Development of interaction models in Geant4-DNA to simulate cosmic rays' effects on ion-molecules reaction in the atmosphere

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Background: Chemical reaction rates can change up to 10 orders of magnitude, depending on the ionization state of the species involved. Therefore, cosmic rays could significantly affect chemical reactions in the atmosphere, considering also that the ions produced are clustered nearby the primary ray. The influence of cosmic rays on atmospheric models is still poorly studied. The amount and states of ionization, and spatial distribution of the produced ions, are open questions for these models [1]. Our project aims to shed light on the rule of ions by exploiting the Track Structure approach of Geant4-DNA and implementing models in it to simulate electromagnetic interactions with molecules of interest for climatology.

Methods: As a starting point, we focused on electron-impact interactions with the two most abundant molecules in the atmosphere, i.e. N_2 and O_2. We reviewed the state-of-the-art models to describe the interactions relevant to our purpose, namely ionization, elastic scattering, and electron excitation cross sections, in an energy range from threshold up to 1GeV [2,3,4].

Preliminary results: We will present a benchmark of the models we selected with experimental data and preliminary results from our implementation in Geant4-DNA. The agreement with the data is very good, except for electronic excitation, for which both theoretical and experimental issues lead to spotty agreement. The extension of Geant4-DNA with models suitable for new molecules, in addition to the potential impact on the physics of the atmosphere, open the way for new space-related studies regarding chemistry and exobiology and be applied to any kind of Geant4-DNA simulation.

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