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Contributions to modelling, simulation and control of chemical reactions based processes

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1. Introduction

Control systems domain has applications in all activity fields of our society. From biology to mechanics, from chemistry to electrical, from food industry to engine run, all processes that govern the industrial applications and not only, require control systems for their functioning. The continuous technical and economic development of these activity fields is asking for permanent optimization of the processes not only related to their concept and structure, but also to their functioning through improved control algorithms. Within the long list of processes, a special attention is driven by the chemical and biochemical based transformations. These types of processes cannot be designed and controlled in the same manner as processes in other industries due to their large scales, nonlinearities, uncertainties, delays and stochastic effects. Extensive efforts must be made in their modelling and control, which require the use of interdisciplinary methods from chemistry and biology to control engineering, applied mathematics and information technology.

This book, based on the Habilitation thesis of the author (University of Craiova, 2018), presents the scientific and technical content structured in 3 chapters, introduction and references. The information is focused and revealed to the reader gradually for a friendly approach of the complexity and is addressed to scientists in the field, young researchers, PhD and Master students.

Opening with Introduction, the book continues with Chapter 2 that describes the current status of the field of interest along with the evolution until now and future trends emphasizing the importance of modelling, control and simulation of chemical reactions based processes together with the difficulties and limitations of current approaches.

Chapter 3 presents the main achievements in the area of modelling and simulation of chemical reactions based processes. The first four subchapters address the modelling and simulation of different types of biosystems, and the last three subchapters are dedicated to the modelling and simulation of thermochemical processes. Subchapter 3.1 approaches the analysis of nonlinear dynamical models of microbial growth processes. Equilibrium points, stability analysis, and structural properties are studied for different biosystems with various kinetics structures. In subchapter 3.2, a novel approach for wastewater treatment bioprocesses modelling, based on pseudo bond graphs is analysed. First, the pseudo bond graph method is applied in order to model some prototype bioprocesses starting from the reactions schemes and taking into account the biochemical phenomena. Then the rules used for the design of these models are applied on two widespread wastewater treatment processes. Several simulations are conducted using 20sim modelling and simulation environment. Subchapter 3.3 presents the modelling and simulation of a baker's yeast process taking place inside a fed-batch bioreactor. The modelling procedure is based on the pseudo bond graph approach, and the simulation is performed, as in previous subchapter, by using 20sim. Subchapter 3.4 presents several results regarding the bond graph modelling applied to cells growing process in pharmaceutical industry. The conducted research is focused on monoclonal antibodies, proteins that are usually produced from mammalian cell cultures and used in biochemistry, biology and medicine. In subchapter 3.5, the fundaments of the bond graph modelling applied to thermochemical processes are presented. The work focused on combustion process kinetics with respect to reactant and reactor input data. The basic reaction between solid carbon and oxygen was considered to model the combustion solid fuel. Subchapter 3.6 addresses a biomass combustion process modelling by using the bond graph methodology. This work considers the oxidation process with heat generation using solid fuels, focused on wood biomass combustion. Results on the combustion process kinetics, especially for the transitory regimes like ignition are here presented. In subchapter 3.7, the research reported in subchapter 3.6 is extended in order to model fast developing processes, such as oxidation reactions applied to

biomass products, useful to quantify the evolution of reactants and reaction products, throughout the entire process. The developed model enables the real time observation of the process, starting with initiation, run and burnout, providing useful information for transitory regimes when the experimental measurements and continuous observation are very difficult, due to sampling and analysing equipment limitation. The pseudo bond graph modelling tool integrates advanced chemical dynamics information (reaction kinetics, formation enthalpy, mass and energy balance) delivering results for fast reacting chemical systems.

Chapter 4 presents the research on estimation and control of chemical reactions based processes. Subchapter 4.1 addresses the on-line estimation of kinetics for a biomethanation process. Two nonlinear estimation strategies are developed for the identification of unknown kinetics of the process. First, an estimator is developed by using a state observer based technique. Second, an observer based on high-gain approach is designed and implemented. The subchapter 4.2 approaches modelling and control techniques for the enzymatic synthesis of ampicillin that is carried out inside a fed-batch reactor. A nonlinear dynamical model of the bioprocess obtained by using the bond graph methodology is used in the design of estimation and control algorithms. First, a high-gain observer is designed for the estimation of the imprecisely known kinetics of the synthesis process. Second, by combining an exact linearizing control law with the on-line estimation kinetics algorithm, a nonlinear adaptive control law is designed. Subchapter 4.3 addresses the design of robust-adaptive control strategies for a lactic fermentation process carried out inside a continuous stirred tank reactor. Under the realistic assumption that the reaction kinetics and the influent flow rates are unknown and time-varying, but lower and upper bounds of the uncertainties are known, two innovative robust-adaptive control structures are proposed. The control structures are designed by combining a linearizing control law with two novel parameter estimators able to estimate the unknown reaction rates. The first structure uses a modified observer based estimator and the second one utilizes an interval parameter estimator. The control objective is to adjust the plant load so as to convert the glucose into lactic acid via fermentation, which is directly correlated to the economic aspects of lactic acid production. By using the proposed control structures the process is maintained at certain operating points. The simulations performed by considering uncertainties and noisy measurement data show that the proposed novel robust-adaptive controllers are suitable to control this kind of fermentation processes.

2. Current issues and challenging problems

Biotechnology is considered to be one of the major sources of advanced business opportunities and creation of jobs in this century. The research and development in all areas of chemical and biochemical systems are subject to fast changes in terms of novelty. These complex systems require careful modelling, design, operation and control to be run in safe and optimal conditions. The importance of chemical reactions based systems modelling, control and simulation is emphasized in the goals of leading professional societies such as IFAC – TC8.4 (International Federation of Automatic Control, Technical Committee 8.4 – Biosystems and Bioprocesses), http://tc.ifac-control.org/8/4/scope; IEEE CSS, TC-SB (IEEE Control Systems Society, TC on Systems Biology), http://systems-biology.ieeecss.org/; IEEE Engineering in Medicine & Biology Society – TC on Computational Biology & Physiome, http://tc-comp-bio-physiome.embs.org/; IEEE Power & Energy Society, http://www.ieee-pes.org/; IFAC – TC6.1 (Technical Committee 6.1 – Chemical Process Control), https://tc.ifac-control.org/6/1;

Understanding, analysis, and control of chemical and biochemical systems are challenging problems due to their large scales, nonlinearities, uncertainties, delays and stochastic effects. From the engineering point of view, the biosystems cannot be designed and controlled in the same manner as processes in other industries. Thus, extensive efforts must be made in modelling and control, which require the use of interdisciplinary methods (from chemistry and biology, control engineering, applied mathematics and information technology). Several approaches from control theory, optimization, and graph theory have been applied to analyse and control a variety of chemical systems (thermochemical processes, biological systems and bioprocesses): from fermentation processes to mammalian cell technology, from pharmaceutical processes to food engineering, from combustion processes to wastewater treatment. The high specificity of these systems needs innovative and advanced modelling, simulation and control techniques to keep up-to-date with the current analytical development.

The modelling and control of chemical and biochemical systems are difficult to implement in comparison with other fields [Bas90], [Sel14], [Gaw16]. The difficulties come especially from the presence of living organisms, the high complexity of the interactions between microorganisms, and also the complexity of metabolic reactions. As a consequence, the resulting models are difficult to handle for monitoring and control.

Generically speaking, the chemical and biochemical dynamical models are either complex or simple. The complex models seem to be exhaustive, but problems such as over-parametrization, structural identifiability, and lack of reliable data for identification may arise (especially when they are used in conditions different than those for which they were designed). In contrast, the simple models are easy to use for control design. Still, due to the simplification, the model may be apparently non stationary. Then, the model parameters that should be constant (yield coefficients, kinetic constants) need to be changing with time to give a suitable prediction of the model dynamics. Another problem is that for monitoring and control applications, only few measurements are available, because the sensors do not exist or are too expensive, or because the measuring devices do not offer reliable measurements under particular conditions.

In conclusion, it can be considered that the main difficulties of the modelling and control of biochemical systems arise from two principal sources [Doc08], [Sel12], [Kon16]: the process complexity (nonlinearity, uncertainties, delays, interconnections) and the frequent lack of reliable measurements of the process biological variables (intra- & inter-cellular concentrations, biomass/substrate concentrations, etc.). The classical modelling and control methods are not able to surmount these difficulties [Doc08], [Gaw16], [Yua16]. Thus, it is necessary to develop innovative modelling and simulation procedures and to design advanced control methods, with application to bioindustry and medicine.

Biochemical systems modelling needs an interdisciplinary effort to understand the interconnections between structures, always accompanied by transfer, propagation or growth. For instance, the growth phenomena are composite processes involving genetic, biochemical, and physical components at different scales and with complex interactions [Mon08]. The recent research trends are focused on the equilibrium, competition and growth modelling, as well as animal cell culture process modelling [Rom13c], [Vaz14], [Sel15], [Gaw16], etc. A research niche is the analysis of time delays in biosystems. Phenomena such as propagation and transport processes are characterized by delays (often time-varying). Even if in delay systems the studies are quite numerous [Gie10], there is a relatively small number of applications concerning the bioprocesses as nonlinear delay systems [Yua16]. Essential for building a model is determining its aim and the goal is to develop models useful for control.

Concerning the modelling methodologies, the methods based on mass/energy conservation balances (classical [Bas90] or bond graph approaches [Rom12a], [Rom16a]), but also the black-box models and Neural Networks are suitable for control design purposes.

H.M. Paynter, founder of bond graph method (1961) [Pay61], stated (preface of International Conference of Bond Graph Modeling - ICBGM 1993): "I remain convinced that bond graph models will play an increasingly important role in the upcoming century, applied to chemistry, electrochemistry and biochemistry, fields whose practical consequences will have an impact similar to that of electronics in this century". The bond graph method initiator proposed to keep contact with the physical world, consequently the Paynter graphs highlighting both the energy flows between different sub-systems and energy conversion, flows transferred through inter-systemic bonds. In other words, fundamental in Bond Graph model construction is the energy conversion investigation, considered to be generated by one or several sources and transferred to all components involved in real physical system functioning [Păs01].

Prof. Paynter collaborators: D.C. Karnopp, D.L. Margolis and R.C. Rosenberg [Kar68], [Kar05] developed the initial graphical representation within a systematic methodology, later characterised by a remarkable progress through formalism and applications. Method success was sustained by the large number of articles, monographs and industrial applications. Some of these works became standard references throughout decades; we refer mainly to works mentioned above and nevertheless to several contributions of J. Thoma, G. Dauphin-Tanguy, O. Păstravanu, R. Ibănescu and other researchers [Tho90], [Tho00], [Dau00], [Păs01], [Bor11], [Rom12a], [Rom16a], [Ibă17], etc.

For industry, bond graph method enables the decrease of design and commissioning time for technological solutions grace to integrated approach (from the technical requirements to concept models, simulation, control laws synthesis and prototypes' tests), and models libraries development for electric, mechanic, hydraulic, thermal systems etc. [Dau00], [Kar05]. An additional argument that states the method importance within the academic and industrial area is given by the implementation of bond graph in dedicated software (20sim, Bondsim etc.) as well as toolboxes in common software (Matlab/Simulink – Kalibond, etc.).

With respect to bond graph applications it has been noticed a progressive increase of modelled physical systems complexity as well as undertake of domains previously considered inappropriate for bond graph approach. Thus, using bond graph modelling (well established for electronic, electro-technical, mechanical, hydraulic and pneumatic systems), methodologies for multiple mechanical systems have been developed [Dau00], [Dam03], [Ers09], [Ibă17]. The initial domain – electro-mechanic and hydraulic systems modelling – is still well represented with a lot of applications in automotive industry, mechatronics, electrohydraulics, etc. [Dam03], [Muk07], [Rom07].

Although bond graph method applicability to chemical and thermochemical processes field wasn't foreseen by the method promoters, yet it has developed in the context of enlargement of

the modelling techniques from “electromechanics” to molecular processes. These processes’ modelling is based on the so-called pseudo bond graph method, in which their description is no longer based on the power variables, or not exclusively [Dau00], [Hen00], [Rom09a,b,c], [Rom12a,b], [Rom16a], but on pseudo-bonds for which the product of corresponding variables has not the signification of power; in thermal domain the entropy flow is replaced by the heat flow, and in chemical domain the chemical potential is replaced by the concentration. Thus, a lot of chemical, thermochemical, thermofluids technological processes were modelled based on pseudo bond graphs [Tho00], [Cou06], [Bal09], [Rom09c], [Rom16a], etc.

The analysis of several published studies revealed that despite current applications of bond graph modelling in the field of chemical and thermochemical processes, there are unsolved problems such as multicomponent chemical reactions, especially the need for a systemic modelling methodology for reactions networks with direct application in thermodynamics, chemistry, biology and biotechnology. For the highly exothermic thermochemical processes, combustion like, the modelling of chemical kinetics at constant temperature – relatively simple and already solved, can be extended for variable temperature within Arrhenius constant, that may be solved by quantifying the heat of reaction and applying interconnected pseudo sub-graphs.

Due to large application domain and complexity, the biological systems and biotechnological processes modelling represents an important challenge for the bond graph approach. The complexity of living world specific structure delayed the extension of bond graph methodology to these processes, although there are some results for biology models. Despite the bond graph progress (incipient research on biological systems in ‘80, recent research on biomolecular systems [Gaw16], pseudo bond graph fermentation models), there exist method limitations for propagation and time-delay biosystems.

Usually, the industrial chemical and biochemical systems operation relies on empirical knowledge, and the improvements are achieved using trial-and-error experiments (time-consuming and costly) [Sel15], [Kon16]. To surmount these limitations, it is of interest to design model-based applications and to achieve accurate dynamical models. Often, the difficulty that arises is related to the computational problems, mainly for distributed, large and stiff systems; the numerical methods used in these cases are of great importance.

An essential problem in dynamic modelling is the so-called parameter estimation. In order to obtain a dynamical model useful for process development, the non-measurable parameters of a chemical or biochemical must to be estimated. Typically, optimization-based techniques are used for the estimation of parameters: quadratic programming techniques, genetic algorithms, orthogonal collocation, particle swarm optimization – PSO (which have been applied mostly on chemical processes or in gene regulatory networks modelling), etc. [Sel15], [Yua16]. A limitation related to the most optimization-based estimation approaches is the considerable computational effort [Yua16].

The design of on-line estimation algorithms for state, parameters and kinetics of biochemical processes is an open research field; it is important because these estimators ensure the implementation of control algorithms when the specific instrumentation is missing. In the present book, the estimation of unknown parameters is mainly addressed. Presently, the research trend is to develop hybrid estimators for state and parameters (e.g. using linear-regressive or high-gain estimators) [Sel12], [Sel14]. Also, for those bioprocesses where the complete knowledge of inputs is not available, a special class of interval observers has been developed (see for example [Alc03], [Moi09], [Pet13], [Pet15], [Pet18]).

The research trends in biosystems control are focused on adaptive, robust, predictive, optimal, and hybrid control [Ren08], [Teb10], [Sel11a], [Rom12c], [Pet18]. The practical implementation of a nonlinear control law is a difficult task when the model is imprecisely known

(model uncertainties); therefore, the simultaneous use of a parameter adaptation law is required. As a result, the control system becomes an adaptive system, which requires reduced a priori information, and it has the capability to modify its structure and/or parameters during operating time, using the current information provided by the process [Åst95]. The present applications of adaptive control can be found in bioindustry [Doc08] and wastewater treatment [Doc01], [Mai04], [Pet10a]. From a theoretical point of view, the current trends consist in applying hybrid control techniques: adaptive-robust, adaptive sliding mode, adaptive-fuzzy, adaptive-neural control, etc. [Dum01], [Teb10], [Sel11a], [Pet13], [Pre15], [Pet18]. Recently, model predictive control (MPC) approaches have been used for biochemical systems, due to the advantages in constraints handling and time-domain formulation [Ola15]. The Nonlinear MPC of biosystems is a powerful control technique with open issues for research (stability and computational issues, distributed parameter and time-delay biosystems, etc.) [Teb10], [Lom12], [Ola15].

Simulation is compulsory in biosystems modelling for a better understanding of their functioning. To simulate biosystems, computational methods are often applied [Mac09]. The aim is to find how biological functions emerge from the behaviour of building blocks, including spatial and temporal organization. Typically, a multiscale method is used to integrate modelling with experiments. Still, the modelling and simulation approached in the present book are focused on developing useful issues for control design. Thus, dedicated software tools will be used: 20sim, Matlab/Simulink, etc. [Rom13b]. Even if the simulation tools are well developed, there are limitations regarding the integration with control design. Specific problems may occur when complex biosystems are simulated (large and stiff systems). The modularity of some modelling formalism (such as bond graph) should be better exploited in simulation.

The current research stage in the field, briefly presented above, and also the existence of a series of open problems (especially for thermochemical and biotechnological processes) represent a strong motivation in finding solutions that lead to results that can be implemented in modelling and design procedures, with direct applicability in chemistry, thermal power engineering, bio-industry and environmental pollution control. The present book is focused on this field, considering the research results published in the last ten years. The next chapters are based mainly on the following list of papers: [Pet18], [Rom10d], [Rom10e], [Rom11b], [Rom11c], [Rom12a], [Rom12c], [Rom13c], [Rom16a], [Rom16b], [Sel10b].