A Percolation Model for Calculating SSB- and DSB-yield

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Motivation

- **Problem**: basic assumption in microdosimetry: $E_{\text{deposited}} \propto (\text{number of ionisations})$.
  
  ... is violated in nanometre-sized volumes (number of ionisations is too small!).

- **Way out** (Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9):

  **Ionisation-cluster size “$v$“** (i.e. number of ionisations [in the volume] per primary particle) should be measured instead of $E_{\text{deposited}}$.

\[
P_1(Q; d) = \sum_{k=0}^{\infty} \left[ f_1^{(1)}(Q; d) \right]^k \frac{\langle k \rangle^k(Q)}{k!} \exp(-\langle k \rangle(Q)) = \text{Probabil. to cause } v = 1 \text{ at } d
\]

\[
F_2 = \sum_{v=2}^{\infty} \sum_{k=0}^{\infty} \left[ f_v^{(1)}(Q; d) \right]^k \frac{\langle k \rangle^k(Q)}{k!} \exp(-\langle k \rangle(Q)) = \text{Probabil. to cause } v \geq 2 \text{ at } d
\]
Motivation


  \[
  P_1 \leftrightarrow \text{single-strand break (SSB)} \\
  F_2 \leftrightarrow \text{double-strand break (DSB)}
  \]

- However, an ionisation cluster with \( \nu \geq 2 \) can also refer to single ionisations caused anywhere in the volume.

- Thus, an ionisation-cluster model would be of advantage!
Motivation

- There has been developed a highly sophisticated realistic DNA target model by Friedland et al. (Radiat. Res. 150 (1998) pp. 170 – 182) up to now which can be used, among many others, for calculating the SSB- and DSB-yield.

- In the following, I propose an alternative (percolation) model which is
  → very simple,
  → very quick,
  → and easy to use.

The model is by far not as powerful as the one of Friedland et al. (see above), but may be used (among others)
  → to analyse the geometry dependence of the cluster distribution.
General remarks about percolation models:

- percolation → percolare (Latin) ⇔ „to trickle through“
  E. g.: liquid trickles through sand (→ clusters arise).

- (simple) statistical models

- known in statistical/solid-state/nuclear/heavy ion physics, polymer chemistry, …

- basic idea:
  - site is occupied with occupation probability „p“
  - occupied neighboured sites are connected with bound probability „q“
The Model

Model formulation:

Scenario (cf. Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9):

Electron beam (homogeneous, monoenergetic)

- Volume: Height as well as diameter: 2.0 nm.
- Liquid water, density: 0.998203 g/cm³
- Molar masses: \( m_a(H) = 1.00794 \text{ u} \)
  \( m_a(O) = 15.9994 \text{ u} \)

⇒ Number of atoms within the cylinder: \( \approx 629 \)
The Model

- Assumptions: - triangular lattice structure

… motivated by H$_2$O molecule and DNA double helix.

- Clustering is dominated by lattice structure
  → 3-dim. lattice can be approximated by a 2-dim. one (25x25 sites)

- DNA molecule can be substituted by H$_2$O molecules.
The Model

- Further assumptions:
  - SSB if 1, 2, or 3 ionisations of the same H\textsubscript{2}O molecule took place.
  - DSB if ionisations belong to 2 or more molecules
  - q = 1
  - $p \Leftrightarrow$ ionisation probability $W$; $W = \omega \cdot \sigma_{\text{ion}}$

number of atoms (sites) per area
The Model

- Cross section for single ionisation of molecules:

![Image: Single ionization of molecules by electron and positron impact](image)

**Results: total cross sections**

**Comparison to experimental measurements**


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**Kinetic energy [MeV]** | **Occupation probability** | **Cross section [$10^8$ b]**
--- | --- | ---
0.05 | 0.1711 | 2.0
0.10 | 0.1996 | 2.3
0.30 | 0.1800 | 2.1
0.50 | 0.1392 | 1.6
2.00 | 0.0365 | 0.4
4.00 | 0.0228 | 0.3

Figure taken from Ch. Champion, GEANT4-DNA, New physics models, from cell to DNA, lecture, KIT - Basic Training Course For Micro- and Nanodosimetry, Oct. 2011.
The Model

Result:

Except for the percolation model, all values above were taken from Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9).

Experiment (irradiation of pBR322 plasmid DNA) was done by Folkard et al., Int. J. Radiat. Biol. 64 (1993), pp. 651 - 658.
Result:

Except for the percolation model, all values above were taken from Bernd Grosswendt, RPD 115 (2005), pp. 1 – 9. Experiment (irradiation of pBR322 plasmid DNA) was done by Folkard et al., Int. J. Radiat. Biol. 64 (1993), pp. 651 - 658.
Result and Conclusion:

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Percolation model values agree similarly well with the experimental values like that of Grosswendt or Friedland et al.

Essential input of the percolation model only was: geometry and \( p \leftrightarrow \sigma_{\text{ion}} \).

CAUTION: Percolation model has not sufficiently been tested up to now!
Thank you!

Ant Nebula (Mz 3)