



# Ion transport in Nitrogen based mixtures

Pedro M.C.C. Encarnação\*, A.F.V. Cortez, Rob Veenhof,  
F.I.G.M. Borges, F.P. Santos, C.A.N. Conde

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

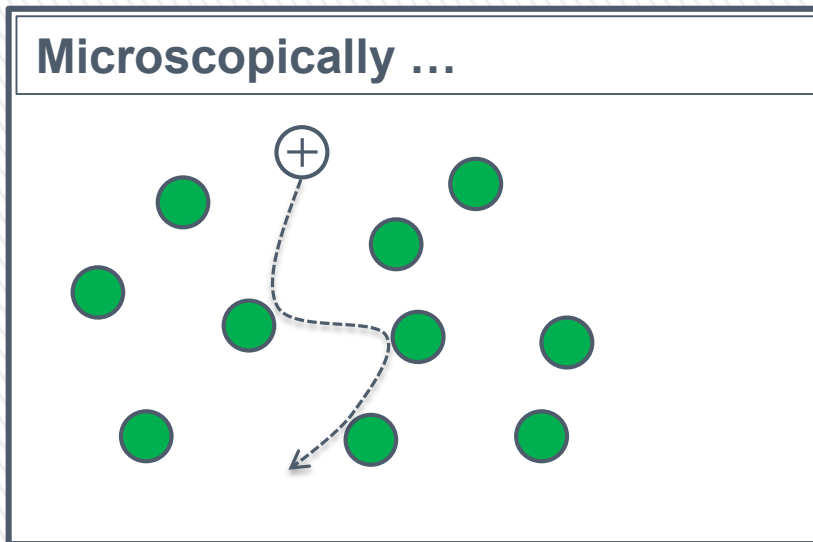
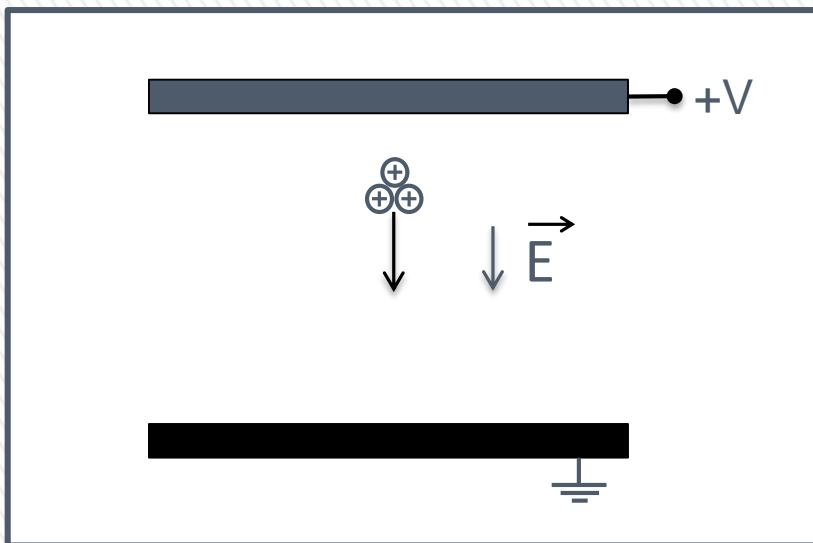




- 1** Basic Concepts
- 2** Experimental Setup and Working Principle
- 3** Ion Identification Process
- 4** Experimental results in:
  - a** Ne, N<sub>2</sub>
  - b** Ne-N<sub>2</sub>
- 5** Reduced Mobility Comparison of mixtures with Nitrogen

# Basics

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



## 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

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

$\mu$  – reduced mass

$\alpha$  – neutral polarizability

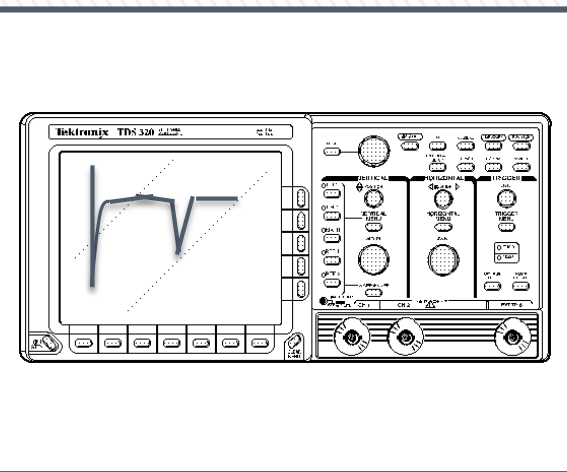
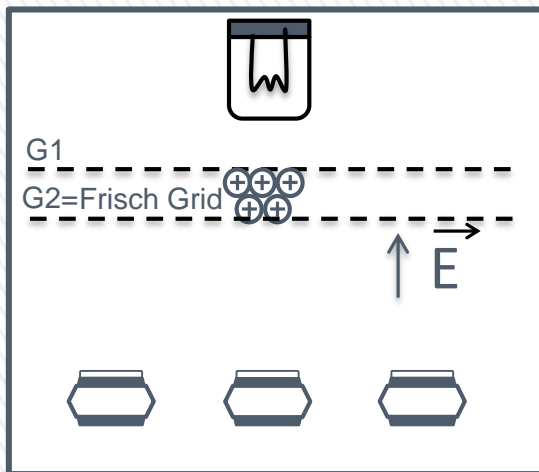
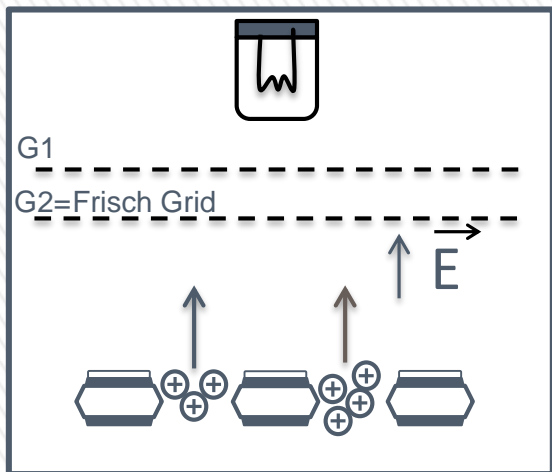
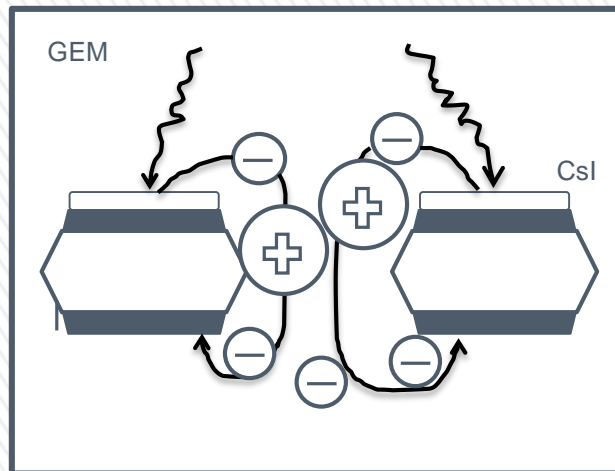
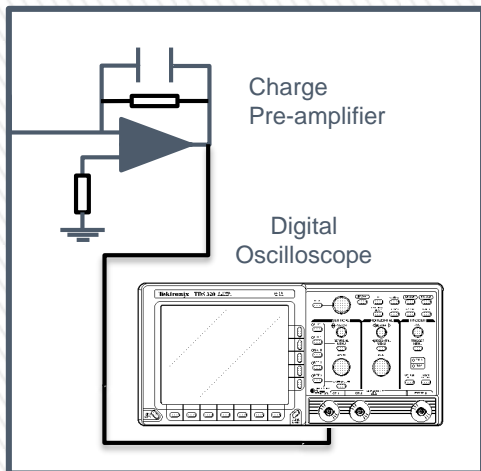
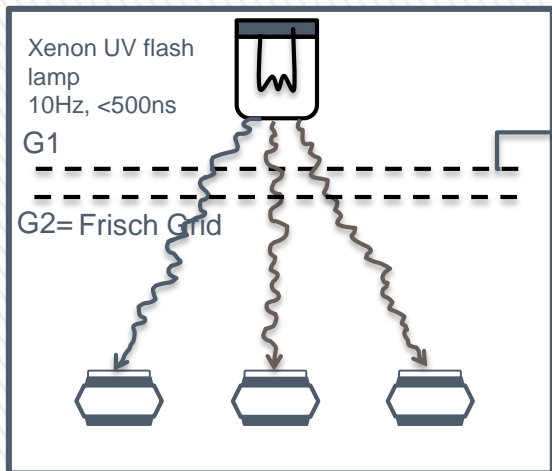
## Blanc's Law

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

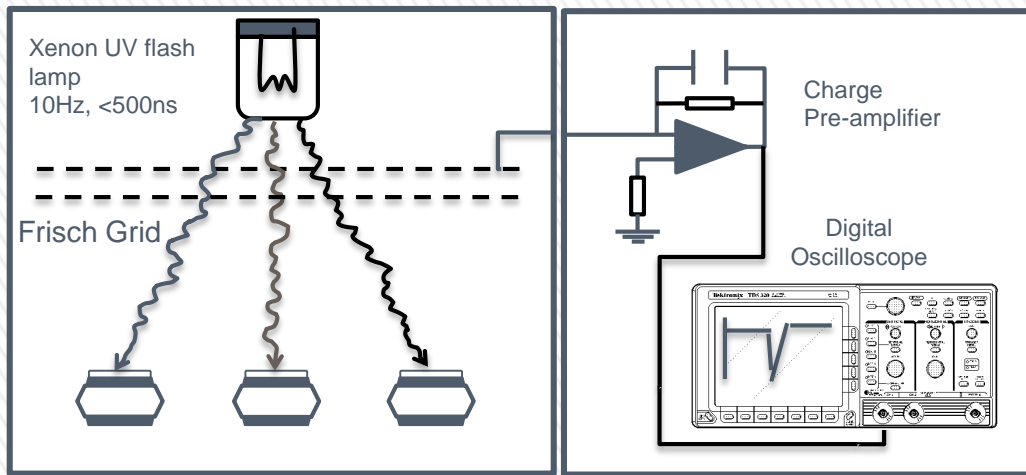
$f_1, f_2$ – molar fraction of gas 1, 2

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

# Experimental Setup and Working Principle



# Experimental Setup and Working Principle



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

Peaks centroids

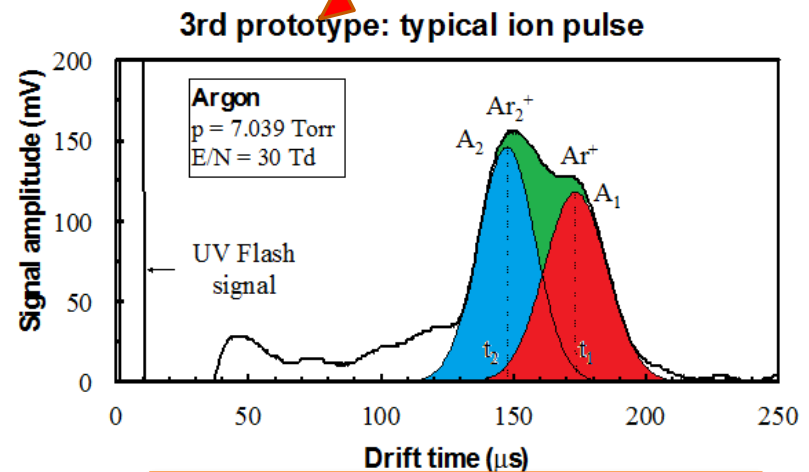


average drift time of the ion's distribution  
( $t_{drift}$ )

$$v_d = \frac{x_{drift}}{t_{drift}}$$



$$K = \frac{v_d}{E}$$



$$K_{01} = 1.57 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} (\text{Ar}^+)$$

$$K_{02} = 1.92 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} (\text{Ar}_2^+)$$

# 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: N<sub>2</sub>

Ionization



Appearance Energies

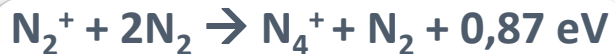
N<sub>2</sub><sup>+</sup> 15,6 eV

N<sub>3</sub><sup>+</sup> 21,1 eV

N<sup>+</sup> 24,2 eV

Above threshold  
15,6 eV

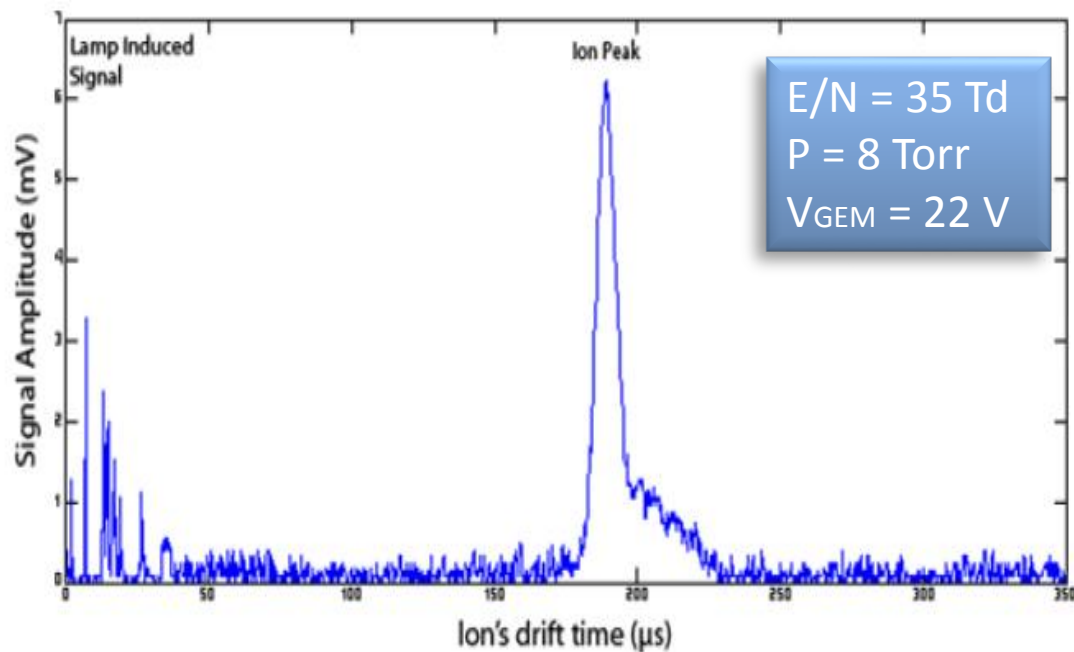
Secondary  
Reactions



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

[1,2,3]

$$K_{01} = 2,37 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} (\text{N}_4^+)$$



# Experimental Results: Ne

Ionization

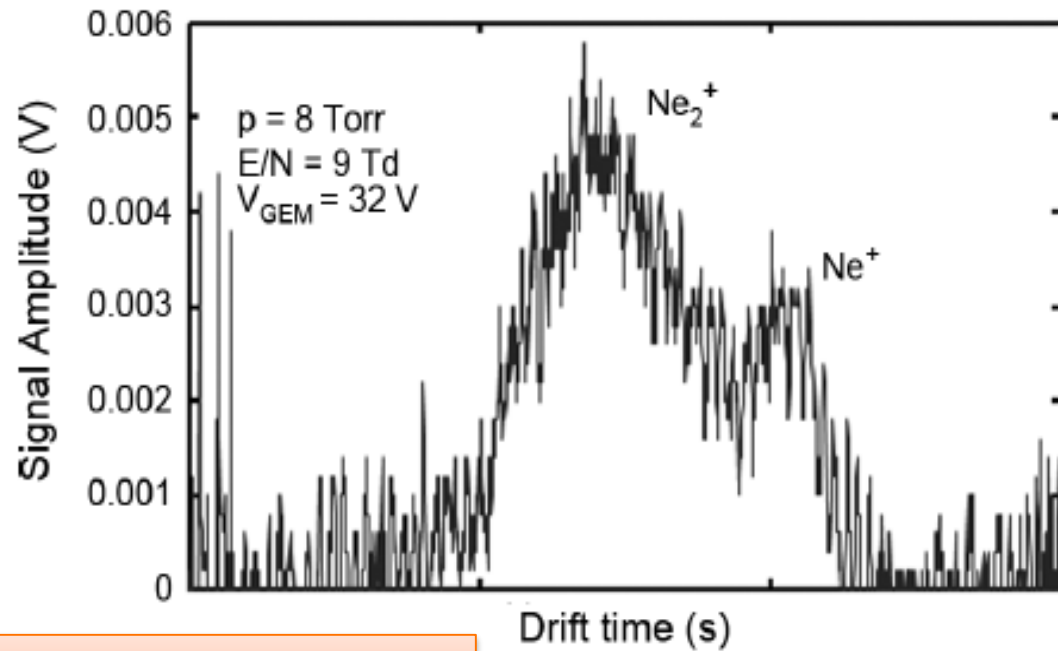


Appearance Energies

Ne<sup>+</sup> 21.56 eV

Above  
21.56 eV

Secondary  
Reactions



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

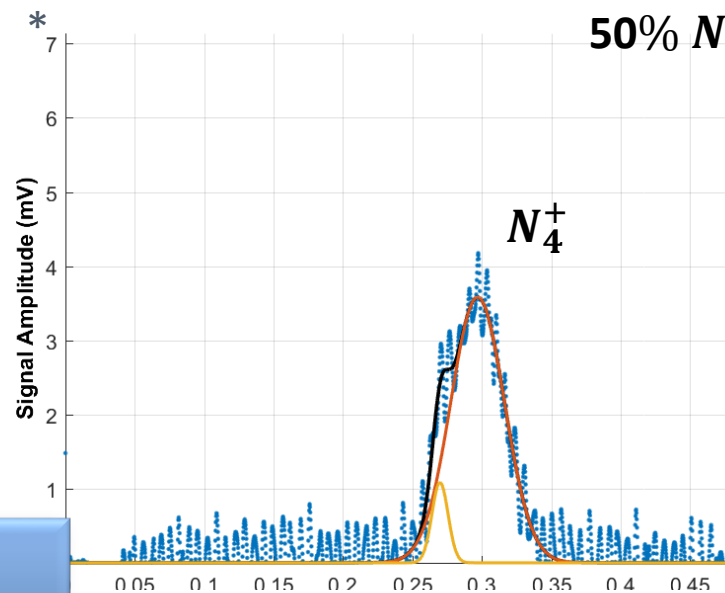
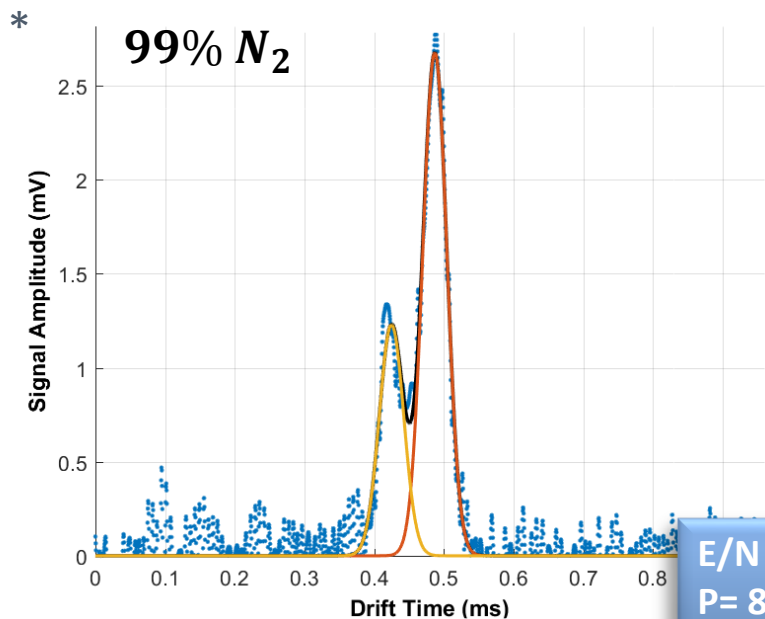
$$K_{02} = 6,2 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} (\text{Ne}_2^+)$$

[5]P.N.B.Neves, 2011, IEEE

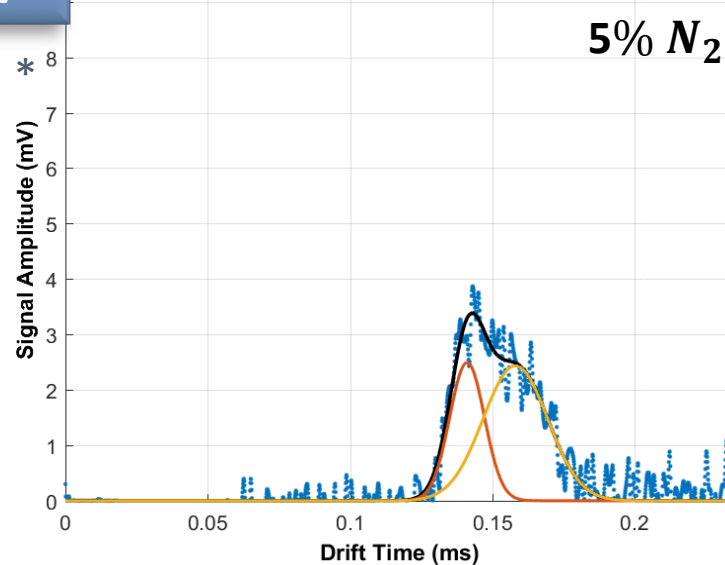
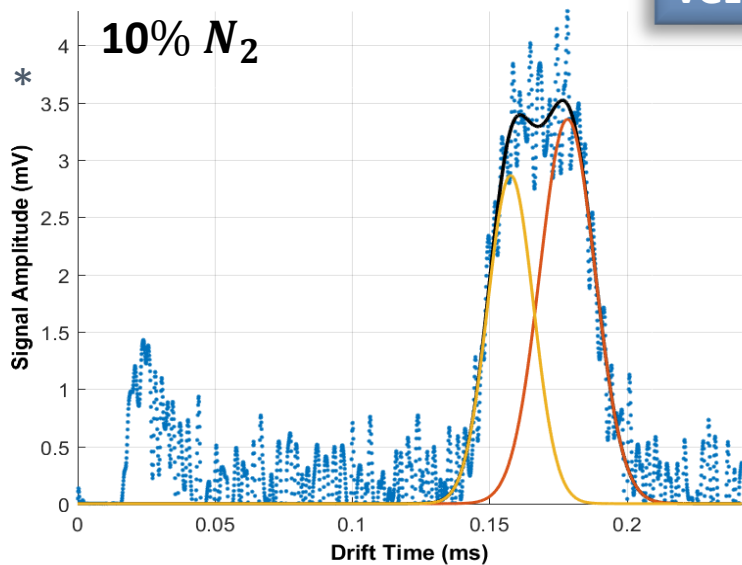


# Experimental Results: Ne-N<sub>2</sub>

\*Not at scale



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



# Experimental Results: Ne-N<sub>2</sub>

Direct Ionization	Cross Section (25V) (10 <sup>-16</sup> cm <sup>2</sup> )	Final Ion
Ne + e → Ne <sup>+</sup> + e	0,20	Ne <sup>+</sup>
N <sub>2</sub> + e → N <sub>2</sub> <sup>+</sup> + e	0,64	N <sub>2</sub> <sup>+</sup>

E/N = 15 Td  
P = 8 Torr (95% N<sub>2</sub> 5% Ne)  
VGEM = 25 V

Secondary Reactions	Rate Constant cm <sup>3</sup> .s <sup>-1</sup> or cm <sup>6</sup> .s <sup>-1</sup>	Final Ion
N <sub>2</sub> <sup>+</sup> + 2N <sub>2</sub> → N <sub>4</sub> <sup>+</sup> + N <sub>2</sub> + 0,87eV	5X10 <sup>-29</sup> [1,2,3]	N <sub>4</sub> <sup>+</sup> ‡
N <sub>2</sub> <sup>+</sup> + N <sub>2</sub> → N + N <sub>3</sub> <sup>+</sup>	1,5X10 <sup>-15</sup> [6]	N <sub>3</sub> <sup>+</sup> *
Ne <sup>+</sup> + 2Ne → Ne <sup>2+</sup> + Ne	5,6X10 <sup>-32</sup> [7]	Ne <sub>2</sub> <sup>+</sup>
Ne <sup>+</sup> + N <sub>2</sub> → N <sub>2</sub> <sup>+</sup> + Ne	1,1X10 <sup>-13</sup> [6]	N <sub>2</sub> <sup>+</sup>

K<sub>01</sub> ~ 2,62 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>  
K<sub>02</sub> ~ 2,32 cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup>

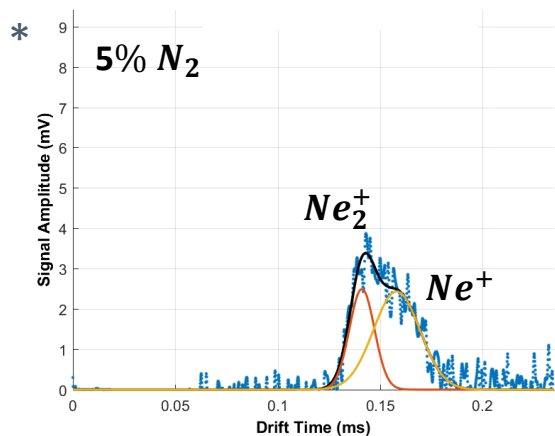
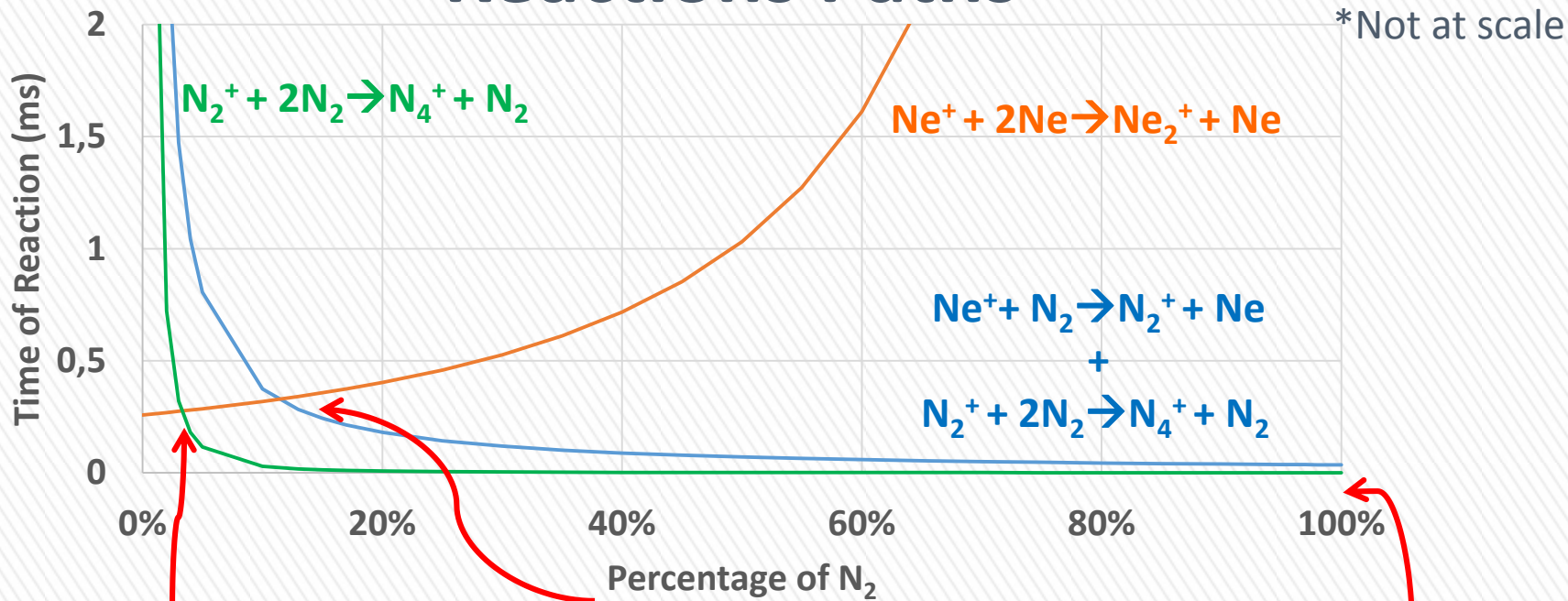


\* Slow reaction

‡ See A. N. C. Garcia work regarding the experimental measurement of the N<sub>4</sub><sup>+</sup> ion mobility [1]

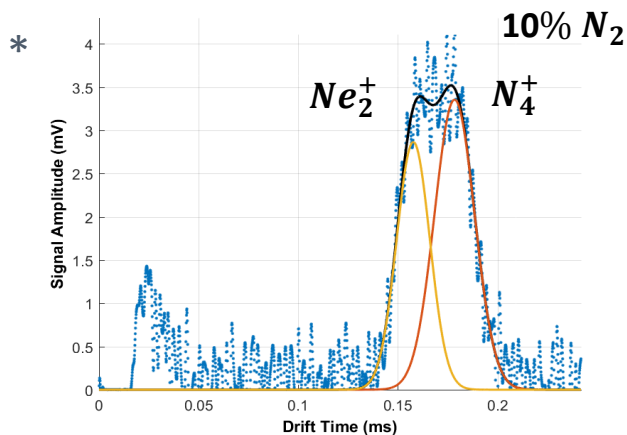


# Reactions Paths



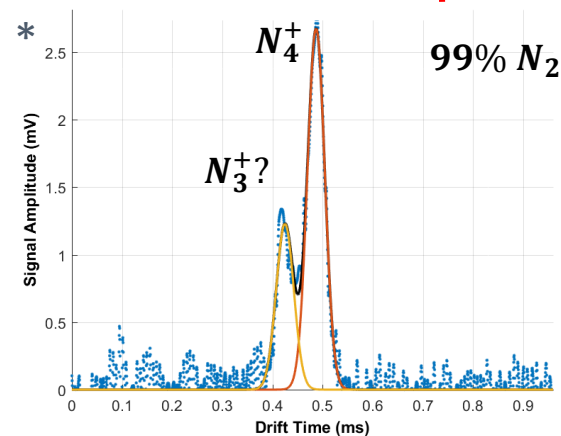
$$K_{01} \sim 7,13 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$

$$K_{02} \sim 6,40 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$



$$K_{01} \sim 6,60 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$

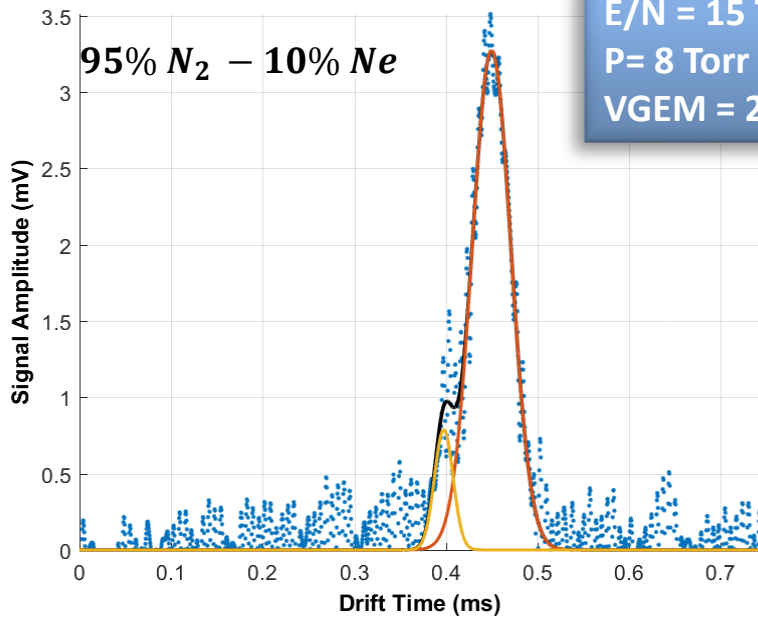
$$K_{02} \sim 5,84 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$



$$K_{01} \sim 2,47 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$

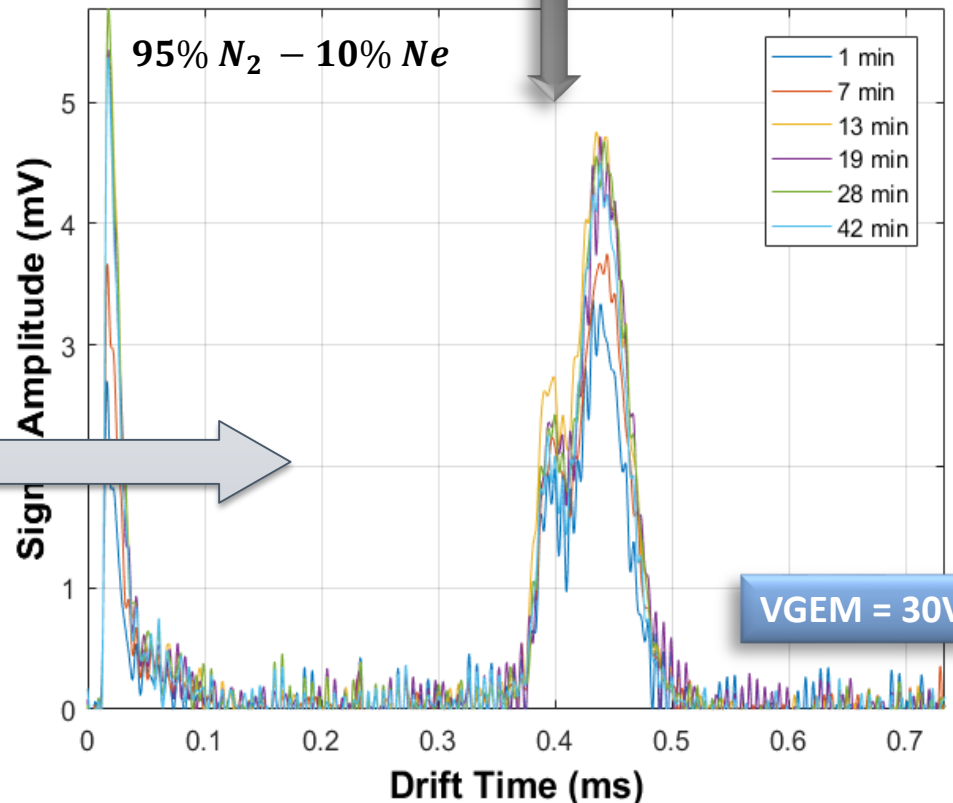
$$K_{02} \sim 2,16 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$$

# Degradation Signal: Ne-N<sub>2</sub>



Both peaks rise with time

The impurities have influence on peak's amplitude

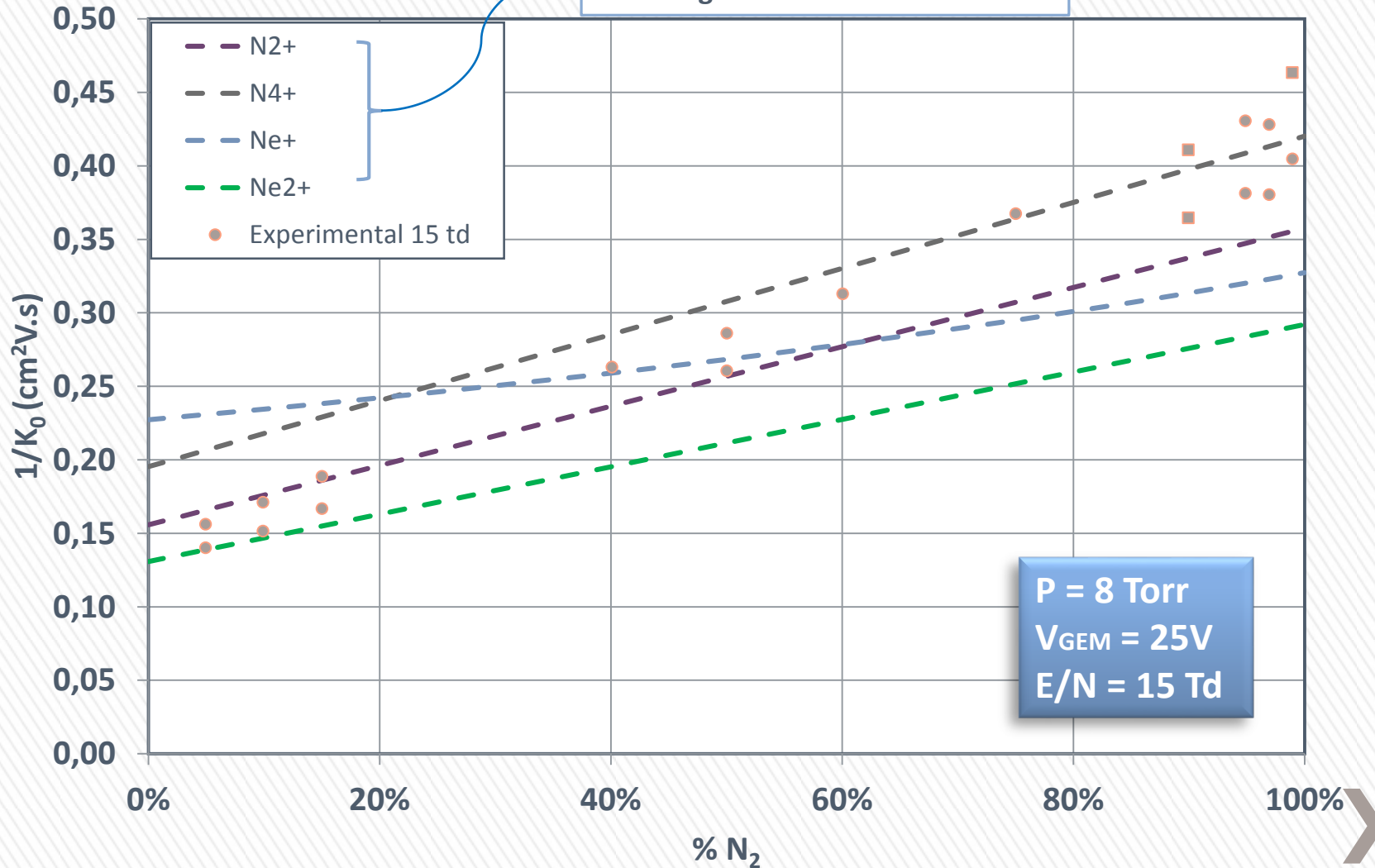


## Causes:

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

# Experimental Results: Ne-N<sub>2</sub>

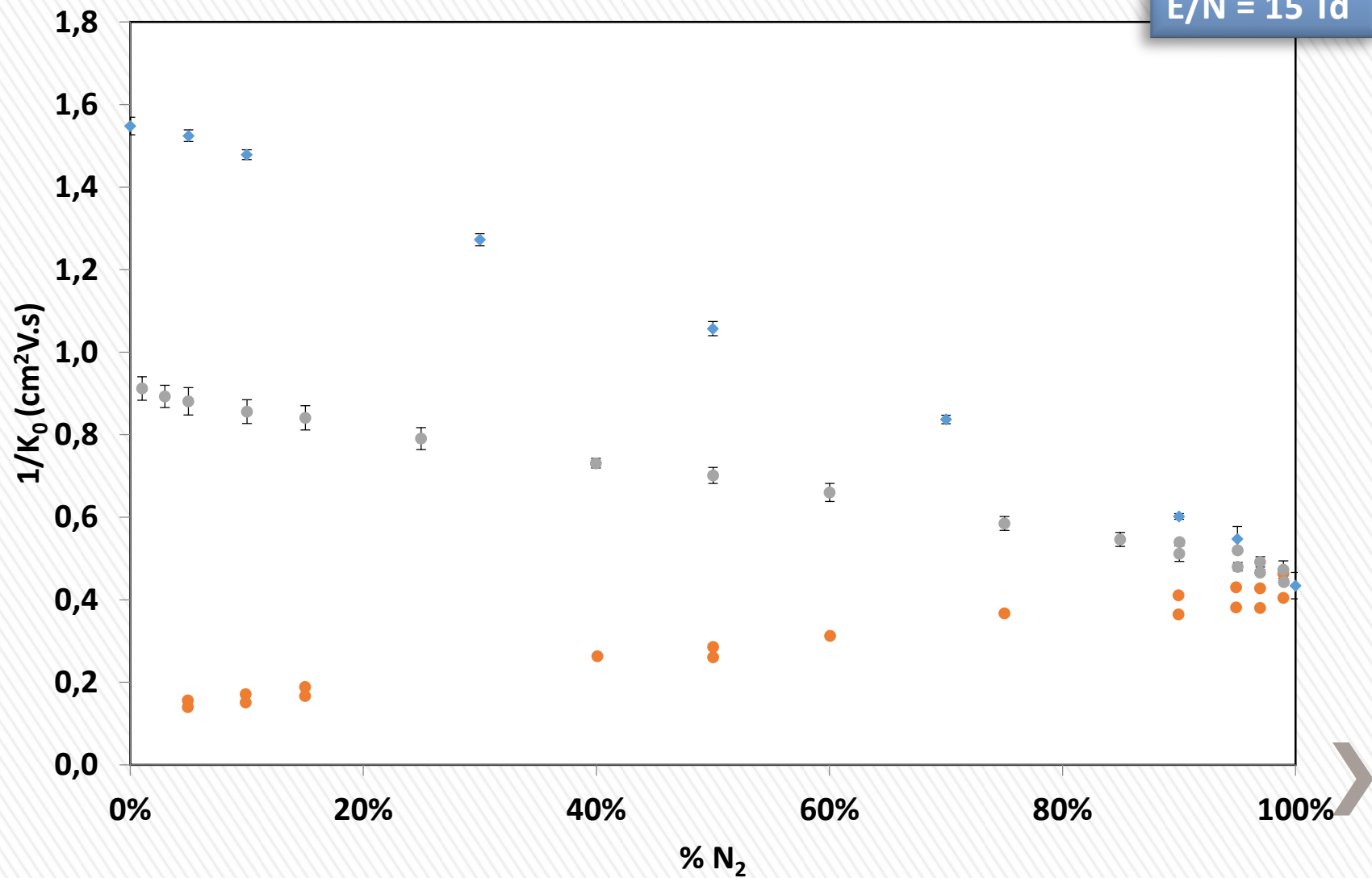
Theoretical values calculated using the Langevin Limit and Blanc's Law



# Comparison of mixtures with Nitrogen

● Ne-N<sub>2</sub>   ● N<sub>2</sub>-CO<sub>2</sub>   ◆ Xe-N<sub>2</sub>

P = 8 Torr  
E/N = 15 Td



# 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).

*Ne-N<sub>2</sub> (started)*

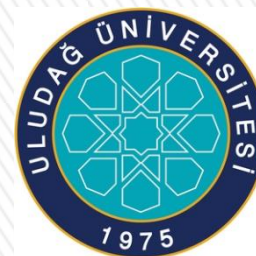
*Ne-CO<sub>2</sub>-N<sub>2</sub> (only preliminary results)*

*Ar-CO<sub>2</sub>-N<sub>2</sub> and Xe-CO<sub>2</sub>-N<sub>2</sub>*

*Ar-CF<sub>4</sub> and Ne-CF<sub>4</sub>*

- Optimization of the detector:
    - *Variable Drift Distance*  
*(Already started -redesigning)*
    - *Higher Pressure*
    - *Measurement of the mobility of negative ions*
  - Study of improved ion-neutral interaction models
- 
- Rate constant influence
  - Study lighter ions (H<sub>2</sub>)
  - Water influence on the ion's mobility
  - (...)

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- CERN/RD51 Collaboration – Common Projects - ‘Measurement and calculation of ion mobility of some gas mixtures of interest’. Participating institutions:



Thank you!



Universidade de Coimbra





# References

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- [2] W. Lindinger et al., Reactions of  $N^+$  with  $O_2$ ,  $CO_2$ ,  $H_2$ , and  $D_2$  and mobilities of  $N^+$  in nitrogen, *J. Chem. Phys.* 68 (1978) 2607.
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- [4] Garcia, A N. C., et al., A new contribution to the experimental measurement of the  $N_4^+$  ion mobility in  $N_2$  at 298K. *Journal of Instrumentation*, 7, P02012–P02012. <http://doi.org/10.1088/1748-0221/7/02/P02012>
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- [6] V.G. Anicich, Evaluated Bimolecular Gas Phase Kinetics of Positive Ions for Use in Modeling Planetary Atmospheres, Cometary Comae, and Interstellar Clouds, *J. Phys. Chem. Ref. Data* 22 (1993)
- [7] A. P. Vitols and H. J. Oskam, "Reaction rate constant for  $Ne^+ + 2Ne \rightarrow Ne_2^+ + Ne$  in *Phys. Rev. A, Gen. Phys.*, 1972, vol. 5, pp. 2618–2622.

# 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.

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

$f_1, f_2$  – 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)



## Possible Reactions

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

## Select Most Probable Ions

## Reaction Time

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

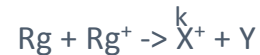
$$\tau = \frac{1}{kN}$$

- Identification the possible ions present.



## Universal decay law

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



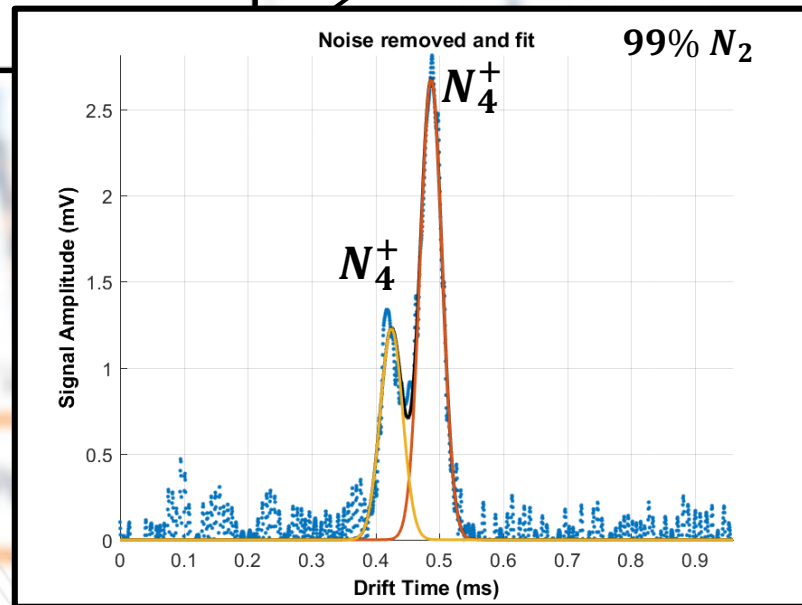
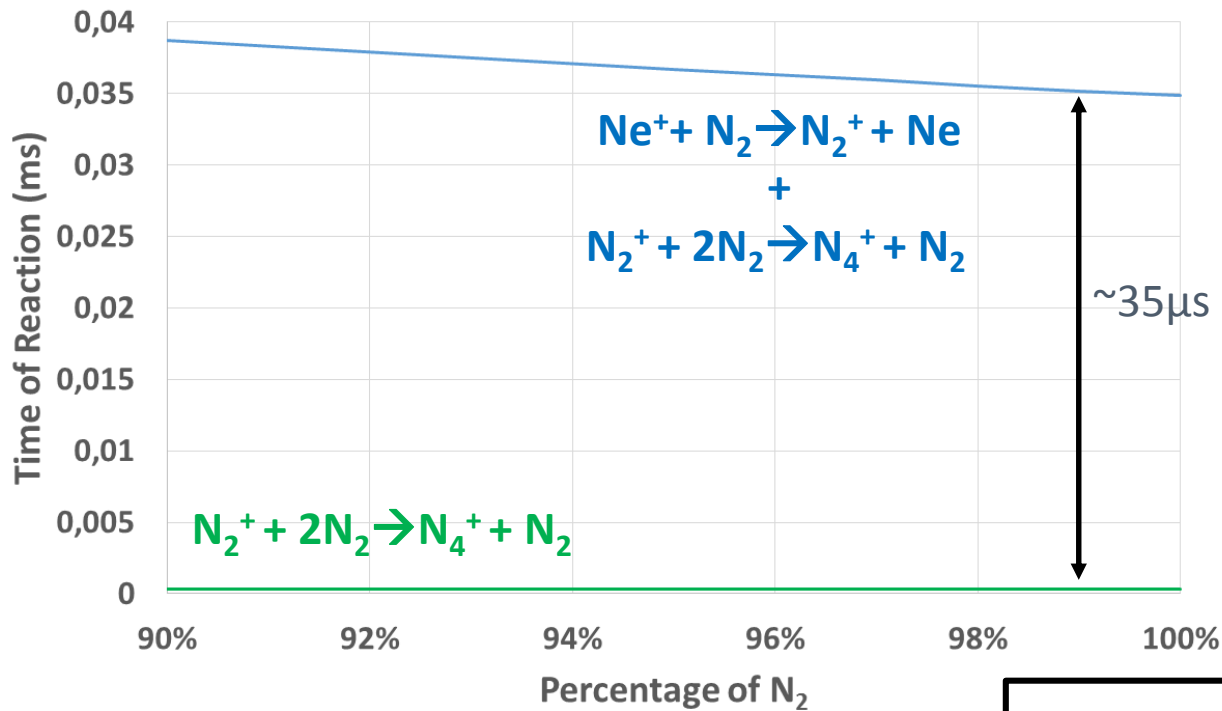
$$\frac{[\text{Rg}^+]}{[\text{Rg}^+]_0} = e^{-\frac{t}{\tau}}$$

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

- Identification the possible ions present.



# Reactions Paths



# Ion mobility results comparison

