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Modeling for plasma medicine: What can we learn from it ?

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Although plasma is very promising for several medical applications, the underlying mechanisms are not yet fully understood. Computer modeling can be very useful for obtaining a better insight. Different types of models can be applied, depending on the system to be studied and the type of information required. In this lecture, I will explain different modeling approaches, relevant for plasma medicine, i.e., both macro-scale and atomic/molecular scale models. In addition, I will present typical results obtained by these models, to illustrate the type of information that can be obtained.

Several different 0D chemical kinetics models and 1D/2D fluid dynamics models have been developed for different types of biomedical plasma sources (i.e., different types of plasma jets and DBDs) and their interaction with liquids. They typically provide information on the important RONS, present inside the plasma, the effluent and/or the liquid. 0D models focus on a detailed chemistry, as they can handle a large number of species and chemical reactions with limited computational cost. On the other hand, they assume a uniform plasma, and only calculate the plasma species densities and other plasma characteristics as a function of time. However, this time-evolution can sometimes be translated into a spatial evolution, i.e., for the species densities in the effluent of a plasma jet, by means of the gas flow velocity. 1D/2D (or in principle 3D) fluid dynamics simulations typically consider a more limited chemistry (due to calculation time), but can be used to model specific plasma devices, and provide full spatial information, e.g., gas and liquid flow profiles, species concentration profiles in the gas and liquid phase (including transport of RONS from the interface to the bulk), and chemical pathways for the various species in gas and liquid phase.

Besides describing the plasma chemistry, chemical kinetics models may also be interesting to study cell signaling pathways, e.g., to better understand the selectivity of plasma for cancer therapy. This is very complicated, but a first attempt for such modeling will be presented as well.

Atomic/molecular scale models have been developed to study the interaction of plasma-produced RONS with biomolecules important in the context of plasma medicine, such as the bacterial cell membrane, the phospholipid bilayer (PLB) as model system for the cell membrane, DNA, and proteins, as well as the effect of these interactions (e.g., oxidation) on structural changes in the biomolecules. To study the interactions, reactive molecular dynamics (MD) simulations are typically used, because they allow to describe bond breaking and formation, and thus chemical reactions. They are however very time-consuming. Thus, if the focus is on studying the effect of e.g., plasma-induced oxidation on structural changes or stability of biomolecules, non-reactive MD simulations are more appropriate, as they are less time-consuming and can thus handle larger systems and longer time-scales. For instance, this type of models can provide insight in the permeability of RONS across both native and oxidized PLBs, as well as in the synergistic effect of plasma oxidation and electric fields on pore formation, the effect of cholesterol present in the cell membrane on the permeability and on the chance for pore formation, and in the different permeability of H_2O_2 (as representative RONS) across AQP channels vs. the PLB, in order to contribute to a better understanding of the selectivity of plasma for cancer treatment.