Energy deposited in the COVID-19/SARS-CoV-2 molecule by beams of low energy electrons

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Abstract. In this work we use the software GEANT4 release 10.6.2 to simulate the experimental setup consisting of a monoenergetic beam of electrons hitting on a molecule of COVID-19/SARS-CoV-2 with protein database identifier: 6vsb. After that we have found the kinetic energy values for the beam, such that the electrons can deposit their maximum amount of energy in the 6vsb molecule. For these kinetic energy values, we have also estimated the electric currents for the beam in vacuum. At the same time, we analysed the fraction of electrons that hit the 6vsb molecule which give us the efficiency of a thought medical treatment. With this early analysis, we aim to understand the physical properties of the coronavirus and set the basis for future analysis involving more molecules from the protein database.

1. Introduction

Up to date, the novel coronavirus COVID-19/SARS-CoV-2 has spread over almost the entire world, becoming the last pandemic in more than 100 years [1]. After the initial misunderstood about the clinical trials [2,3], and worsening when there were another viral and non-viral diseases [4,5] and seeing the seriousness of the matter, we tempted ourselves to try to do an analysis independent of the patient to avoid the combinatoric cases that arise from each individual clinical history and status, we also want to understand a possible mechanism that can benefits the design of electromagnetic devices that could help sanitize the places where people congregate. From this point of view, we arrive at the conclusion that any research that could help other medical and experimental scientists with information to fight this virus must be the pursuit of any interdisciplinary collaborative work in the present. With that spirit, in this work we are focused on to find the kinetic energy values for beams of electrons, such that they can deposit the maximum fraction of energy into the COVID-19/SARS-CoV-2 6vsb molecule, that we have taken from the experimental work [6].

This work is organized thus: section 2 describes the simulation setup for the experiment, section 3 shows the results of a few runs of the beam at different values of energy, we also do a plot of the fraction of absorbed energy and the efficiency, and section 4 are conclusions of the work.

2. Methods

In this work we used the software GEANT4 [7-11] release 10.6.2 For the ROOT [12] platform the release was 6.20.04. This software had been validated by the particle physics community.
2.1. Detector construction
The construction of the COVID-19/SARS-CoV-2 molecule 6vsb as a particle detector is done with help of the pdb file downloaded from the Protein Database Bank webpage; Figure 1 shows its GEANT4 atom representation by spheres of material. This geometry presents the results of an electron microscopy swept on the 6vsb sample and this is the first real sample that accounts for the full atoms in its molecule. The GEANT4 pdb file loader gets 3 loaded chains with 22000 atoms, from which we have 14063 atoms of carbon, 4185 atoms of oxygen, 3651 atoms of nitrogen and 101 atoms of sulfur (Figure 1). The molecule bounding box has dimensions \( l_x = 12.168 \text{nm} \), \( l_y = 12.3843 \text{nm} \), \( l_z = 17.3995 \text{nm} \).

2.2. Physics list
The list of physical processes that can occur in the simulation is set to electromagnetic low energy processes, those that are already incorporated by the geant4-dna collaboration [9] in the geant4 example put on examples/extended/medical/dna/pdb4dna.

2.3. Simulation setup
The geometry of the virus is placed at the origin of the reference system, and the particle gun position \( \mathbf{r}_0 \) is determined in a random way on a sphere with centre at the origin and radius \( r = 12.29 \text{nm} = (s_x^2 + s_y^2 + s_z^2)^{1/2} \), with \( s_{x,y,z} = \frac{1}{2} l_{x,y,z} \). Thus, the random rotational movement of the molecule could be emulated. Let \( \mathbf{b} \) be the vector position of a random point inside the bounding box, thus the initial momentum direction of each beam is set to \( (\mathbf{b} - \mathbf{r}_0)/||\mathbf{b} - \mathbf{r}_0|| \).

2.4. Strategy
As each simulation is the repetition of a beam of one electron going towards the target, where the coronavirus molecule 6vsb is placed, and finalize when the total number of particles in the simulation are launched, then we run a set of simulations each one at a different value for the monoenergetic beam composed of \( n^{\text{launched}} = 100000 \) electrons in the interval \([60, 600]\) eV with steps of at least 60eV. After that we put attention on the low energy interval \([1, 60]\) eV with steps of 1 eV. With \( n^{\text{launched}} = 100000 \) electrons we reach a desired low numerical error (small error bars) compared with, for example 10000 electrons that produce large error bars in the results. We also note that typical electric currents in a cellular membrane involve approx. 11000 electrons.

3. Results
First, when the beam energy ranges between 1 eV and 7.4 eV, we got the 100% of electrons absorption in the COVID-19/SARS-CoV-2 molecule. Second, we show a panoramic view of the COVID-19/SARS-CoV-2 molecule energy absorption distributions for the electron beam in the range \([0, 600]\) eV, this is shown in Figures 2 to Figure 6.
Figures 2 shows a histogram with a distribution that is higher for low energy values. This tendency it maintained in the simulations as the beam energy is lowered until we try the value 360 eV shown in Figure 3, Figure 4, Figure 5, and Figure 6, here the histograms has two peaks being the right peak higher than the left. For interval 240 eV to 18 eV the fraction of absorbed energy is above 0.6 except in 33 eV the fraction is 0.599. We also observe a local maximum at 20 eV and a local minimum at 11 eV, and finally global maximum from 7.4 until 1 eV. This could be seen in Figures 2, to Figure 6.

Figure 2. Energy deposited in the COVID-19/SARS-CoV-2 molecule 6vsb with $E_{\text{beam}} = 600$ eV.

Figure 3. Energy deposited in the COVID-19/SARS-CoV-2 molecule 6vsb with $E_{\text{beam}} = 360$ eV.

Figure 4. Energy deposited in the COVID-19/SARS-CoV-2 molecule 6vsb with $E_{\text{beam}} = 240$ eV.

Figure 5. Energy deposited in the COVID-19/SARS-CoV-2 molecule 6vsb with $E_{\text{beam}} = 60$ eV.
Figure 6. Energy deposited in the COVID-19/SARS-CoV-2 molecule 6vsb by the beam of electrons at 20 eV.

Figure 7(a) and Figure 7(b) show in dark blue the fraction of mean energy deposited by the beam in the molecule $E_{\text{mean}}/E_{\text{beam}}$ and also the ratio of the number of particles absorbed $n_{\text{hits}}/n_{\text{launched}}$. Figure 6 is a plot of the same kind as Figures 2 to Figure 5 with a beam energy of 20 eV. Figures 2, and Figure 3 starting from top left with a beam energy of 600 eV has high frequency for beam's energy values close to zero and also has a smooth right tail. As the energy of the beam decreases, we note the right tail is not smooth but becoming a lump. For beam energy 360 eV the right lump is higher than the left lump, can be noted by its value 0.51472 the blue square is just above 0.5.

At a given beam energy we could calculate the vacuum electron speed by using the relativistic formula $v = \frac{c}{\sqrt{1 - \frac{v^2}{c^2}}}$, for $E_{\text{beam}}$ equals to 1 eV and 20 eV, and for electron $mc^2 = 510998.94$ eV, speed of light in vacuum $c = 2.99792458 \times 10^{17}$ nm/s we have: $v_1 = 5.93 \times 10^{14}$ nm/s, $v_{20} = 2.65 \times 10^{15}$ nm/s the volume is $V = l_1 l_2 l_3 = 2621.96828$ nm$^3$, then the beam current density is $J = n_{\text{launched}} ev/V$, where $f$ is a factor that allow us modify the number of particles in the beam, such that we can get non-lethal values for the electric current, for instance we make $f = 1$ and therefore by using $v_1$ and $v_{20}$, and cross section $A = \pi r^2 = 474.519$ nm$^2$: $I_1 = 3.6241 \times 10^{-3}$ A nm$^2$ = 3.6241 PA/m$^2$, implying the electrical current $I_1 = 1.72$ A; $I_{20} = 16.2073 \times 10^{-3}$ A nm$^2$ = 16.2073 PA/m$^2$, implying $I_{20} = 7.69$ A. We note the value for the cross section is greater than typical membrane ion channel approx. $\pi(0.3$ nm$)^2$.

4. Conclusions
According to the simulations done in this work, the best energy values for the electron beam in the low energy regime in order to get the maximum gain of energy deposited in the molecule are the interval $[1, 7.4]$ eV and alternatively 20 eV. Manipulation of the real number of electrons in the beam can be made through parameter $f$ in such a way to obtain non-lethal values for the electric currents.
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