

BOOK OF ABSTRACTS

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transport properties; *iii*) the precise estimation of kinetic parameters. A simulation model is developed in gPROMS where the micropacked bed reactor is modelled as dynamic plug flow reactor (PFR). The rate laws are formulated based on Eley-Rideal mechanism in which O₂ reacts with HMF adsorbed on the catalyst surface. The framework aims at eliminating unnecessary experimentation and modelling effort as it enables the optimal design of experiments for model discrimination and parameter estimation for the development of a predictive model of the HMF oxidation process.

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APPLICATION OF PARTIAL LEAST SQUARES REGRESSION FOR UNDERSTANDING AND PREDICTION OF FOULING IN THE TRANSFER LINE HEAT EXCHANGER OF A STEAM CRACKER

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Advanced data analysis is crucial to identify hidden information in complex data. Multivariate techniques, such as Partial Least Squares Regression (PLSR), are the preferred data analysis techniques for dimensionality reduction and compression of data structure [1]. The mathematical concepts of PLSR method is able to handle highly correlated (collinear) and noisy data even when the number of measurements highly exceed the number of samples, thereby enabling quantitative multivariate linear modelling. To illustrate the capabilities and limitations, PLSR has been applied for evaluation and prediction of fouling tendencies of gas condensates during steam cracking. The latter is governed by their chemical composition, however, establishing the relation between molecular composition and observed fouling is a challenging task due to the vast amount of compounds in these mixtures. Gas condensates are characterized using two-dimensional comprehensive gas chromatography (GC×GC) indoorsing the high separation power of the technique. Furthermore, pixel based analysis of GC×GC

data enabled a direct unbiased approach for chemical evaluation without loss of information. The large amount of data prevents easy interpretation of variations between the samples and correlating the composition with the experimental observation, i.e. fouling in the steam cracker transfer line heat exchange (TLE). The initial PLRS model is build using complete characterization matrix for seven gas condensate samples and consequently seven pilot scale steam cracking fouling measurements. However, evaluation of root mean square error of cross-validation showed that the model did not give promising predictions. The model focused on describing fouling through correlations with the most abundantly present paraffinic molecules that are not recognized as fouling precursors. By scaling the chromatography data by inverse within-sample standard deviation, the regions with a large amount of random variation have a reduced influence whilst the impact of regions with chemical differences between samples is increased. Next, the regression vector was used as a variable selection method on a logarithmical transformed chromatography and fouling data, providing a prediction model with 20% of error on average. Variable selection indicated that elution regions of aromatic compounds, monoaromatic and naphthenic compounds with a long alkyl chains bonded and paraffin compounds with high boiling point are the best TLE fouling predictors.

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TIME SCALES FOR FREE ENERGY LANDSCAPES

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The connection between rate constants and free energy landscapes is discussed in a context that brings in explicitly a time scale of interest. The free energy of activation is seen to depend crucially on this time-scale. The example of Holliday junction resolution is used to illustrate the arguments.

FINITE VOLUME APPROXIMATION OF TWO-DIMENSIONAL AGGREGATION POPULATION BALANCES ON TRIANGULAR MESH

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A finite volume scheme for approximating the solution of a two-dimensional (2D) aggregation population balance equation on a regular rectangular mesh was introduced by Singh et al. (2016). Recently, Chakraborty and Kumar (2007) proposed a framework known as 'smart discretization' which shows that the accuracy of the numerical scheme highly depends on the choice of the mesh taken into consideration. In this present work, the first application of the finite volume scheme for solving a 2D aggregation population balance equation on a regular triangular mesh is demonstrated. The triangular mesh is generated by slicing the rectangular mesh along the diagonal. To test the accuracy and efficiency of the scheme with the triangular mesh, the numerical results are compared with the sectional method namely Cell Average Technique (Singh et al., 2014) for various analytically tractable kernels. The results reveal that the finite volume scheme is computationally less expensive and predicts the number density function along with the different order moments more accurately than the cell average technique. Furthermore, the numerical comparison is extended by comparing the finite volume scheme with the rectangular mesh. It also reveals that the finite volume scheme using the regular triangular mesh computes the numerical results more accurately and efficiently than the finite volume scheme using a rectangular mesh. In conclusion, the finite volume scheme with regular triangular mesh shows good consistency with the exact results for number density as well as with different order moments and is computationally less expensive.

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MODELING THE ENZYMATIC HYDROLYSIS OF PROTEINS CONSIDERING VARIABLE PRODUCT INHIBITION

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The enzymatic hydrolysis of proteins is an attractive alternative to valorising food residues because it generates functional properties [1]. The reaction has been characterized kinetically and the main mechanisms have been unveiled. The reaction system consisted in the substrate salmon muscle proteins and the enzyme subtilisin [2]. The methodology involved initial reaction rate experiments to estimate the maximum rate (V_{max}), the Michaelis-Menten constant (K_m) and the substrate inhibition constant (K_s). The product inhibition was tested adding hydrolysate at the beginning of reaction and the initial rate experiments repeated at this condition to estimate the product inhibition constants (K_i). Progress curves were carried out to test the product inhibition and its variation during reaction. The mechanisms of uncompetitive substrate inhibition, mixed product inhibition and modulation of the thermal inactivation of subtilisin were verified [2]. The estimated kinetic constants were $V_{max} = 0.581$ mM/min (for 0.6 mAU/ml), $K_m = 4.39$ mM and $K_s = 826$ mM at 40 °C and pH 8.0. Estimated values for competitive inhibition constant K_i and uncompetitive inhibition constant K_2 were 14 mM and 85 mM when a 20 % degree of hydrolysis hydrolysate was used. The product inhibition was the main cause of the dramatic decreasing on the reaction rate during the batch reactor operation due to the low-value of the inhibition constants [2]. A variation of the K_i values was inferred from this results. The variation of K_i values was modelled correlating the inhibition constant with the degree of conversion (X) [3]. A mathematical model was developed and fitted to conversion curves by using least squares method for the calculation of linear functions of both K_i versus conversion. A significant improvement on prediction were achieved with the present approach using functions for both K_i . These results confirmed the variation of both K_i values during the hydrolysis reaction. The quality of prediction with this mathematical model was improved. The model can be used to characterize, evaluate and design the enzymatic hydrolysis of proteins in batch reactor.

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POSTER PRESENTATIONS

Multiscale modeling

QUICK WAY TO COMPUTE THE AXIAL DISPERSION COEFFICIENT USING LAPLACE TRANSFORM AND MAPLE®

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The Laplace transform is applicable in many disciplines like mathematics, physics, mechanics, process control, chemical engineering and biosciences. It is a useful *tool of mathematics* in solving of many problems which are described by a system of differential equations. In many complex cases, an analytical transform to the time domain can be difficult or even impossible to obtain, so numerical methods have to be used. According to literature reports, there are many methods for numerical inversion of the Laplace transform. According to literature reports, and authors own experience, different algorithms can be recommended for solution of a specific type of problem, e.g. dispersion problem [1, 2].

In this paper, we presented the application of the Laplace transform to solve the model of gas flow describing dispersion of a gas tracer pulse in a real measurement system. We used the Gaver-Stehfest algorithm of inverse Laplace transform to obtain the solution in the time domain. Axial dispersion coefficients D_L were estimated by comparing model solution with recorded TCD signal (inverse method). The values of parameter D_L was determined using an optimization procedure of the program Maple® (*NLPSolve*).

The results show that the Laplace transform is very effective tool for solving the inverse boundary value problems associated with the diffusion equation. The axial dispersion coefficients can be easily determined. The values of axial dispersion coefficients indicate that under operational conditions, neither plug-flow nor perfect mixing can be assumed.

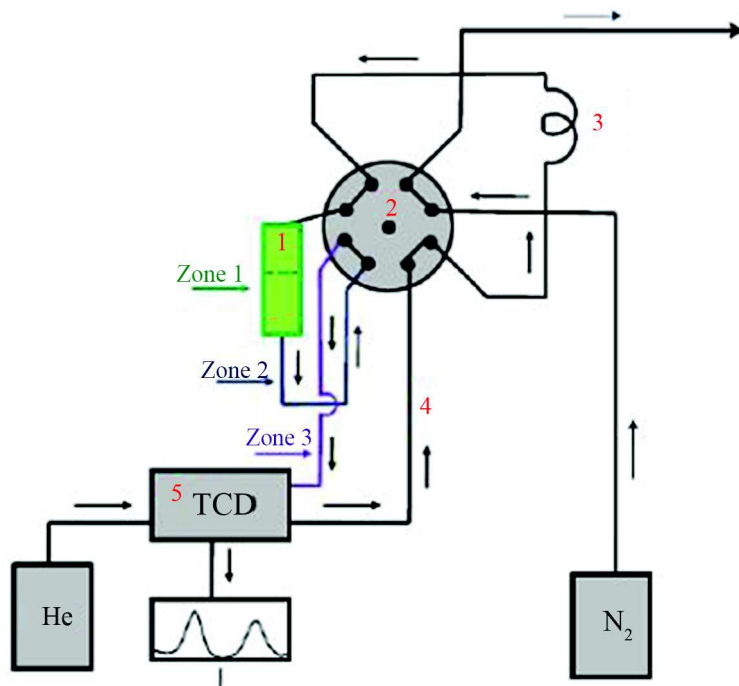


Fig. 1. The simplified schematic representation of apparatus (Micromeritics' AutoChem 2950HP): 1 – a unit called vessel, which consisting of two steel pipes, 2 – the 8-way valve, 3 – the sample loop, 4 – pipes, 5 – the thermal conductivity detector (TCD).

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Stochastic kinetics and simulation

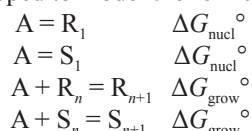
CHIRAL SYMMETRY BREAKING IN CRYSTALLIZATION EQUILIBRIUM

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Chiral symmetry breaking during the crystallization of non-chiral chemicals in forming structures belonging to enantiomorphic symmetry groups is an experimentally detected phenomenon. The best known example is the case of solid sodium chlorate. [1]

To following model was developed to model the formation of chiral crystals:



In this model, A is the non-chiral substance in solution, whereas R_n and S_n mean crystals of opposite chirality containing n units. Only two different standard free energies are used in the model: that of nucleation ($\Delta G_{\text{nuc}}^\circ$) and that of crystal growth ($\Delta G_{\text{grow}}^\circ$). It is assumed that this latter energy is independent of the size of crystal (n).

The system was fully characterized from a combinatorial point of view: the number of possible states and the state multiplicities were determined. Equilibrium calculations were carried out based on the methods of statistical thermodynamics. The expectation for the overall enantiomeric excess was calculated as a function of the two standard enthalpies in a small system where all the possible states could be handled within reasonable computation time.

Acknowledgements

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Reaction-diffusion systems

SIMULATION OF REACTION-DIFFUSION PATTERNS IN AN INITIALLY SEPARATED LANDOLT-TYPE PH OSCILLATOR*Brigitta Dúzs – István Szalai*

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Pattern formation in reaction-diffusion systems has been widely investigated owing to its theoretical and practical importance in geological and biological systems. It is known that the initial and boundary conditions determine the basic properties of the developing pattern. Now we use a general reaction-diffusion model of the well-known Landolt-type pH oscillators,¹ and simulate the effect of a special initial condition: namely when the reactants are spatially separated at the initial moment.² Our one-dimensional calculations show the time development of the reaction-diffusion patterns perpendicular to the interface.

The general mechanism of the Landolt-type pH oscillators includes a positive and a negative feedback concerning on the H⁺ autocatalytic species. This ensures the possibility of bistability and periodicity even in continuously fed homogeneous media, or in reaction-diffusion systems where the concentrations are fixed at one of the boundaries.¹ In our setup the reaction-diffusion system is divided into two parts, which are filled homogeneously with different reactants at the initial moment: the OX part contains the oxidant (the partner of H⁺ in the autocatalytic reaction) and the ACID part contains extra H⁺ (in bonded form). The initial concentrations of the other reactants are equal in both parts. There is no external reagent supply.

The initially separated reactants diffuse due to the cross-gradient of the concentrations, and the autocatalytic reaction results in a narrow acidic band in the counter-diffusion zone. In the presence of the H⁺-consumer species the width of the acidic band remains constant. Depending on the initial concentrations, the behaviour of the band changes dramatically. We present a phase diagram to show the following dynamical behaviours:

- 1) propagation of the acidic band towards the OX part or towards the ACID part;
- 2) damped oscillation (forming needles) at the beginning of the acidic band;
- 3) spatial separation of the autocatalytic region (the acidic band splits up).

We analyse qualitatively the spatial/temporal concentration profiles and the reaction rate profiles to understand how the diffusion and the autocatalytic reaction interact to form these nonlinear phenomena. We conclude that the appropriate autocatalytic kinetic is crucial for the oscillation, while the kinetic of the H⁺-consuming step has less importance.

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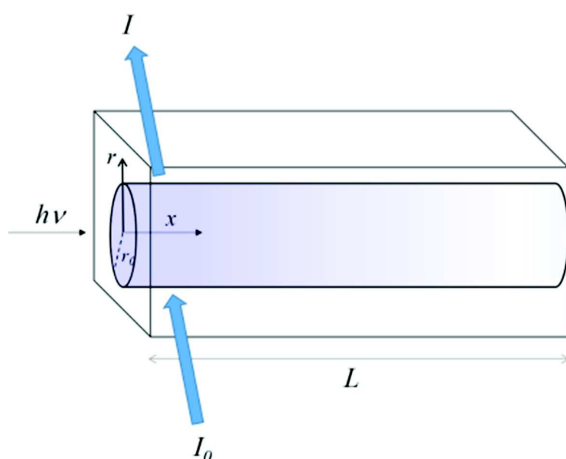
A REACTION-DIFFUSION APPROACH TO THE INHERENT INHOMOGENEITIES DURING LASER FLASH PHOTOLYSIS EXPERIMENTS

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Laser flash photolysis (LFP) is an experimental method for generating highly reactive intermediates, transient species or free radicals by a very short, high energy laser pulse. The concentrations of the transients reach a sufficient level to apply spectrophotometric detection.



This work presents a detailed mathematical study of the effect of inhomogeneities in LFP studies, which are of two different kinds: the first arises from diffusion, whereas the second one has geometric origins (the shapes of the excitation and detection light beams). Both of these are taken into account in our reported model, which uses reaction-diffusion type partial differential equations to describe the chemical process between sulfate ion radical and iodide ion using cylindrical coordinates to match the symmetry properties of the system:

$$\frac{\partial c_s}{\partial t} = D_s \left(\frac{\partial^2 c_s}{\partial x^2} + \frac{1}{r} \frac{\partial c_s}{\partial r} + \frac{\partial^2 c_s}{\partial r^2} \right) - k c_s c_1$$
$$\frac{\partial c_1}{\partial t} = D_1 \left(\frac{\partial^2 c_1}{\partial x^2} + \frac{1}{r} \frac{\partial c_1}{\partial r} + \frac{\partial^2 c_1}{\partial r^2} \right) - k c_s c_1$$

These equations were solved by a specially developed finite volume method. The results showed that diffusion is too slow to influence the kinetic curves on the usual time scales of LFP experiments. However, the use of the absorbances measured requires very detailed mathematical consideration and the full knowledge of the geometrical details. The pseudo-first order approach could be used to evaluate the kinetic traces successfully even if the large excess condition was not met in the reaction cell locally. [1]

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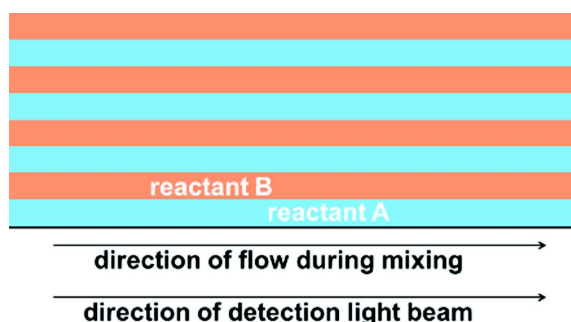
A REACTION-DIFFUSION APPROACH TO MICROMIXING DURING STOPPED-FLOW EXPERIMENTS

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The stopped-flow technique is the state-of-the-art instrumental method for measuring the kinetics of reactions for processes where mixing of two solutions is unavoidable. The performance of this method is limited by the efficiency of mixing. [1]



In this work, a stopped-flow experiment was modelled by assuming that thin layers of solutions form in the cell as a result of macromixing, but then the homogeneous state is achieved through the diffusion of reactants (micromixing). This process is described by a one-dimensional diffusion-reaction equation for two substances (A and B), which react in a mixed second order process:

$$\frac{\partial A(t,x)}{\partial t} = D_A \frac{\partial^2 A(t,x)}{\partial x^2} - kA(t,x)B(t,x)$$

$$\frac{\partial B(t,x)}{\partial t} = D_B \frac{\partial^2 B(t,x)}{\partial x^2} - kA(t,x)B(t,x)$$

$A(t,x)$ and $B(t,x)$ are the concentrations of the two reactants, D_A and D_B are the diffusion coefficients, whereas k is the second order rate constant.

This equation was solved numerically and attempts were also made to find approximate analytical solutions by Fourier transformation. It is shown that the approximate analytical solutions are in excellent agreement with the numerical calculations. The simulation results were compared with experiments done in the calibration process of the stopped flow instrument.

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DYNAMICS OF PH OSCILLATORS IN A TWO SIDE FED REACTOR

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Pattern formation in chemical reaction–diffusion systems with positive and negative feedback serve as a prototype of non-equilibrium self-organization. Hydrogen ion autoactivated systems with appropriate negative feedback, pH oscillators, are preferably used to study reaction-diffusion phenomena.¹ These systems are capable to show a wide range of spatiotem-

poral phenomena from spatial bistability and oscillations to the formation of stationary patterns. The experiments are typically performed in open spatial reactors, which allow to feed all space points of a porous material (e.g a hydrogel) in order to maintain the system far from equilibrium, without introducing macroscopic fluid motion. The feed can only be made by diffusive exchanges of matter with the environment at the boundaries of the system. The spatiotemporal dynamics of pH oscillators have been mostly explored in one-side-fed-reactors, where all reagents are fed through a unique continuous-flow stirred tank reactor (CSTR) and the feed composition at the CSTR/gel boundary relies on the chemical state of the CSTR. Here, apply a two side fed reactor (TSFR) geometry, where complementary sets of chemicals are provided at opposite faces of the gel. This configuration induces cross composition ramps of the chemicals between the feed boundaries. This asymmetric feeding mode avoids the development of the temporal instabilities in the feed tanks and allows us to study pattern formation in presence of cross gradients. It is widely accepted, that the graded distributions of morphogens play important roles in biological pattern generation.² By using numerical simulations with a general model of the pH oscillators we observed spatial bistability and oscillations in a presence of counter gradients of the chemicals. The nonequilibrium phase diagram of the system shows a typical cross shaped topology. Two types of spatiotemporal oscillations have been found, one with large and the other with small amplitude. The interaction of them leads to the formation of mixed mode oscillations. We discuss the role of gradients of the chemicals in the development of the observed phenomena.

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Chemical reaction networks and chemical reactor network theory

ANALYSIS OF BIOCHEMICAL ADAPTATION

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We study two specific measures of quality of chemical reaction networks, Precision and Sensitivity. The two measures arise in the study of sensory adaptation, in which the reaction network is viewed as an input-output system. Given a step change in input, Sensitivity is a measure of the magnitude of the response, while Precision is a measure of the degree to which the system returns to its original output for large time. High values of both are necessary for high-quality adaptation. We focus on reaction networks without dissipation, which we interpret as detailed-balance, mass-action networks. We give various upper and lower bounds on the optimal values of Sensitivity and Precision, characterized in terms of the stoichiometry, by using a combination of ideas from matroid theory and differential-equation theory. Among other results, we show that this class of nondissipative systems contains networks with arbitrarily high values of both Sensitivity and Precision. This good performance does come at a cost, however; since certain ratios of concentrations need to be large, the network has to contain many species and reactions, or the network should show strongly different time scales.

UNCERTAINTY QUANTIFICATION FOR QUANTUM-CHEMICAL MODELS OF COMPLEX REACTION NETWORKS

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For the quantitative understanding of complex chemical reaction mechanisms, it is, in principle, necessary to accurately determine free energies for all elementary processes, and to solve the corresponding continuous-time reaction-rate equations, which are generally highly coupled and spread over several time scales. It is computationally hard to fulfill these two requirements. However, it is possible to approximately address these challenges in a physically consistent way. On the one hand, it may be sufficient to consider approximate free energies if a reliable uncertainty measure can be provided. On the other hand, a (quasi-)continuous-time evolution may not be necessary to still determine quantitative fluxes in a reaction network if one is interested in specific time scales.

Here [1], we present discrete-time kinetic simulations for a coarse-grained state space taking free-energy uncertainties [2] into account. The method builds upon thermo-chemical data obtained from electronic-structure calculations in a condensed-phase model. Our ap-

proach supports the analysis of complex chemical reaction networks [3] spanning multiple time scales, which is here demonstrated at the example of the formose reaction. An important application of our approach is the detection of regions in a reaction network which require further investigation, given the uncertainties introduced by both approximate electronic structure methods and kinetic models. Such cases can then be studied in greater detail on the basis of more sophisticated first-principles calculations and reaction-rate theories.

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INTERMEDIATES, ENZYMES, BINOMIALITY AND MULTISTATIONARITY

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In this poster we consider reaction networks with intermediates (as described in [1]), with enzymes (as described in [2]) and networks with toric steady states (as considered in [3]). Specifically, given a core reaction network and an extension of it obtained by adding intermediates or enzymes, we study how the Gröbner bases of the steady state ideal of the core reaction network relate to the Gröbner bases of the steady state ideal of extended networks. We use this to (1) find Gröbner bases of large networks from Gröbner bases of simplified versions of them, thereby reducing substantially the computational cost; (2) infer when extensions of networks with toric steady states also have toric steady states; (3) pinpoint what/whether intermediates can be target as responsible for multistationarity.

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STRONG REACHABILITY OF CHEMICAL REACTIONS

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Controlling chemical reactions is important both for chemical engineering, pharmacology and in some other parts of chemistry, as well. Studying strong reachability is necessary to decide if we can have any effect on the states (described by the vector of concentrations) of the system. As a first step we have chosen temperature and the inflow rates of some species as control input. The analysis is based on the Lie-algebra generated by the vector fields related to the induced kinetic differential equation of the reaction.

First we give conditions for strong reachability with temperature input. It turned out that the chemical reactions are strongly reachable on a subspace that has the same dimension as the number of independent reaction steps in every point except where the concentration of reactant species is zero. Next we analysed the continuously stirred tank reactors. We have shown that the same result holds for these cases, as well. Finally, we analyse a simple model of polymer electrolyte membrane fuel cells, using the inflow rates as control.

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TIME-PROGRAMMED SELF-ASSEMBLY

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We present a general concept to drive the self-assembly of various building blocks from molecular level to nanoscopic level by combining a pH clock reaction and lactone hydrolysis in a closed system. The time scale separation of these two processes (fast pH jump provided by the clock reaction and a delayed decrease of pH by lactone hydrolysis) ensures the existence of a transient alkaline state. This chemical system can be used to control and drive autonomously the self-assembly of pH switchable self-assembling components: fatty acid molecules, carboxyl group terminated gold nanoparticles and amine functioned polymer chains in a network. We demonstrated that the proper control over the electrostatic interaction between the building blocks can govern and induce reversible transformation of vesicle-to-micelle, dispersion/aggregation of nanoparticles and contraction/reswelling of gel filaments.

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KINETICS OF THE REACTION BETWEEN 2,5-DICHLORO-1,4-BENZOQUINONE AND SULFITE ION

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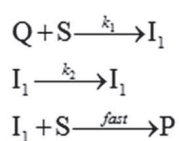
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The reaction between variously substituted quinones and sulfite ion in water is a special type of the quinone-bisulfite addition reactions.[1] The kinetics of the reaction was investigated under slightly acidic conditions (pH 3.8 and 4.5 in acetate buffer). Both the rate and

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the stoichiometry of the reaction depend on the substituents of the quinone derivative. This process clearly involves intermediates[2], the existence of which can be proved by UV-vis spectroscopy.

The observed absorbance-time traces showed a very fast (stopped-flow time scale) absorbance increase and decrease in a wide wavelength region (380-500 nm) for 2,5-dichloro-1,4-benzoquinone (Q). The kinetic traces can be fitted well to a double exponential function in a wide concentration range: $c(2,5\text{-dichloro-1,4-benzoquinone}) = 0.5 \text{ mM}$, $c(\text{SO}_3^{2-}) = 0.02\text{-}50 \text{ mM}$. The kinetic traces measured at 420 and 320 nm were simultaneously fitted to the following mechanism using the multipurpose program package ZiTa:[3]



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QUANTITATIVE KINETIC DESCRIPTION OF THE REDOX (PHOTO)REACTION BETWEEN CERIUM(IV) AND WATER

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The acidic aqueous solutions of Ce(IV) salts give Ce(III) and dioxygen gas when illuminated by polychromatic light, even if it comes from the detection beam of a diode array spectrophotometer (total photon flux of $1.7 \times 10^{15} \text{ s}^{-1}$). [1] This reaction is part of the photocatalytic

water splitting cycle which gives O₂ and H₂ gas when an acidic aqueous Ce(III) solution is illuminated by UV light.[2]

The rate of the photoreaction and also the spectrum of the reactant and product Ce complexes depend on the chemical identity of the strong acid. A detailed mathematical evaluation was developed to interpret the experimental findings in perchloric acid of different concentrations, based on the general quantitative description of photoreactions assuming a single initial excitation process, which leads to the following differential equation:

$$\frac{d\xi}{dt} = \frac{\Phi}{Vc_0} \int \left(1 - 10^{-(1-\xi)\beta A_\lambda^{ini} - \xi\beta A_\lambda^{fin}} \right) \frac{q_{P,\lambda} (1-\xi) A_\lambda^{ini}}{(1-\xi) A_\lambda^{ini} + \xi A_\lambda^{fin}} d\lambda$$

$$A_{det} = (1 - \xi) A_{det}^{ini} + \xi A_{det}^{fin}$$

In this formula, ξ is the extent of reaction (*i.e.* the reaction coordinate), Φ is the differential quantum yield, $q_{P,\lambda}$ is the spectral photon flux at wavelength λ , c_0 is the sum of the initial concentrations of cerium(III) and cerium(IV), V is the volume, A_λ is the *initial* and *final* absorbance at wavelength λ , A_{det} is the absorbance at the wavelength of detection and β is the ratio of the path length of illumination and detection.

The rate of the reaction in the absence of light is also investigated using not only diode array but also scanning double beam spectrophotometer (total photon flux < 1% compared to a diode array spectrophotometer).

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EXPERIMENTAL AND MODELLING STUDY OF SYNTHESIS GAS PRODUCTION FROM CATALYTIC STEAM REFORMING OF METHANE

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In the latest years, the environmental problems derived from useful energy generation sources and from the increment of fossil fuels prices, have enhanced the development of new technologies for energy production. Steam reforming of methane produced by biomass gasification is one of the most employed processes to produce hydrogen and synthesis gas. Synthesis gas, constituted by different quantities of carbon monoxide and hydrogen, can also be used to produce high purity hydrogen streams and chemical products. In this research, experimental and theoretical studies of steam methane reforming reactions with different amount of hydrogen sulfide in the feed gas are presented. A two dimensional pseudo-heterogeneous model is developed to simulate methane steam reforming reactions in a packed bed tubular reactor. This model is based on mole and energy balance equations for the catalyst and the fluid phases. Attention is given to the analysis of sulfur negative effects on methane conversion when Ni-based catalysts are used. A parametric study is done and effects of different steam to carbon ratios, space velocities, temperatures on methane conversion and temperature distribution within the reactor are investigated. The results are verified comparing to the experimental results. It is shown that even presented in the gas at very low concentration levels (ppm), sulfur drastically decreases the conversion of methane. The obtained results play a key role in design and optimization of an actual reactor.

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APPLICATION OF VARIOUS MATHEMATICAL METHODS ON MODELING OF FULLEROLE DEHYDROXYLATION

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Fullerols, derivatives of fullerenes with hydroxyl group, possess number of extremely important properties, such as: antioxidant [1], antimicrobial [2] and anti-cancer [3] activity. It is well-known that physical, electronic and functional properties, as well as reactivity of a ful-

lerols are strongly dependent on number of hydroxyl group attached per surface [4]. Thus, it is important for one to develop methods by which fullerol with certain number of OH groups can be obtained. With that in mind, we investigated non-isothermal kinetics of $C_{60}(OH)_{27}$ dehydroxylation. Fullerol dehydroxylation thermogravimetric curves were recorded at different heating rates ranging from 5 K min^{-1} to 25 K min^{-1} . Dependence of energy activation on dehydroxylation degree was calculated by Vyazovkin's method [5], from which it is clear that investigated reaction has complex kinetic mechanism consisting of a few reaction steps. Reaction rate curves were further decomposed by Suzuki-Fraser method [6] and two reaction steps were distinguished. It has been concluded that in reaction step which dominates at lower temperatures 14 OH groups leave fullerol surface, whereas dehydroxylation of the rest of OH groups takes place in other step (i.e. one which dominates at higher temperatures) and that temperature program by which fractions with high content of fullerol with desired number of OH groups may be designed.

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