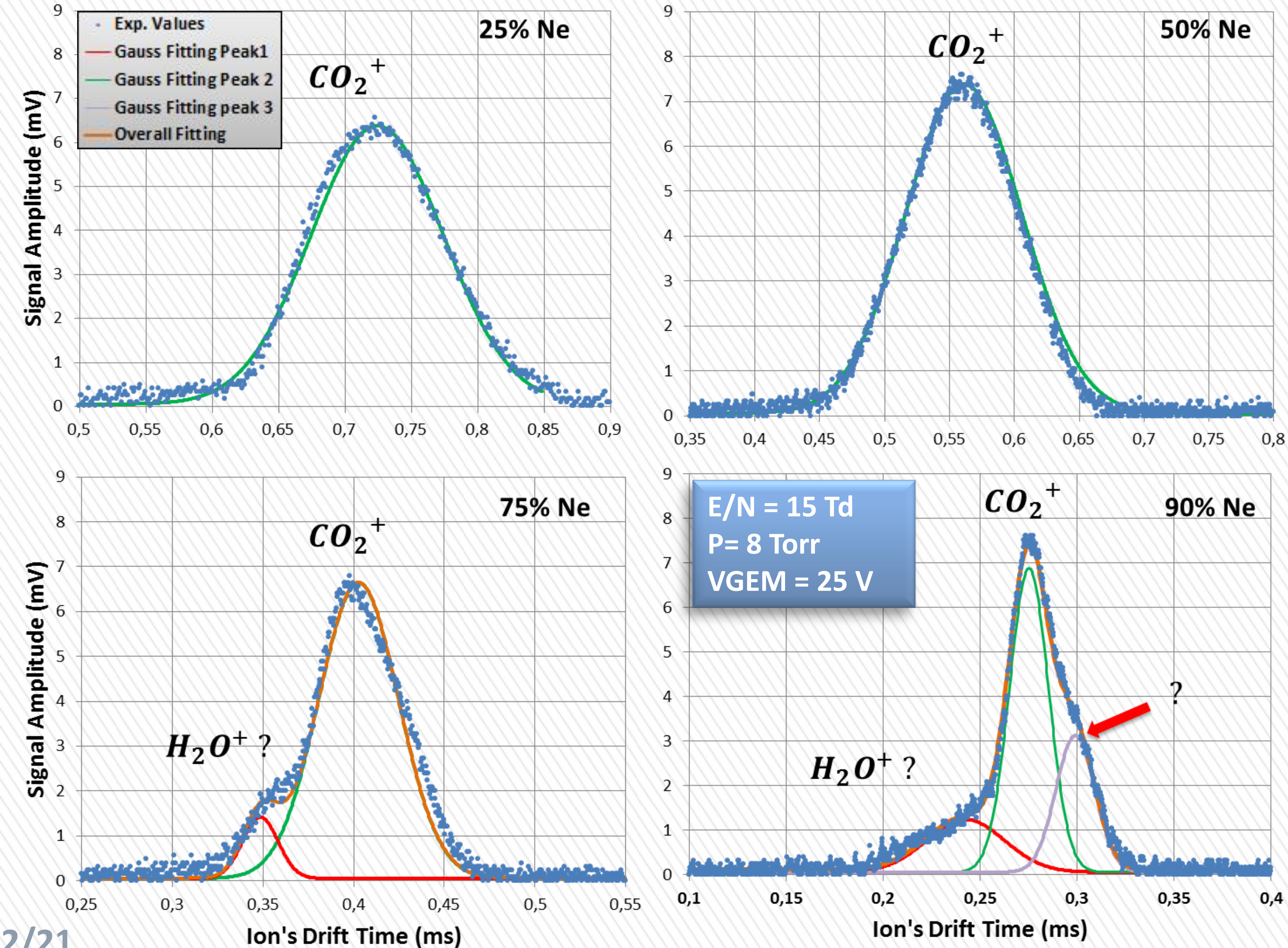
Rate constant $\rightarrow 5\mathrm{X}10^{-29} cm^6 s^{-1}$




$K_{01} = 2{,}37\ cm^2V^{-1}s^{-1}$ ($N_4^{+}$)

A.N.C. Garcia, 2012, JINST

# Experimental Results: Ne-$CO_2$



# Experimental Results: Ne-$CO_2$

| Direct Ionization | Cross Section (25V) ($10^{-16}$ $cm^2$) | Final Ion |
|---|---|---|
| $CO_2 + e \rightarrow CO_2^+ + e$ | 0,969 | $CO_2^+$ |
| $CO_2 + e \rightarrow CO^+ + 1/2O_2 + e$ | 0,0279 | $CO^+$ |
| $CO_2 + e \rightarrow O^+ + CO + e$ | 0,0419 | $O^+$ |
| $Ne + e \rightarrow Ne^+ + e$ | 0,02 | $Ne^+$ |

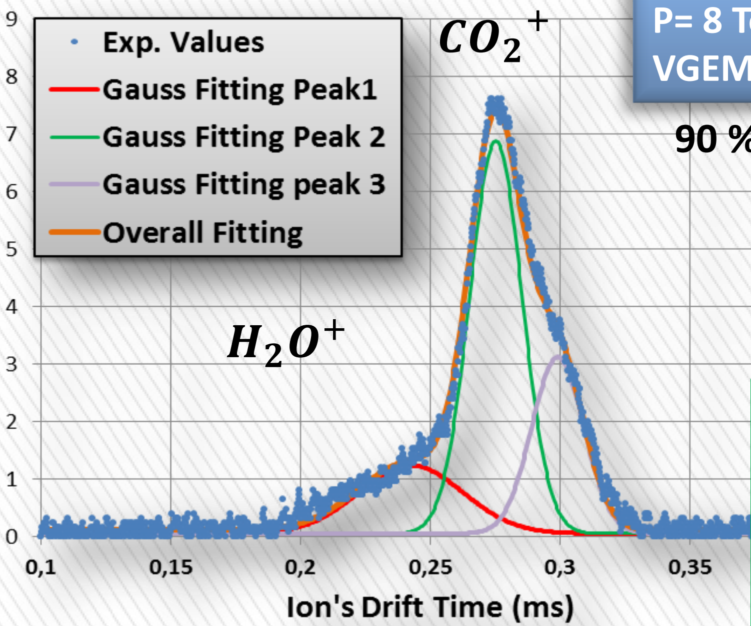
E/N = 15 Td
P= 8 Torr (90% Ne 10% $CO_2$)
VGEM = 25 V

| Secondary Reactions | Rate Constant $cm^3.s^{-1}$ or $cm^6.s^{-1}$ | Reaction Time (s) | Final Ion |
|---|---|---|---|
| $CO_2^+ + CO_2 \rightarrow CO_2 + CO_2^+$ | 3,7E-10 | 1,03E-07 | $CO_2^+$ or Cluster |
| $CO^+ + CO_2 \rightarrow CO_2^+ + CO$ | 1,1E-09 | 3,45E-08 | $CO_2^+$ |
| $O^+ + CO_2 \rightarrow O_2^+ + CO$ | 1,1E-09 | 3,45E-08 | $O_2^+$ |
| $Ne^+ + Ne \rightarrow Ne + Ne^+$ | 6,2E-10 | 6,81E-09 | $Ne^+$ |
| $Ne^+ + 2Ne \rightarrow Ne_2^+ + Ne$ | 5,8E-32 | 2,91E-06 | $Ne_2^+$ |
| $Ne^+ + CO_2 \rightarrow CO^+ + Ne + O$ | 6E-11 | 7,04E-08 | $CO^+$ |

$K_{03}$ ~ 3,51±0,05 $cm^2V^{-1}s^{-1}$
(Suggestions? Clusters?)
$K_{02}$ ~ 3,85±0,04 $cm^2V^{-1}s^{-1}$
($CO_2^+$?)
$K_{01}$ ~ 4.61±0,19 $cm^2V^{-1}s^{-1}$
($H_2O^+$?)

# Experimental Results: Ne-$CO_2$

E/N = 15 Td
P= 8 Torr
VGEM = 25 V

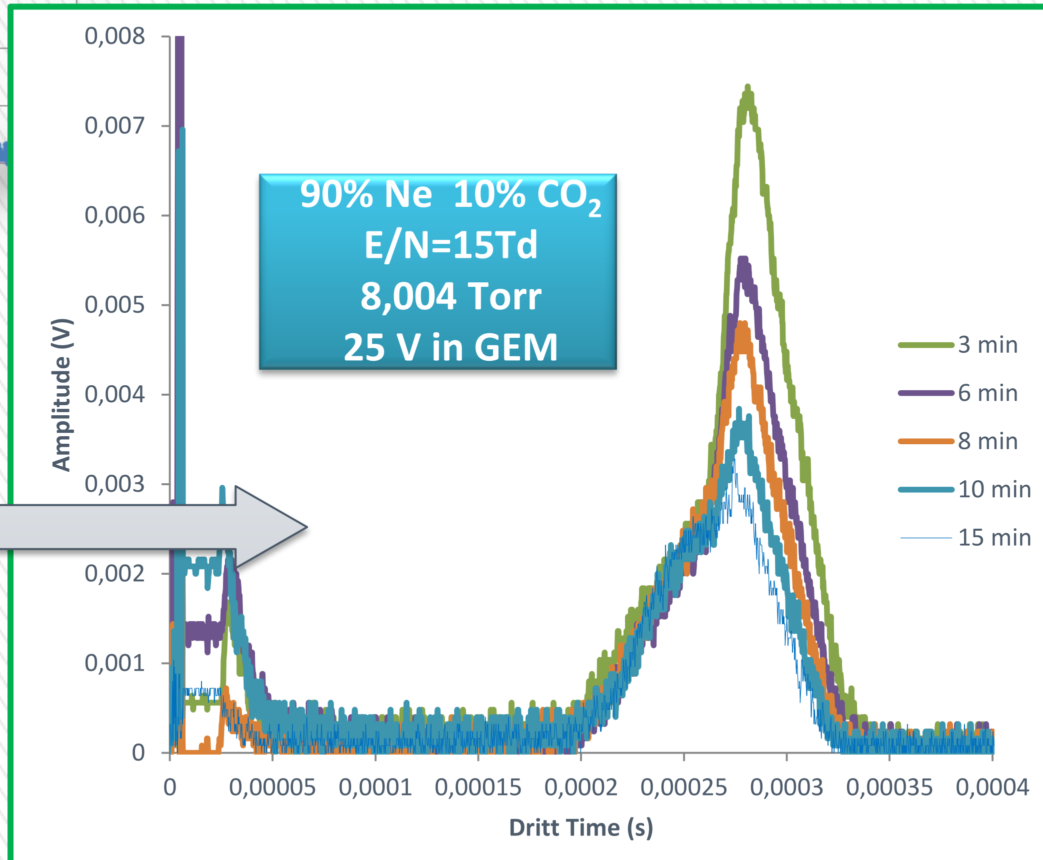



**Why is the first peak caused by impurities?**

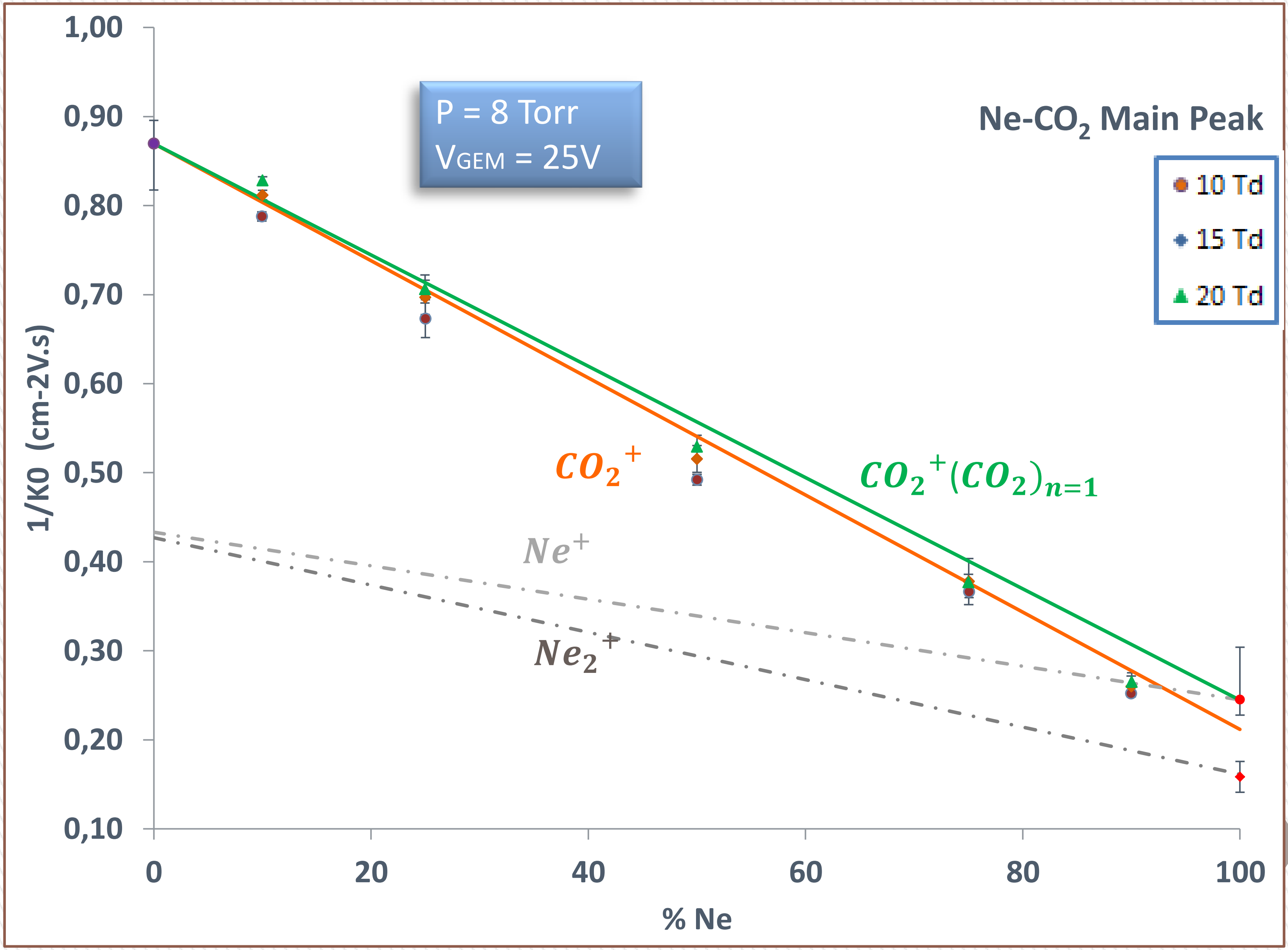
- The small bump appears even for lower VGEM (18 V).
- Even for 25 V, $O_2^+$ has a small probability to being formed

**Causes:**

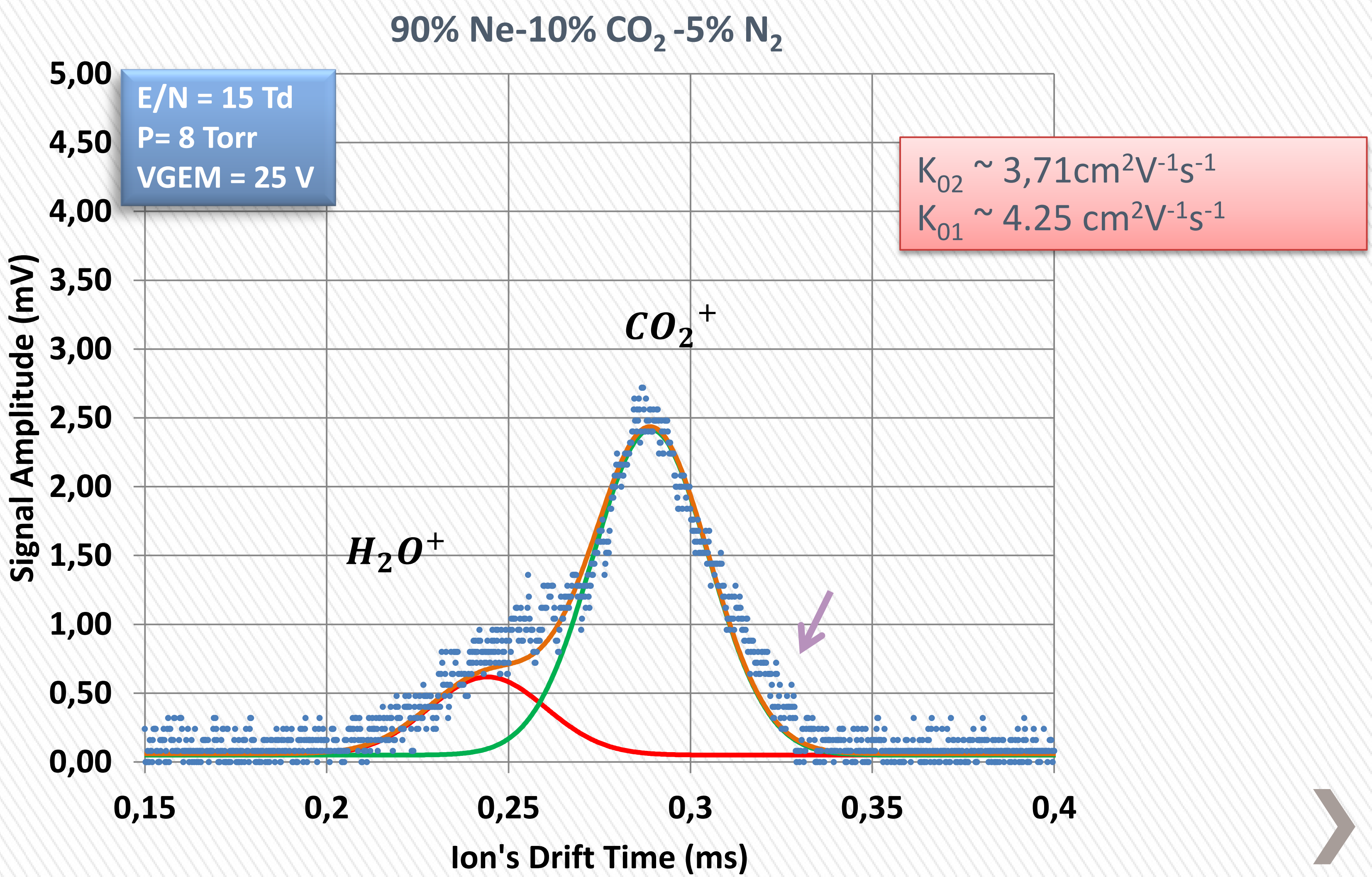
- Gas purity (99,99997%) (HP)
- Outgassing process (LP)
- Contribution of the GEM



# Experimental Results: Ne-$CO_2$



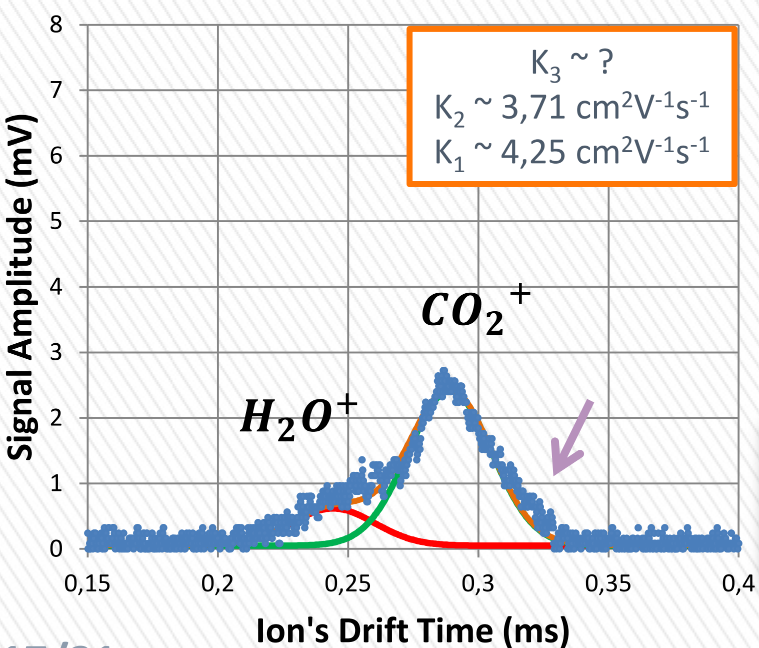
# Experimental Results: Ne-$CO_2$-$N_2$



# $K_0$ Experimental Results: $Ne$-$CO_2$-$N_2$

| E/N | 4 Torr | 6 Torr | 8 Torr | 10 Torr |
|---|---|---|---|---|
| 10 Td | 3,81 | - | 3,90 | 3,86 |
| | 4,37 | 4,10 | 4,38 | 4,38 |
| 15 Td | 3,83 | 3,90 | 3,71 | 3,71 |
| | 4,39 | - | 4,25 | 4,33 |
| 20 Td | 3,77 | 3,69 | 3,66 | 3,65 |
| | - | 4,12 | 4,21 | 4,26 |

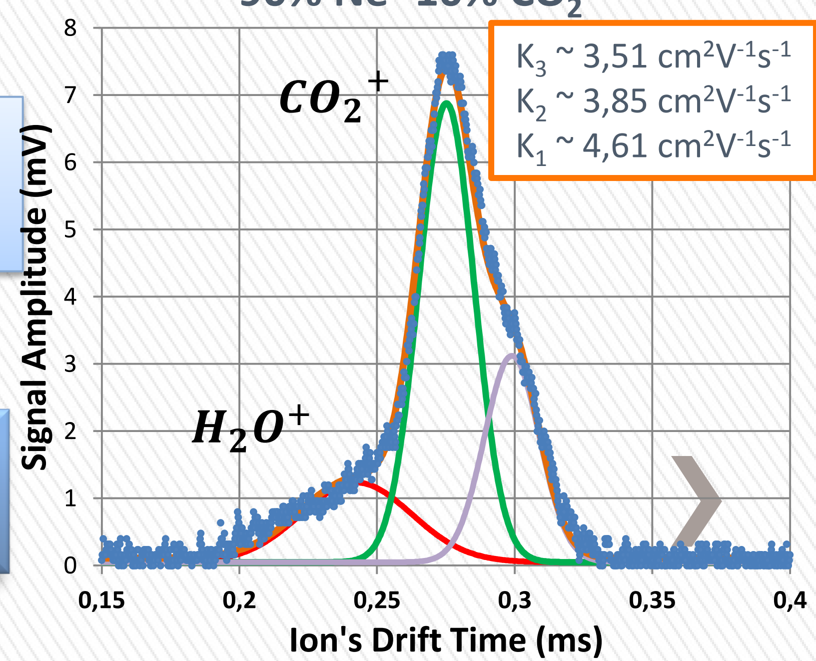
**90% Ne-10% $CO_2$ -5% $N_2$**




**Probably the same ion distribution**

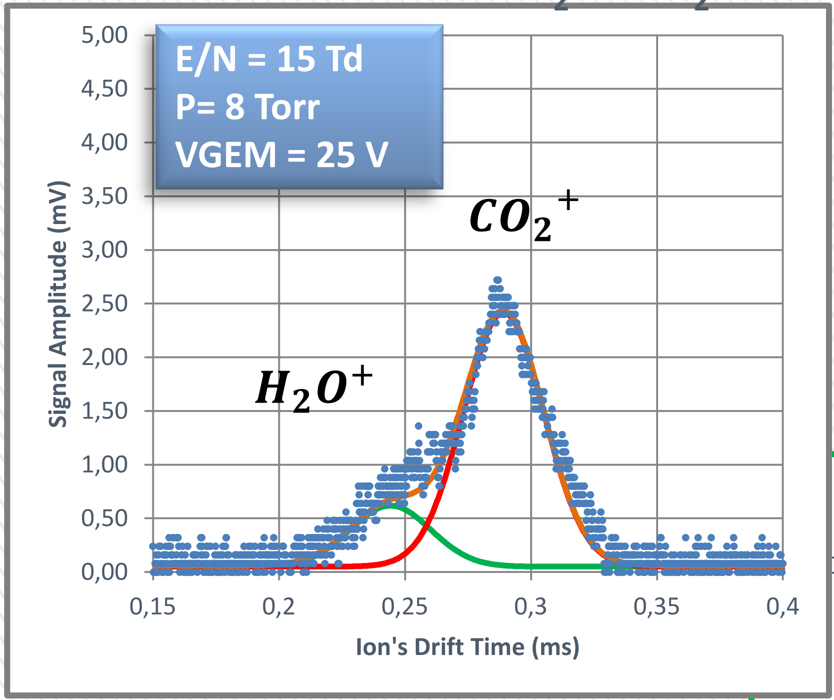
**E/N = 15 Td**
**P= 8 Torr**
**VGEM = 25 V**

**90% Ne- 10% $CO_2$**



# Experimental Results: $Ne$-$CO_2$-$N_2$

90% Ne-10% $CO_2$ -5% $N_2$

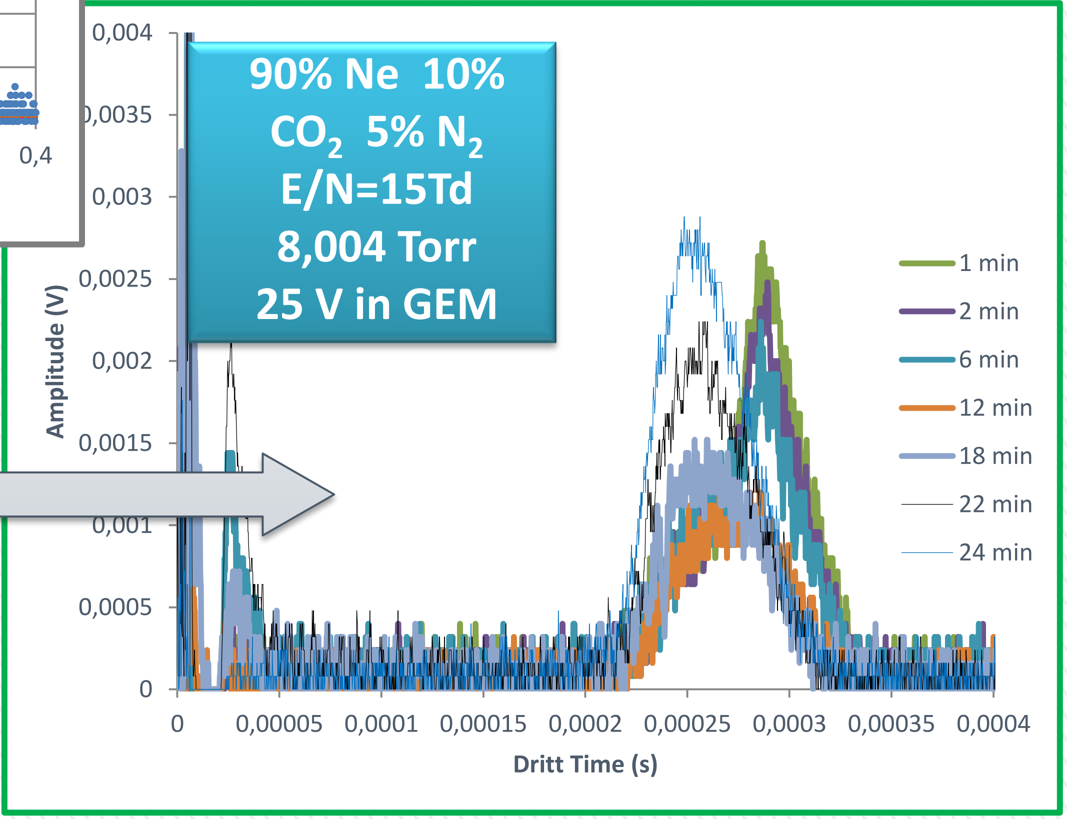



## Why is the first peak caused by impurities?

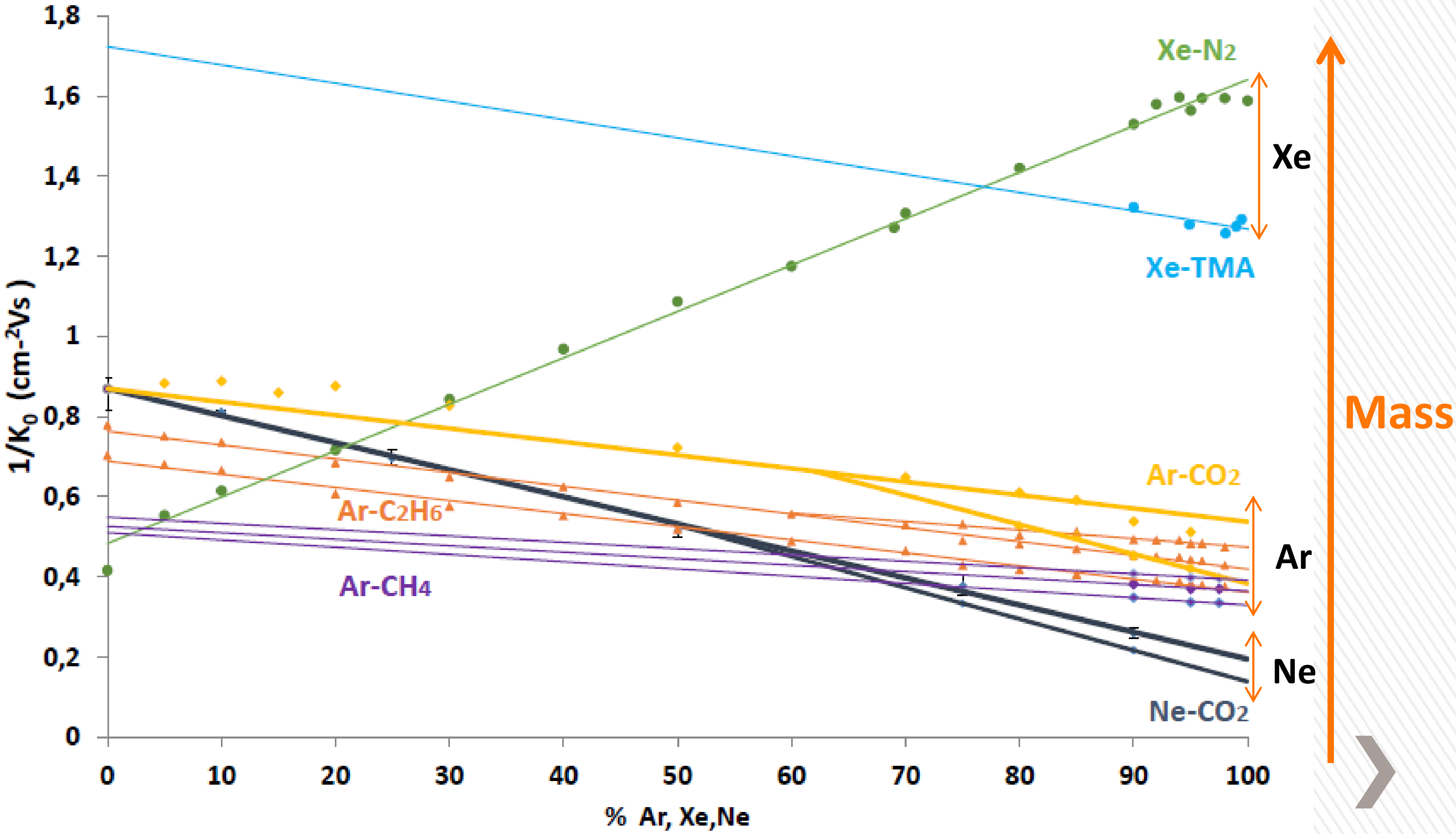
- The small bump at the left of the main peak appears even for lower VGEM (18 V).
- Even for 25 V, $O_2^+$ has a small probability to being formed

**Causes:**

- Gas purity (99,99997%) (HP)
- Outgassing process (LP)
- GEM



# Ion mobility results comparison



# Present Status and Future Work

- Pursuit the investigation of the mobility of ions in different gas mixtures of practical use (if you have any suggestions feel free to contact us).
  - In the scope of the RD51 common project submitted with GSI (Germany), Uludag Univ. (Turkey) and VECC (India).

  *Ar-$CO_2$ (was concluded and a paper recently published)*
  *Ne-$CO_2$ (to be concluded soon) – ($CO_2$-$N_2$ and Ne-$N_2$)*
  *Ne-$CO_2$-$N_2$ (just started)*
  *Ar-$CF_4$*
  *Ne-$CF_4$*

- Optimization of the detector: →
  *Variable Drift Distance*
  *Higher Pressure*
  - Rate constant influence
  - Study lighter ions ($H_2$)
  - Water influence on the ion's mobility
  - (...)

- Study of improved ion-neutral interaction models

A special thank to FCT-Fundação para a Ciência e Tecnologia for supporting this work through the National funds in the frame of the Project QREN n.4825, Rad for Life.

**I would like to thank also A.F.V. Cortez, P.N.B. Neves, A.M.F. Trindade, F.I.G.M. Borges, F.P. Santos, C.A.N. Conde, J. Escada, Yalçin Kalkan, Chilo Garabatos and Rob Veenhof for their help and contribution to this work.**

# Thank you!

**Universidade de Coimbra**

# Mixing Langevin Limit with Blanc's Law

## Langevin Limit

To determine the mobility of an ion within a gas (not the parent).

$$K_p = 13.88\left(\frac{1}{\alpha\mu}\right)^{\frac{1}{2}}$$

$\mu$ – reduced mass
$\alpha$ – neutral polarizability

## Theoretical Mobility Values

## Experimental Ion Mobility Values

Mobility of an ion within his parent gas (if known).

## Blanc's Law

Used to calculate the mobility of an ion in a gas mixture.

$$\frac{1}{K_{0mix}} = \frac{f_1}{K_{0g1}} + \frac{f_2}{K_{0g2}}$$

$f_1$ , $f_2$ – molar fraction of gas 1 and 2

**Mobility of an ion in a mixture**

# Candidate ions identification

## GEM Voltage

- Maximum energy gained by electrons.
- Primary ions possible to be formed.

Rg (pure)

$Rg + e \rightarrow Rg^+ + 2e$

## Possible Reactions

Ions formed through reactions of the primary ions with neutral atoms or molecules from the medium.

## Reaction Time

Used to calculate the mobility of an ion in a gas mixture.

$$\tau = \frac{1}{kN}$$

- Identification the possible ions present.

## Universal decay law

Used to calculate the variation of the concentration of a specific ion in a mixture.

$$Rg + Rg^+ \xrightarrow{k} X^+ + Y$$

$$\frac{[Rg^+]}{[Rg^+]_0} = e^{-\frac{t}{\tau}}$$

$$\frac{[X^+]}{[X^+]_0} = 1 - \frac{[Rg^+]}{[Rg^+]_0}$$

- Identification the possible ions present.

## Select Most Probable Ions