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Preface

Mathematical modeling of controlled drug delivery

Mathematical modeling of controlled drug delivery can help provide a scientific knowledge base concerning the mass transport mechanisms which are involved in the control of drug release. In addition, if an adequate mathematical theory is identified for a particular pharmaceutical system it can be used to simulate the effect of the device design parameters (e.g., geometry and composition) on the resulting drug release kinetics. In an ideal case, the system formulation parameters required to achieve a certain, desired drug release profile can be predicted. Thus, mathematical modeling can significantly facilitate the optimization of existing and the development of new pharmaceutical products.

When developing new controlled release systems or elucidating drug release mechanisms, the choice of the appropriate mathematical model strongly depends on the type of drug, type of excipients and composition of the device. Various mechanisms can be used to control drug release. Diffusion, water-triggered transport (swelling) and degradation/erosion are the most important ones. Other phenomena, such as osmotic, magnetic, or electric effects may be involved.

Very often, polymers are added to control or modify the release step of the drug. The chemical nature of the polymers commonly used for pharmaceutical purposes differs significantly. Some of them are freely water-soluble, others completely water-insoluble. They vary in the rate and extend of swelling, bioerosion/biodegradation and their potential to interact with the drug.

There is no overall mathematical model covering all the possible chemical and physical processes that can occur. Thus, it is crucial to identify or develop an adequate mathematical theory for a specific drug delivery system.

This special issue provides comprehensive review articles on the current state of the art of mathematical modeling approaches of various types of devices (controlled by diffusion, dissolution, swelling and/or erosion/degradation). As polymer dissolution plays a crucial role in many drug delivery systems, a review article describing theoretical approaches to quantify this complex phenomenon is included, focusing on the consequences for drug release. For the therapeutic efficiency of a pharmaceutical product, the resulting drug concentrations at the site of action in the human patient are decisive. For this reason, two papers are included dealing with mathematical modeling approaches describing the pharmacokinetics of a drug in the body. Both major approaches are represented: compartment and non-compartment-based theories. Furthermore, the importance of the administration route is emphasized. One article deals with transdermal drug release modeling, another with the mathematical treatment of drug transfer through mucus. Finally, a review on control-relevant modeling in drug delivery is presented.

A large spectrum of mathematical theories describing drug release from controlled delivery systems and modeling approaches to quantify the pharmacokinetics of the drug in the human body is available. For those involved in the design and development of new drug delivery systems the choice of the appropriate model for a particular purpose depends on various aspects. Of course, the route of administration, type of drug and excipients to control the resulting release rate are important criteria to be considered. The desired/required predictive ability and accuracy of the model are of major importance. Yet, in many cases, the literature relies on the use of simple empirical or semi-empirical models which are not truly sufficient to predict

the exact behavior of a drug. When reliable, detailed information are required, more complex, mechanistic theories must be applied. Hopefully, one of the long term goals of this special volume will be to show how exact modeling can be done and what its implications are.

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