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Low-energy electron and positron transport in gases and soft-condensed systems of biological relevance

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HIGHLIGHTS

- Detail differences in electron/positron transport in water in gas and liquid states.
- Emphasizes the importance of swarms as a test of accuracy/completeness of cross-sections.
- Emphasizes the importance of swarms for benchmarking Monte-Carlo simulations.
- Demonstrates the sensitivity of low-energy positron thermalization to cross-sections.

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ABSTRACT

We present a study of electron and positron transport in water in both the gaseous and liquid states using a Boltzmann equation analysis and a Monte-Carlo simulation technique. We assess the importance of coherent scattering processes when considering transport of electrons/positrons in dense gases and liquids. We highlight the importance of electron and positron swarm studies and experiments as a test of the accuracy and completeness of cross-sections, as well as a technique for benchmarking Monte-Carlo simulations. The thermalization of low-energy positrons (<150 eV) in water is discussed and the sensitivity of the profiles to the form of the cross-sections in this energy region, and assumptions in the microscopic processes, is considered.

1. Introduction

The study of electron and positron transport in biological matter is a key area of research in a variety of medical fields. Positrons, the antiparticle of the electron, are now a routinely used tool in imaging technologies such as positron emission tomography (PET) (Cherry et al., 2003) and in new therapeutic treatments such as positherapy and ion-beam therapy. In the latter, nuclear fragmentation of incident ions can often generate positron emitting particles, which can then provide a measure of the dose depth distribution for the ion beams (Enghardt et al., 2004). Positrons are emitted typically at hundreds of keV and must thermalize in human tissue down to a few hundred eV or less, before they can form positronium (Ps) or annihilate directly. The observation of the emitted back-to-back gamma rays arising from the annihilation is the key physics associated with these tools. Consequently, the source of the gamma rays is displaced from the source of positrons. Understanding the positron thermalization process is essential to optimizing the technologies and informing the development of positron dosimetry models. There is also a second issue of ionizing radiation involved in many imaging and therapeutic technologies, which by definition liberates copious numbers of secondary electrons along its path. Typically these electrons are produced with energy distributions less than 20–30 eV. These low-energy electrons thermalize in human tissue through a variety of energy deposition processes. Although low in energy, these electrons have recently been shown to be a source of DNA damage (Boudaiffa et al., 2000) and hence understanding the transport of low-energy

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secondary electrons is key to understanding radiation damage and informing dosimetry models.

Water is often used as a surrogate for modeling human tissue. Modeling charged particle transport in human tissue is dependent on, amongst other things (i) an accurate microscopic picture involving a complete and accurate set of cross-sections for positrons and electrons in water, and (ii) an accurate transport theory/simulation linking the microscopic and macroscopic scales. This is the focus of our program and the current paper.

Compilation of the best available set of cross-sections for all collisional processes (e.g. elastic, rotations, vibrations, etc.) is generally based on a critical assessment of available experimental studies and theoretical calculations (Itikawa and Mason, 2005). A key question, however, is establishing the completeness and accuracy of the resulting cross-section sets, and it is here that experimental swarm physics continues to play an important role (Huxley and Crompton, 1974; Petrovic et al., 2009). The reader is referred to recent studies of electron swarms in water (Robson et al., 2011; Ness et al., 2012), where the consistency of electron–water cross-section sets with experimental swarm data has been investigated. The ability of swarm experiments to discriminate on the consistency or otherwise of the cross-section sets demands the most accurate transport theory to analyze the data. There is a large body of literature for swarm transport theory focussed on establishing such accuracy through benchmarking transport codes and simulations (Ness and Robson, 1986; Raspopović et al., 1999; Petrovic et al., 2002), including a recent study of positrons in water (Banković et al., 2012b). Our program aims to apply such theories and codes to the field of radiation damage modeling.

Often human tissue is simply treated as a gas at liquid densities in the field of radiation damage modeling, thus facilitating the use of the highly accurate gas-phase cross-sections that are available. Electron swarm measurements in liquids and dense gases generally indicate that such an assumption is questionable, however, particularly at low energies. We have recently developed a theory that combines the binary collision (gas-phase) cross-section data with information on the structural properties of the soft-condensed matter, thus allowing us to consider multiple (coherent) scattering effects (White and Robson, 2009, 2011). We believe that experimental swarm studies in liquids and dense gases provide key benchmarks required for accurately accounting for the soft-condensed nature of media in any transport theory or simulation used in modeling charged particle thermalization in human tissue. We explore this procedure further in this paper.

In this paper, we present the current status of our program of modeling low-energy electron and positron transport in water. In Section 2 we present two independent techniques for transport modeling—Boltzmann equation and Monte-Carlo simulation treatments. The key role of swarm physics in establishing the accuracy and consistency of cross-section sets is considered in Section 3 along with a discussion of the differences between electron and positron transport in water vapor and the differences between gas and liquid phase transport. We finish with a study of the thermalization of low-energy positrons (<150 eV) in water in Section 4.

2. Transport models: Boltzmann equation and Monte-Carlo simulation techniques

The analysis of charged particle motion in matter can be treated semi-classically by Boltzmann equation or Monte-Carlo simulation techniques. Both effectively follow an ensemble of particles as they move through phase-space (combined configuration $\boldsymbol{r}$ and velocity $\boldsymbol{c}$ spaces) under the action of forces and collisional processes. Boltzmann equation methods solve directly for the phase-space distribution function $f(\boldsymbol{r},\boldsymbol{c},t)$ (Boltzmann, 1872)

$$\frac{\partial f}{\partial t}+\boldsymbol{c}\cdot\nabla f+\frac{qE}{m}\cdot\frac{\partial f}{\partial \boldsymbol{c}}=-J(f). \tag{1}$$

Here $\boldsymbol{r}$ $\boldsymbol{c}$ denotes, the electric field while q and m are the charge and mass of the particle, respectively. Also, $J=J_{elas}+J_{inel}+J_{Ps}+J_a+J_{ion}$ is a linear collision operator representing the various collisional processes with the medium. The collision operator J_{elas} describes elastic scattering processes and the operator describing Ps formation, $J_{Ps}=n_0 c\sigma_{Ps}(c)$, where n_0 is the number density of the molecules of the background medium, and $\sigma_{Ps}(c)$ is the Ps formation cross-section. The positron annihilation operator J_a is similarly defined in terms of an annihilation cross-section $\sigma_a(c)$, while J_{inel} is taken here to be the semi-classical inelastic collision operator (Wang-Chang et al., 1964). For ionization processes, we implement the ionization collision operator J_{ion} detailed in Ness and Robson (1986). This is the microscopic picture. Solution for the phase-space distribution function $f(\boldsymbol{r},\boldsymbol{c},t)$ enables calculation of macroscopic measurable quantities through appropriate averages, e.g. the local charged particle density at time t is given by

$$n(\boldsymbol{r},t)=\int f(\boldsymbol{r},\boldsymbol{c},t)\,d\boldsymbol{c}. \tag{2}$$

Monte-Carlo simulation methods follow event by event the trajectory of each charged particle in the system. By considering an ensemble of such charged particles, one can then approximate (simulate) the charged-particle phase-space distribution function. Measurable macroscopic quantities are formed from appropriate averaging over the members of the ensemble.

In what follows, we briefly discuss the methods of solution and simulation used in this study. These independent techniques have been exhaustively tested against each other and against experiments for various benchmark systems. This is necessary to ensure the validity of the techniques.

2.1. Boltzmann equation treatment—a "multi-term" solution

Solution of the Boltzmann equation (1) requires decomposition of $f(\boldsymbol{r},\boldsymbol{c},t)$ in velocity space as discussed below. The first step in any analysis is typically the representation of the distribution function in terms of the directions of velocity space through an expansion in spherical harmonics (Robson and Ness, 1986)

$$f(\boldsymbol{r},\boldsymbol{c},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_m^{(l)}(\boldsymbol{r},c,t)Y_m^{[l]}(\hat{\boldsymbol{c}}), \tag{3}$$

where $Y_m^{[l]}(\hat{\boldsymbol{c}})$ are spherical harmonics and $\hat{\boldsymbol{c}}$ denotes the angles of $\boldsymbol{c}$. While common practice is to set the upper bound of the l-summation to 1 (i.e., the two-term approximation) and consider only $m=0$ (i.e., a Legendre polynomial expansion), we do not make any such restrictive assumptions in this theory, thus avoiding serious error (Ness and Robson, 1986; White et al., 2002). In best practice, the integer $l_{\max}$ is successively incremented until a prescribed accuracy criterion is met, as considered below. Combining (1) and (3) leads to the following hierarchy of coupled integro-differential equations for $f_m^{(l)}$:

$$\partial_t f_m^{(l)}+\sum_{l'm'}\left\langle lm\left|\boldsymbol{c}\cdot\nabla+\frac{e\boldsymbol{E}}{m}\cdot\frac{\partial}{\partial\boldsymbol{c}}\right|l'm'\right\rangle f_{m'}^{(l')}=-\sum_{l'm'}\langle lm|J|l'm'\rangle f_{m'}^{(l')}. \tag{4}$$

Expressions for the matrix elements of the streaming operator on the LHS are given in Robson and Ness (1986) and Ness and Robson (1986). The collision matrices e.g. $\langle lm|J|\,l'm'\rangle=[J_{elas}^{l}+J_{inel}^{l}+J_{Ps}^{l}+J_a^{l}+J_{ion}^{l}]\delta_{l',l}\,\delta_{m',m}$ are all diagonal in l and m, since the collision operators are all scalars. Details of the numerical schemes required for the solution of (4) are presented in the Appendix.