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Calculations of recombination in ion beams

EPTN WP2 Aarhus, April 2022

Overview

Introduction

Where do we stand?

- The use of Monte Carlo particle transport codes
- Recombination in single ion tracks (*initial* recombination)
  - solved analytically by G. Jaffé in 1913
  - limited prediction capabilities
  - not generalised to multiple tracks

Bulk recombination simulations

Open-source project `IonTracks`

- Extends the Jaffé theory with amorphous track structure theory
- Includes track interactions (*initial* + *general* recombination) $\Rightarrow$ beam simulations

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Calculations of ion recombination

Semi-empirical approaches

- Three-voltage linear method [1]
- or separation of components [2–4]

$$k_s \approx 1 + \underbrace{\frac{c_1}{V}}_{\text{initial}} + \underbrace{\frac{c_2}{V^2} I_V}_{\text{general}}$$

1 Rossomme S *et al* (2019) *PMB* **65** 045015

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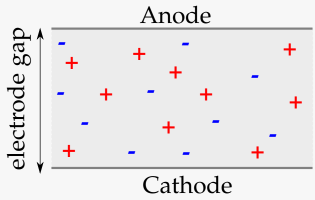
Theoretical approach

(1) Bulk movement and recombination of charge carrier density $n_\pm$ in an electric field:

$$\frac{\partial n_\pm}{\partial t} = \underbrace{D_\pm \nabla^2 n_\pm}_{\text{diffusion term}} \mp \overbrace{\mu_\pm \vec{E} \cdot \vec{\nabla} n_\pm}^{\text{drift term}} - \underbrace{\alpha n_+ n_-}_{\text{recombination}}$$

(2) Uniform charge carrier distribution (e^- / γ):



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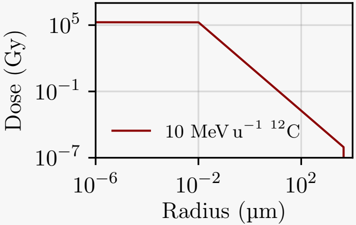
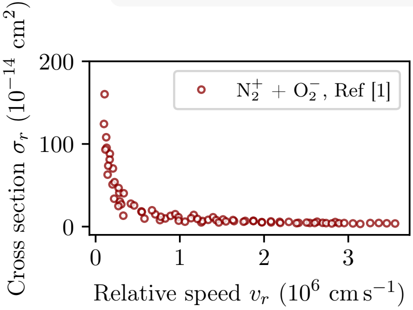


Recombination cross section

Monte Carlo simulations with particle transport codes?

Limited by the recombination cross sections and bulk behaviour



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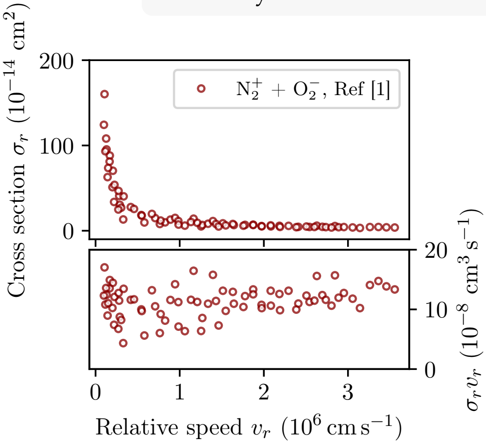

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with recombination rate coefficient

$$\alpha \equiv \sigma_r v_r \approx 10^{-7} \mathrm{cm}^3\,\mathrm{s}^{-1}$$

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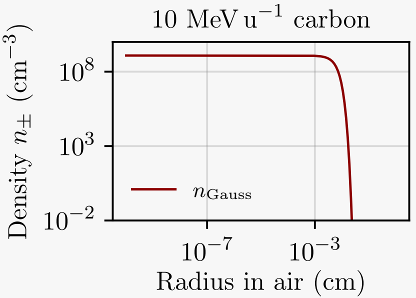
Recombination in a single track (Jaffé theory)

The Gaussian radial distribution

$$n_{\text{Gauss}}(r) = \frac{\text{LET}}{W} \frac{1}{\pi b^2} \exp\left(-\frac{r^2}{b^2}\right)$$



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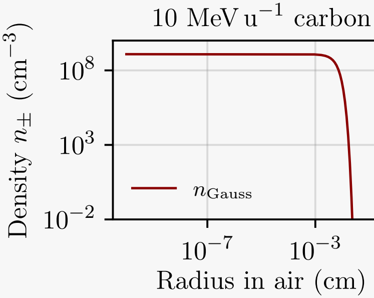
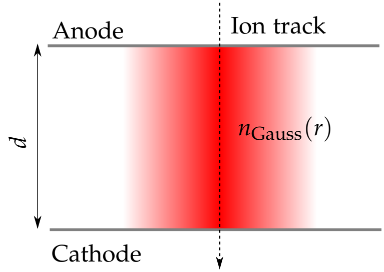


Given the initial condition:



Solve:

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Recombination in a single track (Jaffé theory)

Jaffé theory (1913, 1929)

Collection efficiency:

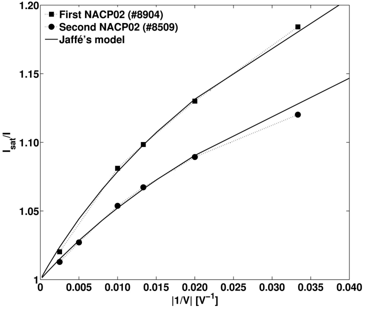
$$f = y_1 \frac{\mu E b^2}{2Dd} \exp\left(-y_1\right)\left[\mathrm{E}_i(y_2) - \mathrm{E}_i(y_1)\right],$$

$$y_1 = \frac{8\pi W}{\alpha\,\mathrm{LET}}, \quad y_2 = y_1 + \ln \frac{4D\dfrac{d}{2\mu E} + b^2}{b^2}$$

Problems

- Limited predictions (*a priori* knowledge of *b*)
- the Gaussian distribution is an approximation
- Only for a single track, no inter-track interactions

Initial recombination in carbon ions [2]:



Validation:

[1] Kanai T *et al* (1998) *PMB* **43**(12) 3549

[2] Rossomme S *et al* (2016) *Med Phys* **43**(7) 4198

Scholz-Kraft radial dose distribution (RDD)

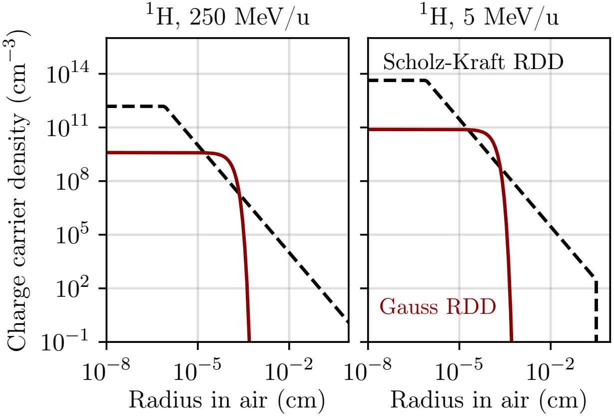
Example RDD: Scholz-Kraft (SK)

$$D_{SK}(r) = \begin{cases} \frac{C}{r_c^2}, & r < r_c \\ \frac{C}{r^2}, & r_c \leq r \leq r_{max} \\ 0, & r_{max} < r \end{cases}$$

with

$$r_{max}(E) = 4 \cdot 10^{-5}\ E^{1.5}, \quad r_c = 10\,\text{nm}.$$

$$\int_0^{2\pi} \int_0^{\infty} D(r)\, r \,\mathrm{d}r \,\mathrm{d}\theta = \frac{\text{LET}}{\rho}$$



Brief summary

Recombination in a single ion track

The case of an ion track in a parallel-plate chamber

- ✓ Solved analytically assuming a Gaussian distribution (Jaffé theory)
- ✗ No (analytical) solution for *real* track structure models
- ✗ No generalisation to multiple track interactions

Recombination in multiple tracks (e.g. continuous beam)

- Solve the equations numerically
  - For different amorphous track structure models
- Generalise the solution for N tracks
  - for continuous beams
  - or pulsed beams

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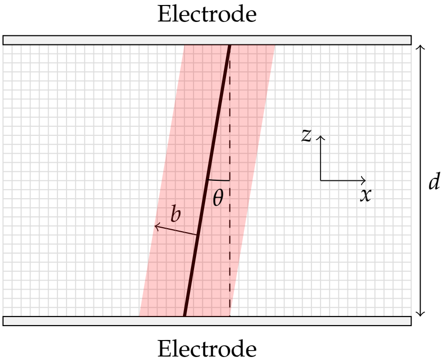
Numerical solutions (`IonTracks` project)

Solve:

$$\frac{\partial n_\pm}{\partial t} = D_\pm \nabla^2 n_\pm \mp \mu_\pm \vec{E} \cdot \vec{\nabla} n_\pm - \alpha n_+ n_-$$

Defined on the grid:



The software project IonTracks [1]

- Completely open source (`python`)
- Calculate ion recombination numerically
- Extends the Jaffé theory to multiple tracks

`github.com/jbrage/IonTracks`:

```
from IonTracks import ks_initial

# single ion track
ks = ks_initial(gap_d_cm=0.2,
                voltage_V=200,
                particle="carbon",
                energy_MeV_u=62,
                RDD_model="Gauss")
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[1] Christensen JB, Heikki T, Bassler N (2016) *Med Phys* 43(10) 5484

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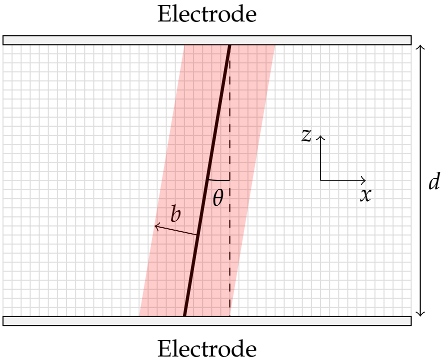

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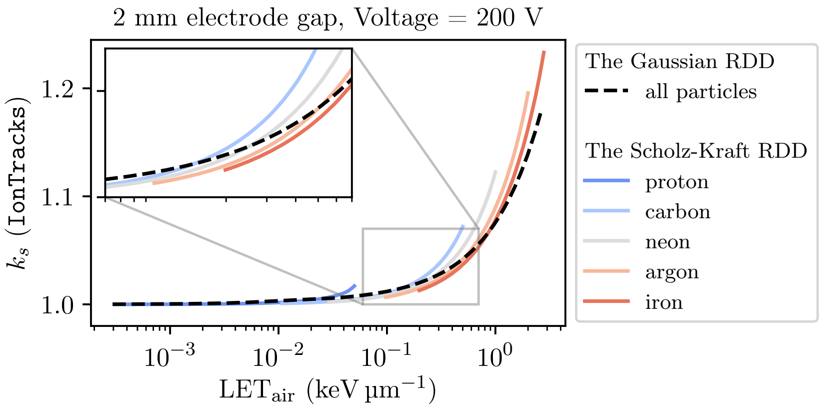
Radial dose distributions (RDDs)

The Gaussian track structure model

- Appears to be a good approximation
- Predicts the same k_s for two different ions (z) with same LET ($\Rightarrow$ wrong)



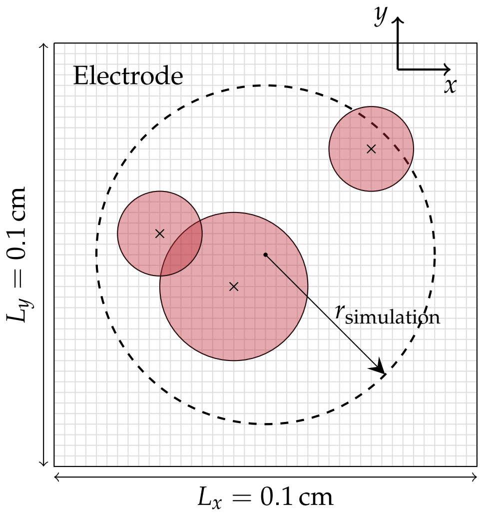
IonTracks simulation of a continuous beam

Input parameters

- Dose-rate $\dot{D}$
- electrode gap d, voltage V
- particle type (^{1}H, ^{4}He, ...) and energy E

Track sampling

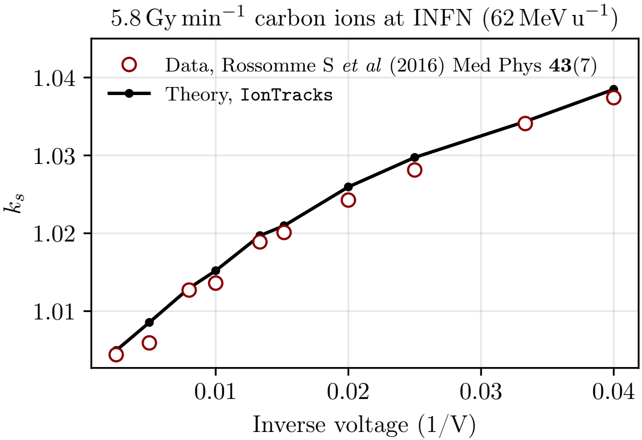
- Beam along $\hat{z}$
- Fluence-rate $\dot{\Phi} = \dot{D}/S_{\mathrm{air}}(E)$
- Track-rate $\dot{N} = \pi r^2_{\mathrm{simulation}}\dot{\Phi}$



Example: Low dose-rate carbon beam

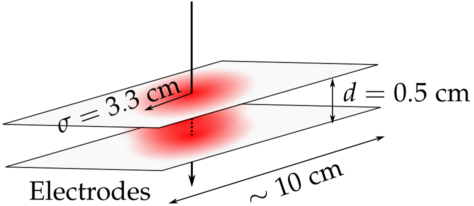
```python
from IonTracks import beam

# continuous beam
ks = beam(gap_d_cm=0.2,
          voltage_V=200,
          particle="carbon",
          energy_MeV_u=62,
          D_rate_Gy_min=5.8)
```



Courtesy: Marina Orts Sanz,
UCLouvain, Institute for Experimental and Clinical Research, Belgium

Recombination in ultra-high dose-rates (protons)



Conditions

- Wide chambers, narrow beam:
  - Beam sigma $\sigma = (3.3 \pm 0.3)$ cm
  - Electrode width $\gg \sigma$
- $k_s \propto \dfrac{\text{Ionization chamber signal}}{\text{Faraday cup signal}}$

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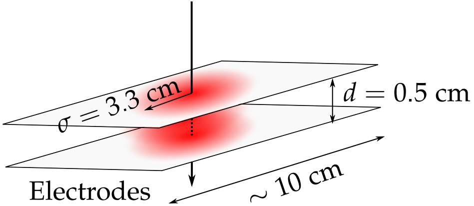

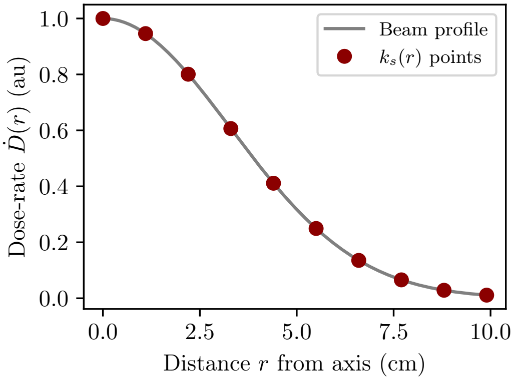

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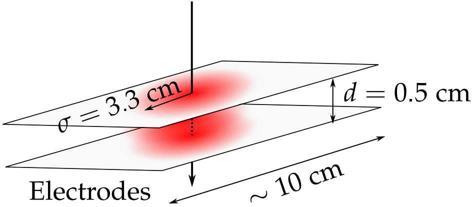

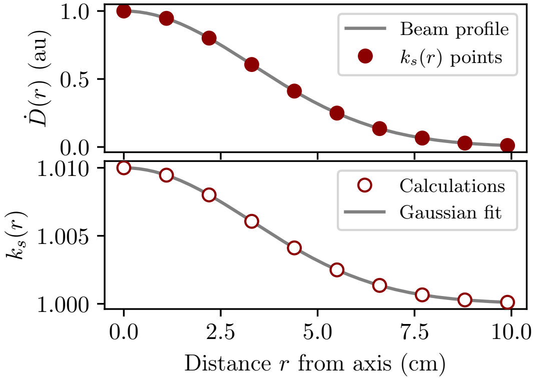

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$$k_{s,\text{total}} = \frac{1}{\int \dot{D}(r)\mathrm{d}r} \int k_s(r)\, \dot{D}(r)\, \mathrm{d}r$$

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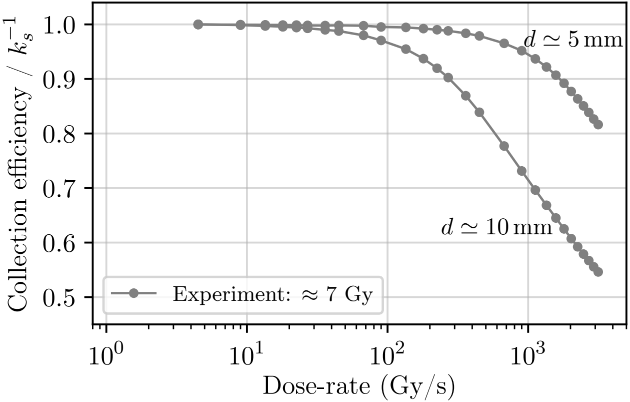

Irradiations

- Relative to a Faraday cup
- 250 MeV protons
- $d \simeq (5, 10)$ mm
- 2000 V

Measurements at CPT (PSI):
Robert Schäfer, Michele Togno, Sairos Safai

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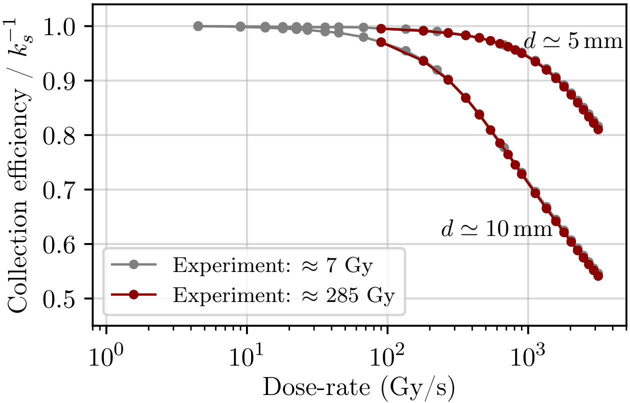

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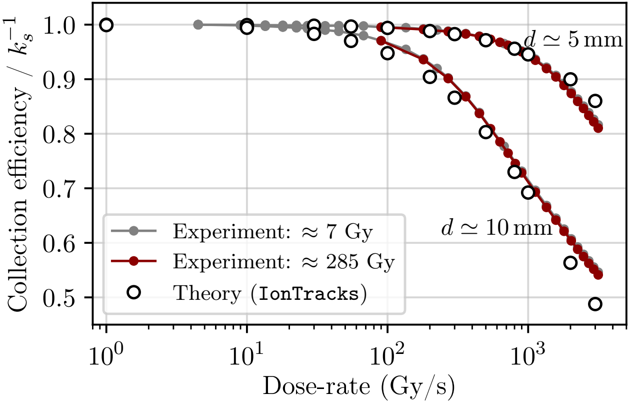

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  - Gaussian radial dose distribution (RDD)
- Generalised with `IonTracks`
  - any RDD

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Recombination between multiple ions (beams)

- semi-empirical models
  - three-voltage method
  - separation of initial-general recombination
- `IonTracks` for
  - not only mono-energetic fields! (sample tracks from a spectrum)
  - mixed particle fields
  - free-electron components
  - ...

Summary II

Data and code availability

- check out `github.com/jbrage/IonTracks`
- source code, data, scripts, this slideshow, . . .

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Next steps

- (More) user friendly interface!
- Benchmarking for heavier ions

A special thanks to

DCPT, DK

... Niels Bassler, Anne Vestergaard, Liliana Stolarczyk

UCLouvain, BE

... Marina Orts Sanz, Séverine Rossomme

PSI, CH

... Robert Schäfer, Michele Togno, Sairos Safai

Institute of Nuclear Physics, Kraków, PL

... Krzysztof Retkiewicz, Leszek Grzanka

... and many others!

Appendix

The Gaussian radial charge carrier distribution

The Jaffé theory works, but

- radius b should vary with E
- not a *real* amorphous track structure model
- e.g. ^{12}C and ^{16}O with same LET $\Rightarrow$ same k_s

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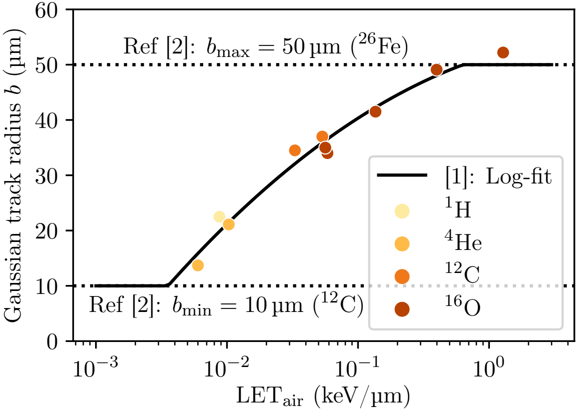

[1] Rossomme S *et al* (2017) *PMB* **62** 5365

[2] Kanai T *et al* (1998) *PMB* **43**(12) 3549