

EXECUTIVE SUMMARY

A human body simulator that mathematically models the concentration levels of a drug in the blood and in 23 tissues was developed. The model consists of over 1,100 simultaneous ordinary differential equations and two-hundred parameters. Case studies were performed which compared the model to experimentally obtained drug concentration data for two different drugs and showed that the model could reproduce experimental results extremely well.

Developing a human body model is critical to the pharmaceutical industry where \$70 billion is spent every year on research and development of new drugs. This money is mostly used for in vitro and in vivo testing of large numbers of compounds with potential medical applications, most of which are later found to be unsuitable for further development. A human body simulator should refine this process by allowing pharmaceutical companies to screen more compounds using simulations as opposed to expensive lab testing. Additional applications include allowing doctors to make customized, optimized dosages for each of their patients that produce the exact desired effects of a drug.

Although sophisticated drug distribution models are available commercially, the model developed here is a significant advancement in models currently discussed in academic literature and thus can serve as a stepping stone for future work. The model includes the latest theory about the most critical organs in the body, a novel distribution system that integrates each body system at the level of the capillary, and a method to account for differences in concentration along spatial dimensions inside each tissue within the body.

To make the model truly predictive, two important elements should be developed in the future. Firstly, the model should be able to predict all the parameters of the drug which will affect its behavior inside the body. Currently, parameters are obtained from literature when possible and estimated when necessary. Secondly, the model should account for variations between persons. In order to do this, the predictive algorithms for estimating the parameters would need to consider genetics, body type, and other factors. Developing a mathematical model of the human body is a prerequisite for these other developments and thus was the focus of our work.