Extremum Seeking-Based Output Regulation Using Time-Scale Transformation for Nonlinear Systems

Maryam Azhdari

This work presents an approach that integrates Extremum Seeking Control (ESC) with timescale transformation to estimate the internal model required for output regulation in dynamical systems. The proposed method aims to track a desired trajectory despite the presence of unknown disturbances and uncertainties, particularly in nonlinear systems with unknown optimal equilibrium points. The combination of ESC with time-scale transformation enables adaptive regulation without the need for a precise system model, making it particularly suitable for complex nonlinear systems where only output measurements are available. Simulation results, conducted on a nonlinear dynamic system, validate that this strategy effectively regulates the system output and maintains the desired performance under external disturbances. The combined ESC and time-scale transformation scheme achieves steady-state regulation with minimal overshoot and improved convergence. A stability analysis confirms the robustness and theoretical soundness of the proposed model-free control technique for practical output regulation applications.

Keywords: Extremum Seeking Control; Output Regulation; Nonlinear Systems; Model-Free Control; Internal Model; Time-Scale Transformation

KKL Observer Design for Bioreactors with Unknown Kinetics and Limited Measurements

Joel Bartlett

Effective feedback control of bioprocesses requires knowledge of the full system state vector. Since full online state measurements are not available due to limited reliable sensor availability, state observers are required to reconstruct the unmeasured states. The Kazantzis-Kravaris-Luenberger (KKL) observer extends the Luenberger observer to nonlinear systems by embedding the system dynamics into a set of linear coordinates through a mapping that satisfies a partial differential equation (PDE). The state vector is recovered through the inverse mapping. However, enforcing the PDE requires knowledge of the system dynamics and full state measurements. In addition to limited measurements, the system dynamics are governed by growth kinetics that are often unknown.

In this work, we propose a two-step framework to design a KKL observer for a bioprocess with unknown kinetics and limited measurements. First, the kinetics are learned from the available measurements. Second, the PDE is reformulated in the transformed linear coordinates enabling enforcement using only output measurements. The inverse mapping is then directly approximated using a neural network. The proposed method is demonstrated on a three-state bioreactor with online biomass measurements and offline substrate samples.

Separation of isotopic water mixtures using graphene oxide membranes: the influence of membrane fabrication method and filtration mode on separation efficiency

Alireza Bagherzadeh Hosseinabad

Nuclear plants, especially those employing Canada Deuterium Uranium (CANDU) reactors, need an efficient tritiated water removal technology. The reactors utilize D2O as coolant and generate tritiated heavy water as a byproduct. The removal of tritium (existing as T2O, DTO, and/or HTO) from D2O is necessary before the latter can be reused or recycled. Existing methods, such as chemical exchange and water distillation are energy intensive, cost-inefficient and not environmentally friendly. Therefore, there is a tremendous need for new, safe, cost-effective and energy efficient methods for separating isotopic water. Recently, GO membranes have been studied for this purpose and shown to produce promising results.

To investigate the effect of GO membrane fabrication methods on the structure of the membrane and subsequent separation performance, GO membranes were prepared through vacuum and pressurized filtration (ΔP=1-4 bar). The produced membranes were examined by SEM, XRD and XPS. The results showed that pressurized filtration was a more efficient membrane fabrication process and allowed the production of thicker membranes. The membranes produced at ΔP=4 bar (maximum pressure used) had the most compact structure and slightly lower interlayer spacing than other membranes.

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To gain an understanding of how the filtration mode can influence separation performance, the GO membranes were tested for separation of isotopic water (H2O/D2O mixture) using two different filtration modes: vapor-phase and liquid-phase filtration. The results showed that GO membranes produced through pressurized filtration at ΔP=4 bar gave the highest separation efficiency (7.86%) in vapor-phase filtration experiments (T=110oC). In liquid-phase, the same GO membranes led to 4.72% separation efficiency. Despite its better performance, the vapor-phase process is highly energy-intensive. Moreover, part of the separation is due to the contribution of the VLE (vapor-liquid equilibrium) effect, which is not related to the GO membrane selectivity. On the other hand, liquid-phase filtration is a facile process that can take place at room temperature, which makes it environmentally friendly and more suitable for large-scale applications. Overall, our results provide significant insights and pave the way for the utilization of GO membranes in real world applications of hydrogen isotopic separation.

Key words: Graphene oxide, Membranes, Separation, Isotopic water

Engineered Chitosan Platforms for Canadian Freshwater Remediation: Targeting Ibuprofen and Dyes

Amir Hossein Behroozi

The efficient removal of anionic contaminants from water requires adsorbents that simultaneously provide high surface accessibility and abundant active sites. In this work, a series of chitosan-based adsorbents were rationally engineered through crosslinking, templating, and amine functionalization to elucidate structure–property–performance relationships governing adsorption. Protonated epichlorohydrin-crosslinked chitosan beads exhibited high structural stability (~98% mass retention) and achieved a maximum ibuprofen (IBP) adsorption capacity of 232 mg/g, with adsorption governed by a combination of electrostatic interactions and hydrogen bonding. To address limitations in active-site accessibility, polyethylene glycol (PEG)-templated chitosan aerogels were developed, generating interconnected mesoporous networks (surface area up to 188.8 m2/g) that enabled rapid adsorption kinetics (<45 min) and selective removal of anionic dyes (>97%), primarily driven by electrostatic ion-pairing interactions. Building on these insights, amine-functionalized chitosan aerogels with tunable surface chemistry were synthesized using ethanolamine (ETA), triethanolamine (TEA), triethylenetetramine (TETA), and polyethyleneimine (PEI) to systematically vary amine density and pore structure. Adsorption studies under unified conditions demonstrated that optimal performance arises from a balance between high amine density and preserved mesoporosity, with PEI- and ETA-modified aerogels achieving >97% dye removal, up to 76% phosphate removal, and 89% IBP uptake. This integrated study establishes design principles for tailoring chitosan-based adsorbents, highlighting the critical interplay between surface functionality and pore accessibility for selective and multifunctional water purification.

Modeling of a Fluidized Bed Gasifier

Yun Woo Choi

Syngas is an important intermediate used for electricity generation, producing hydrogen for fuel cells, and as a reductant in steel manufacturing. Almost 99% of syngas production is currently derived from fossil fuels. Natural Resources Canada (NRCan) operates a fluidized-bed gasifier (FBG) for generating syngas, using biomass as a feedstock. They are interested in the development of a mathematical model to complement their experimental work and learn how their reactor should be operated to achieve economical syngas production.

A new model has been developed to describe the operation of NRCan's FBG. This model is one-dimensional, steady-state, and assumes instantaneous biomass pyrolysis within the reactor. The resulting char and tar are gasified via 6 reactions. The reactor model considers heterogeneous and homogeneous reactions that occur in the dense bed and in the freeboard region above the fluidized bed. The dense bed is assumed to be isothermal, but temperature variation within the freeboard is considered.
Material balance differential equations within the dense bed and the freeboard are solved as a boundary value problem (BVP. The model gives reasonable predictions of the resulting syngas composition obtained in 2 experimental runs. In future, parameter estimation will be required to ensure reliable quantitative predictions from the model.

Sacrificial Anode-Free Alkyne Electrocarboxylation

Dante Flores

Carboxylic acids are high-value chemicals used extensively in the pharmaceutical, textile, and cosmetic industries. Electrocarboxylation, an electrolytically driven reaction wherein a carbon-carbon bond between CO2 and another organic molecule is formed to yield the corresponding carboxylic acid, offers a sustainable alternative to traditional carboxylation methods and an opportunity to diversify CO2 valorization. Alkynes represent an important feedstock for industrial organic processes, given their wide availability and synthetic versatility. While the electrocarboxylation of alkynes to cinnamic acids has been demonstrated in literature, the scalability of this chemistry is limited as it utilizes a sacrificial anode and suffers from low faradaic efficiency. This work aims to develop an innately scalable electrochemical process that converts terminal alkynes to carboxylic acids devoid of sacrificial anodes.

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Phenylacetylene was chosen as a model substrate for system optimization. Preliminary screening of metal foil working electrodes using constant current electrolysis showed nickel as the strongest candidate for selective electrocarboxylation to cinnamic acid. Constant current electrolysis has achieved comparable faradaic efficiencies to previously reported values in the literature, without the need for a complex transition metal catalyst or sacrificial anode. Historically, sacrificial anodes have played a critical role in electrocarboxylation reactions, as metal ion dissolution into the electrolyte stabilizes reaction intermediates and restricts parasitic anodic reactions. To address this challenge, previous work has demonstrated highly efficient electrocarboxylation without a sacrificial anode by employing inorganic salts as electrolyte additives.

The successful development of this scalable electrocarboxylation process could enable the chemical manufacturing industry to both reduce its carbon footprint and capitalize on clean technology financial incentives. This approach contributes to environmental sustainability and economic growth by using CO2 as a low-cost renewable carbon feedstock to produce ubiquitous value-added chemicals.

Inertial microfluidic platform for micro and nanoplastic detection via Surface Enhanced Raman Scattering sensor

Aldo Gonzalez Lopez

Microplastics (MPs) and nanoplastics (NPs) contamination is a growing concern due to their abundance and intrinsic negative impact on the environment. Detection of MPs and NPs is inherently challenging; however, vibrational spectroscopic methods are well-suited to enable their detection and identification in real-time. Raman spectroscopy is a nondestructive method that can chemically identify a wide variety of polymers; nevertheless, Raman is often limited by weak signal intensities and reproducibility. Surface-enhanced Raman Scattering (SERS) is a technique that boosts the Raman signals through the enhancement of the local electromagnetic field from metallic nanostructures, which can be used to overcome Raman limitations. This work presents an inertial microfluidic-sensor platform for the detection and identification of MPs and NPs through an integrated using SERS technique. Our approach enables the growth of SERS-active nanodendritic metallic structures in situ and in real-time, with the possibility of being regenerated on demand. In the context of MP pollution – a current critical worldwide challenge– the nanodendritic structures were used to successfully detect polystyrene (PS), polypropylene (PP), and polyethylene terephthalate (PET) MPs and NPs with average diameters of between 1 and 10 µm. These results confirm that the SERS-active nanodendritic structures presented in this work are effective for the detection of PS MPs and NPs, offering great potential for in-situ deployment and portable MP and NP detection applications, and are amenable for integration with readily available microfluidic platforms. The nanodendritic structures, using different microelectrode shapes, are being investigated for the detection of different types of MPs and NPs.

Enhancing Sugar Recovery from Poplar Residues Using Combined Acid–Thermal and Enzymatic Processing

Nimaat Salami

The sustainable production of biofuels depends on efficient recovery of fermentable sugars from renewable feedstocks. Lignocellulosic biomass is abundant and often considered waste, making it an attractive resource. Poplar hardwood residues are generated in large quantities in Canada, and rich in cellulose and hemicellulose. However, these polysaccharides are embedded in a rigid lignin–carbohydrate matrix which limits their accessibility. To overcome this, a two-stage approach is used: acid–thermal pretreatment to disrupt biomass structure and release hemicellulose, followed by enzymatic hydrolysis to convert the remaining cellulose into fermentable sugars.

Acid pretreatment experiments were structured using a Box–Behnken design to evaluate the effects of acid concentration (0.3–1.5 wt/v%), temperature (150–190 °C), and reaction time (30–90 min) at a fixed solid–liquid ratio of 10 wt/v%. Hydrolysates were analyzed for carbohydrates, chemical oxygen demand (COD), and volatile fatty acids (VFAs) to assess sugar release, solubilization, and byproduct formation. Temperature was identified as the dominant factor influencing carbohydrate recovery, with up to 66% recovery achieved. Comparable results under milder conditions indicate potential for reduced process severity.

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Based on these results, a representative pretreatment condition (0.3 wt%, 170 °C, 30 min) was selected for enzymatic hydrolysis. The resulting pretreated solids were subjected to enzymatic hydrolysis under varying solid loading (5–15% g/mL), enzyme dosage (10–30 FPU/g solid), and hydrolysis time (0–72 h). The hydrolysates were similarly analyzed for carbohydrates, COD, and VFAs. Preliminary results show that enzymatic treatment increases carbohydrate release by up to 30%, with most sugars liberated within 24–48 h.

Overall, the results highlight the effectiveness of acid–thermal pretreatment in enhancing carbohydrate recovery from poplar residues, while enzymatic hydrolysis further improves
the recovery. Additional experiments are underway to complete evaluation across the full range of studied conditions.

Effect of Delignification on Biogas Production from Poplar Wood Residues

Varsha Sharma

Despite the abundance of lignocellulosic biomass (LCB) worldwide, much of it remains underutilized. Specifically, in Canada, forest residues such as poplar represent an untapped resource for integrated bioenergy and bioproduct recovery. Anaerobic digestion (AD) provides a sustainable pathway for converting these residues into biomethane; however, the recalcitrant nature of LCB, particularly due to lignin, limits microbial access and biogas yields, making pretreatment essential. Among the various pretreatment strategies, alkali pretreatment is particularly attractive, as it disrupts lignin–carbohydrate complexes, enhances carbohydrate digestibility, and enables lignin solubilization, thereby improving the overall economic feasibility of biomass conversion. This study investigated microwave-assisted and room-temperature alkali pretreatments of poplar residues for biomethane production through anaerobic co-digestion of solid residues and wastewater sludge. Poplar residues were ground and sieved (mesh #10) and pretreated at a solid-to-liquid ratio of 1:10 under microwave-assisted heating using 1–3% (w/v) NaOH at 110–150 °C for 30–180 min, and room-temperature using 1–5%(w/v) NaOH at 22 ± 2 °C for 24 h. After pretreatment, solid and liquid fractions were separated; the liquid fraction was analyzed for soluble chemical oxygen demand (measures the organic matter), carbohydrates, volatile fatty acids (VFAs), and solubilised lignin. The solid fraction was used in a batch anaerobic co-digestion.

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Among the evaluated conditions, the highest cumulative methane yield of 270 mL CH_4/g VS was achieved under two conditions: 110°C for 30 min with 2% NaOH, and 150°C for 90 min with 2% NaOH, corresponding to synergistic enhancements of 83.5% and 85.7% respectively, compared to only 36.7% for untreated poplar co-digested with sludge. Notably, the pretreatment at 150 °C resulted in a substantially higher lignin removal of 61%, whereas the 110 °C condition achieved 37% lignin removal. Despite this difference, both conditions produced identical methane yields, indicating that beyond a certain threshold of delignification, further structural disruption does not lead to proportional improvements in anaerobic digestion performance.

Overall, these results demonstrate that while increased pretreatment severity enhances lignin removal and biomass solubilization, moderate-severity alkali pretreatment provides a more favorable balance between delignification and preservation of readily digestible substrates, enabling enhanced biomethane production as a valuable product.

Achieving Well-Defined Methacrylate Polymers via Low-Copper Semi-Batch Reversible Deactivation Radical Polymerization

Baris Topcuoglu

Cu-mediated reversible deactivation radical polymerization (RDRP) is a controlled radical polymerization technique that uses transition metal catalysts to synthesize polymers with well defined structures. Previous studies utilized a two-step RDRP process where methacrylate macroinitiators were first synthesized in a copper tubular reactor and then chain-extended with acrylates in a semi-batch reactor. While prior research has shown success with chain extending with acrylates, methacrylates demonstrated slower reaction rates and diminished initiation efficiency. The process was simplified by having the dissolved catalyst and initiator in a solution in the reaction flask, while the monomer and reducing agent were fed into the system via a syringe pump. Therefore, it is of a particular interest to polymerize 2-(dimethylamino)ethyl methacrylate (DMAEMA) and methyl acrylate (MA) copolymers via the simplified RDRP process, as these were previously produced using conventional radical polymerization. In addition to the DMAEMA-MA system, this simplified approach was extended to the polymerization of glycidyl methacrylate (GMA), with the goal of producing well-defined polymers.

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In this work, both GMA homopolymers and DMAEMA-MA copolymers were synthesized while investigating the influence of different parameters such as ligand loading, copper level, reducing agent loading, and temperature. Current findings demonstrate that well-defined DMAEMA-MA copolymers were achieved with a twofold reduction in copper loading compared to initial conditions, ultimately resulting in a final loading of ~ 20 ppm. In addition, the knowledge and experience gathered from the DMAEMA-MA copolymer system were utilized to synthesize well-defined GMA homopolymers. The GMA homopolymer system achieved > 90% conversion with dispersity approximately 1.3 within 2 hours, paving the way for future copolymerization applications with various acrylates and methacrylates.

Optimizing facility siting, technology selection, and feedstock allocation for plastics recycling using life cycle assessment integrated with mixed-integer linear programming

Abdul Yaeesh Yaish

In this talk, we present an optimal technology siting tool utilizing mixed-integer linear programming for plastics recycling in Canada. The tool selects between 19 process configurations with 7 unique recycling technology families across 7 polymers. Polymer bale sourcing from 34 regions in Ontario is considered, along with transport distances to each of the 7 candidate industrial parks. The objective is to minimize a weighted life cycle assessment environmental burden score by selecting technology-siting combinations that satisfy the annual product/service requirements. Initial results indicate that the optimal configurations combine mechanical recycling facilities with incumbent virgin processes to meet the product/service demands. Different scenario analyses, including policy- and market driven constraints, were conducted. For example, when further constraining the system to include nonmechanical technologies, the optimal solution included the newly innovated polyethylene terephthalate enzymatic recycling process1 . Future work will include expanding the current scenario analysis set to include a wider range of realistic scenarios useful for stakeholders. Additionally, expansion of the tool into a multi-objective optimization problem by introducing life cycle costing parameters is a future goal for development. This will add an extra dimension to the tool’s capabilities by enabling quantification of the trade-offs between environmental and economic sustainability.

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Keywords: Plastics recycling, mixed-integer linear programming, life cycle assessment, optimization, process design, process simulation

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