Abstract No: PO-09

A mathematical model for the description of the drug distribution in the human body

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In pharmaceutical industry, various researches have been carried to discover new drugs and to find effective ways of transporting drugs into target parts of the human body. Oral administration, intravenous and inhalations are the commonly used methods in administering drugs. This research study mainly considers oral administration of a drug in tablet form. Determining the absorption processes of a drug after oral administration to the body is a complicated problem. But mathematical modeling can provide the optimal solutions to various complex problems. The compartment model is the mathematical representation of human organs, created to study the drug distribution. This study describes a four-compartment model for drug distribution in the oral mode. In this study, stomach, small intestine, blood and tissues were used as four compartments. In oral consumption of a drug, absorption into the bloodstream occurs in the stomach and small intestine. The blood carries medicine from the site of absorption to the targeted sites and also to sites of metabolism or excretion, such as the kidneys, the liver. Finally, the drugs are excreted through urine after the metabolic process. Drug absorption rate and drug flow rate were used in developing this mathematical model. The rate of drug movement between compartments was described by first-order kinetics. The drug is absorbed through the stomach when drugs are taken orally but has been neglected in this study because of its small amount of absorption compared with other absorption constants. The formulation of this model is based on the principle of continuity and first-order kinetics. First the mathematical interrelationships between the drug concentration were derived with distribution time and rate constants. Then the first-order differential equation system was derived. This first-order differential equation system was solved using the Laplace transform method to avoid the complication raised while finding the eigenvector in the eigenvalue method. Existing rate constants in the mathematical model take different values for different drugs. The rate constants needed for this study were taken from the clinical trial conducted for paracetamol. The drug used in the current mathematical model was paracetamol. The mathematical model for paracetamol distribution was solved using the 4^{th} order Runge-Kutta method and the solutions were plotted using MATLAB. Here, with higher absorption rate constants, the drug is absorbed faster into the body and with lower absorption rate constants, the drug will be retained within the body as a residue, thereby causing side effects. Hence, when the second dose is administered after six hours, the residual drugs from the first dose were also calculated. The present study helps to estimate the relationship between drug absorption, distribution, and the elimination processes.

Keywords: absorption, compartment model, drug distribution, Laplace transform, Runge-Kutta