Modelling gold nanoparticle biodistribution <u>Tahmineh Azizi¹¹</u>

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Abstract

Nowadays, nanoparticles have a growing use in industry specially medicine. There are some studies about applications of NPs in therapeutic areas, however, the number of these studies is not a lot. Increasing the importance of studies about tumors and concentration of drugs and NPs in tumors or other tissues has enhanced the role of in vitro models to simulate absorption process of drugs and NPs. Pharmacokinetic and physiological models are useful means to demonstrate the relationships between different drug administrations, and drug exposure or concentration.

A mathematical model for drug or NP distributions is a structural model, consisting of compartments such as adipose, tissues, brain, gut, heart, kidney, liver, lung, muscle, spleen, skin, and bone and gastrointestinal tract including mouth, esophagus, and abdomen which are connected by the cardiovascular system. In mathematical perspective, they describe biological systems by converting into mathematical and theoretical equations and parameters and then using computer code to solve the model system computationally. To check the accuracy of any mathematical model, we need to use different methods and because of existence of uncertainty in experimental data, it can be often complicated. Uncertainty and sensitivity analysis are useful techniques which help us to identify these uncertainties in data and then control them.

Pharmacokinetic models are mathematical models which provide insights into the interaction of chemicals with biological processes. During recent decades, these models have become central of attention in industry that caused to do a lot of efforts to make them more accurate. Current work studies the process of drug and nanoparticle (NPs) distribution throughout the body which consists of a system of ordinary differential equations. We use a tri-compartmental model to study the perfusion of NPs in tissues and a six-compartmental model to study drug distribution in different body organs. We have performed global sensitivity analysis by LHS Monte Carlo method using PRCC. We identify the key parameters that contribute most significantly to the absorption and distribution of drugs and NPs in different organs in body.

Keywords: Global Sensitivity Analysis, Latin Hypercube Sampling (LHS), Partial Rank Correlation Coefficient (PRCC), Physiological Systems, Drug and NPs Distribution

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