University of Ljubljana
Faculty of Computer and Information Science

Maja Somrak

Computational modelling of treatment with *in situ* biological drug production

ABSTRACT

Computer modelling is increasingly important part of drug development process. It helps to reduce the number of required experiments and provide initial evaluation of therapy outcomes.

In this thesis, we focus on modelling pharmacokinetics of therapeutic substances for different therapy approaches. We present a physiologically based compartmental pharmacokinetic model, which quantitatively describes drug processes in the body using a system of ordinary differential equations. We develop a model for standard types of drug administration and expand it to include the process of production. With the expanded model we can simulate therapy, which uses a drug delivery system for *in situ* production of a specific biological drug. The expanded model predicts the necessary drug production rate for the therapy to ensure the desired therapeutic effect.

We develop both the basic and the expanded model for two study cases. The first study case evaluates treatments of hepatitis C; the second treatments of ischaemic heart disease. A result comparison enables quantitative and qualitative therapy evaluation in terms of efficiency, drug localization and degree of systemic adverse effects.

Key words: pharmacokinetics, physiological model, compartmental model, model with *in situ* production, Matlab