Preface

The principles of optimality govern our everyday life. Any natural or artificial system, which surrounds us or influences our closest vicinity, tends to operate optimally, i.e. it tries to maximise or minimise some given function under present constraints. This can be seen even in such microscopic phenomena as the bonding of atoms to form molecules in order to minimise the overall potential energy (function). The primary neural network in humans is the brain, in which the neurons use the minimum of wiring material (neuronal connections) necessary to comply with the constrain imposed by the amount and rate of information transfer. Seeds in sunflowers are collocated in order to maximise their number subject to the given area and the seed shape. In these cases, it is nature which decides, using evolutionary (trial and error, survival of the fittest) principles, about the optimal design of the systems.

Artificial systems, such as traffic, electricity, or logistic networks, are designed by engineers who express the objective and constraints in mathematical form of functions and equations. If only this were true—just look at the traffic congestion around oxford. Using such a mathematical model of reality, actual design problems can be then solved by exploiting tools (e.g. algorithms) provided by mathematics and computer science. The solution is then given by a set of discrete values of decision (optimisation) variables. Once this is done, we are sure that nothing better is possible to achieve for the actual form of objective and constraint functions and for the actual state of the system.

But what if the system state or any of these functions involved in the optimisation problem are changing over time? Then, we obviously need to repeat the whole optimal design procedure at each time instant. From the practical point of view, we no longer speak about discrete decision (control) actions but we consider the corresponding time-dependent trajectories. We attribute all dynamic changes happening at the observed system to an entity that we call process. Again, since our goal is the optimisation of the system, we need to devise a mathematical model of the reality, a dynamic (process) model.

It is interesting to note that a variety of problems of the design of optimal process operation (i.e. optimal process control) arise in fields of engineering (chemical, mechanical, electrical,…), computer science, economics, finance, operations research and management science, space exploration, physics, structural and molecular biology, medicine and material science. Such problems include finding of an optimal control strategy which minimises energy or raw material consumption during the production processes, maximises production profit, or leads to optimal process model identification (optimal experiment design, parameter estimation). Although similar concepts from static design apply for this optimisation problem, the situation is complicated by the presence of dynamic forms of system state and objective and constraint functions.

Tools for solving static optimal design problems date back to the end of the first half of the last century. Development of linear programing methods, followed soon by nonlinear programming (NLP) ones, enabled effective computer solution of various engineering problems arising in many fields. Dynamic optimisation (DO) represents a mathematical approach for solving problems of open-loop optimal process control.

The techniques utilised to solve DO problems in the class of deterministic approaches fall under two broad frameworks: variational (indirect) methods and discretisation (direct) methods. Variational methods address the DO problem in its original infinite-dimensional form exploiting the classical calculus of variations together with dynamic programming or Pontryagin's maximum/minimum principle. A big advantage of this is that we look for an exact solution to the problem without any transformations. On the other hand, use of these approaches can become difficult if we want to solve DO problem for more complicated systems. Then discretisation plays an important role since the original infinite-dimensional problem is transformed to a nonlinear programing problem. Once transformed into static form, the DO problem can be solved approximately by means of static optimisation just as in static optimal design. It is then only a matter of utilised degree and form of discretisation as to how close the obtained solution will be to the original problem. Discretisation methods can be subdivided into two broad classifications known as simultaneous and sequential.

The simultaneous method is a complete discretisation of both state and control variables often achieved via collocation. While completely transforming a dynamic system into a system of algebraic equations eliminates the problem of optimising in an infinite-dimensional space, simultaneous discretisation has the unfortunate effect of generating a multitude of additional variables yielding large, unwieldy NLPs that are often impractical to solve numerically.

Sequential discretisation, usually achieved via control parameterisation, is a discretisation approach in which the control variable profiles are approximated by a sum of basis functions in terms of a finite set of real parameters. These parameters then become the decision variables in a dynamic embedded NLP. Function (functional) evaluations are provided to this NLP via numerical solution of a fully determined initial value problem (IVP), which is given by fixing the control profiles. This method has the advantage of yielding a relatively small NLP and exploiting the robustness and efficiency of modern IVP and sensitivity solvers.

In this monograph, we deal with membrane processes which stand for an emerging technology in the chemical and bioprocess industry, used both in production and downstream processing. Membrane processes, such as membrane distillation, pervaporation, membrane purification, diafiltration, and processes exploiting membrane-equipped reactors, are receiving growing attention mainly due to reduced energy demands and higher efficiency of the achieved separation or processing goals. These systems, however, did not receive much attention from the process optimisation community and that is why they provide many opportunities, for example, the development of optimal operation design.

Purification of a solution can be achieved by employing a semi-permeable membrane which retains or concentrates (in) valuable species. A diafiltration process combines two possible ways of treating a solution to concentrate its valuable components and to dilute (dispose of) present impurities. It can be performed continuously or discontinuously. This depends on several physical factors and on properties of initial solution as well as the final product. The process can be controlled, either in continuous or batch set-up, by influencing concentrations through an addition of solute-free solvent (diluant). Utilisation of this diafiltration buffer can be dynamically adjusted to optimise the process performance, e.g. minimum time or minimum diluant operation can be attained.

This monograph concentrates on finding a general optimal operation strategy for batch diafiltration processes which are a particular class of membrane separation/purification processes. The existing operating practice is explored and improved operation, based on the optimal control theory, is provided. The results presented summarise the research outcomes of our group since 2009, which have been published in journals and at various IFAC, IEEE, and membrane-process-oriented conferences.

The monograph is organised as follows. The first part (Chaps. 1–3) introduces the theory of membrane processes, optimal control, and dynamic optimisation in a way to provide tools that are exploited in the second part for finding an optimal operation of batch diafiltration processes. The theory of membrane processes includes the definition of separation problems, the derivation of dynamic mathematical models of batch membrane processes, and the introduction of typical cost specifications. The part on control theory involves an introduction to the problems of dynamic optimisation mainly from a chemical engineering point of view. It is followed by an explanation of methods (analytical and numerical) that can be exploited to treat the problems of optimal control of membrane processes.

The second part (Chaps. 4–8) then builds upon the theoretical basis and uses it to establish a solution to treated problems. It is divided into sections treating membrane models with increasing complexity. First, the limiting flux model is treated. The next chapter deals with perfect separation of solutes with arbitrary flux models. A further generalisation is studied when the macro-solute is perfectly rejected or if both rejection coefficients are constant. Finally, Chap. 8 discusses the most general model. Each chapter starts with a derivation of optimal operation and continues with selected case studies that present various aspects of considered optimal control problems and discuss the possible advantages and drawbacks of real implementation of optimal operation of diafiltration processes.

The objectives of the monograph can be summarised as follows:

- to introduce the reader to the field of dynamic optimisation and optimal control of (chemical) processes,
- to survey analytical and numerical methods for solving problems of optimal control,
- to present a study of optimal control for general diafiltration processes,
- to derive analytical solution for most common classes of batch diafiltration processes,
- to propose a simple numerical approach to treat the general case of optimal operation for batch diafiltration processes,
- to present a comparison of the resulting optimal operation with the standard industrial control techniques and discussion of advantages of optimal operation and of future challenges for optimal operation of diafiltration processes.

Some of the programs and figures of the examples presented in the monograph are freely available at the web page:

http://www.kirp.chtf.stuba.sk/~fikar/books/mem/index.htm.

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