Postgraduate Symposium

Hosted by the Department of Chemical Engineering
at Stellenbosch University

Welcome to the Postgraduate Symposium!

Prof Robbie Pott

Postgraduate Coordinator

To live the life of the mind is a privilege - and the corollary to this privilege is the duty to share what you've learned.

Every year I am always so enthused by the postgraduate symposium. This is a wonderful annual event, showcasing the really excellent work which our postgraduate candidates, postdocs, academics, and researchers have engaged with. The department is a hub for inventive, innovative, insightful, and intriguing research, and here is an opportunity to hear much of it laid out in detail by our enthusiastic postgraduates.

Through presentation, discussion, debate, and collaboration the work we do as researchers is improved and made more impactful and useful to society. Making a space for these interactions is important and can be extremely fruitful. I encourage you, as attendee, to make the most of this time. Listen with curiosity to the speakers, and consider how their work might impact your own. Engage in discussion with poster presenters, so that you might learn something new about our discipline. Everything is interesting once you start to look at it closely.

A special word of thanks to the following individuals who assisted with arranging the symposium: Paula-Ann, Veronica, and Thaakira, for helping to arrange the event, Heinrich, Alvin, Ollie, and Ayanda for assisting with set-up, and the whole postgraduate student council. A thank you to our poster and oral presenters as well – thank you for the work you have put in here.

I trust you will find the day's proceedings stimulating, interesting and fruitful!

All the best,
Prof Robbie Pott

Keynote presenter

Mr Donald Mjonono

Head of Engineering at Afrigen
Biologics and Vaccines

**Future-Forward Pharma Factories:
Innovations in Modular Plant Designs**

Mr Donald Mjonono currently serves as the Head of Engineering at Afrigen Biologics and Vaccines, a biotechnology company committed to advancing biologics and vaccines for global health. His leadership has been instrumental in steering the engineering team towards innovative solutions that align with Afrigen's commitment to sustainability, quality, and technological excellence. He holds a MSc in Chemical Engineering, specialising in bioprocessing from the Centre for Bioprocessing Engineering Research (CeBER) at the University of Cape Town. Before joining Afrigen, he held key positions at Unilever, where he spearheaded notable projects in process optimisation and biotechnology. His success has been largely attributed to his proficiency in the design, operation, and intensification of biotechnology plants as well as the scaling up of nanotechnology processes.

He is a member of the International Society of Pharmaceutical Engineers (ISPE) and South African Institution of Chemical Engineers (SAIChE), where he actively engages with peers, shares insights, and stays abreast of the latest developments in the field. His commitment to advancing healthcare through innovative engineering solutions continues to position Afrigen at the forefront of technological advancements in the industry.

Poster presentations

All posters can be viewed online <u>here</u>

Optimisation of protein content during spray drying of Black Soldier Fly larvae protein
D Chakawa & Prof NJ Goosen

The effect of feed and recycle rates on the performance of an up-flow anaerobic filter at ambient temperatures treating synthetic winery wastewater
WF Fleming & Prof AJ Burger

Aspen® simulation and techno-economic analysis of fractional condensation and distillation of plastic waste pyrolysis oil for sustainable aviation fuel production
N Hanekom, Prof CE Schwarz & Prof JF Görgens

Effect of organic solvent structure on ternary liquid-liquid equilibria of (water + short-chain alcohol + organic solvent) systems
I Hayes, Ms DL de Klerk & Prof CE Schwarz

Constrained Bayesian methods for sensor validation
W Horak, Prof SM Bradshaw & Prof TM Louw

Decomposition and carbon storage of selected paper products in pilot scale landfills under optimal anaerobic conditions
T Jabaar, Prof TM Louw, Prof JF Görgens & Prof E van Rensburg

Advanced immobilisation strategies for the biological production of hydrogen using the phototrophic bacterium, Rhodopseudomonas palustris
G Keet & Prof RWM Pott

The extraction and identification of antioxidant bioactive compounds from endophytic bacteria
R Kholumo & Prof SL Tai

Development of economically viable waste tyre pyrolysis technologies that will yield liquid fractions that meet commercial fuel standards
M Khosa, Prof JF Görgens & Prof CE Schwarz

Enhancing anaerobic digestion of organic wastes through micro-aeration
J Kuyler, Mr Mamphweli, Prof JF Görgens & Prof E van Rensburg

Investigating the feasibility of chlorinated resin for water disinfection in developing countries
T Mtimuni & Prof VL Pillay

Recovery and purification of mannosylerythritol lipids using aqueous two-phase extraction
M Ncube, Prof E van Rensburg & Prof RWM Pott

Development of a bench scale bioreactor system for alginate lyase production
M Noach, Prof E van Rensburg, Prof RWM Pott & Prof NJ Goosen

Enhancing delivery of biopharmaceutics classification system class II drugs through a novel carrageenan-alginate-oleogel matrix: a case study on praziquantel for improved therapeutic efficacy
CN Nsanzubuhoro & Prof SL Tai

An investigation into production strategies for large-scale microbial oil production to maximise economic viability
D Nunes, Prof E van Rensburg, Prof VL Pillay & Prof RWM Pott

The extraction and depolymerisation of lignin from grape stalks using green and sustainable methods
N Scholtz, Dr HC Pfhukwa & Prof AFA Chimphango

Scale up and process development of recombinant enzymes used for RNA vaccine manufacturing
JI Tanyanyiwa, Prof JF Görgens, Prof RWM Pott & Prof SL Tai

The effect of carbon source and trace elements on the fed-batch production of mannosylerythritol lipid-A from hydrophilic carbon sources
AD Valkenburg, Prof E van Rensburg & Prof RWM Pott

Enhanced ethanol production from paper sludge waste under high-solids conditions with industrial and cellulase-producing strains of Saccharomyces cerevisiae
J van Dyk, Prof JF Görgens & Prof E van Rensburg

Lipopeptide separation and purification in an aqueous two-phase system
KJ van Niekerk & Prof RWM Pott

Enhancing the biomethane production of alkaline pre-treated lignocellulosic waste through bioaugmentation of anaerobic digestion
J van Wyk, Mr NS mamphweli, Prof Görgens & Prof E van Rensburg

Effects of consolidation and compression of biofouling layer on the performance of a membrane bioreactor
SA Yala & Prof VL Pillay

Oral presentation abstracts

Classical actor-critic for the online, continuing adaptation of PI control policies

EH Bras, Prof SM Bradshaw & Prof TM Louw

Keywords: Model-free Controller Design and Tuning, Nonlinear Process Control, Safe Reinforcement Learning, Average Reward Setting, Actor-Critic

Reinforcement learning (RL) is a computational technique in which an "agent" makes a series of decisions in a dynamic, interactive environment, where each decision is associated with a scalar reward. RL aims to maximise the rewards that the agent receives over time. The agent consists of an algorithm and a function approximator with adjustable parameters which are learnt through trial-and-error. The output of the RL training process is a policy which suggests a distribution over possible actions based on the current state that the agent finds itself in. The adoption of RL in the chemical process industries as process control strategy is currently hindered by black-box decision making, the exploration-exploitation dilemma, and high sample complexity. In this work, PI control was used to generate training data for the initialisation of the RL agent's adjustable parameters. Providing such a warm start to the RL agent ensures that the subsequent search for the optimal control policy during RL agent training can be visualised and improves the safety and efficiency of the training process. The classical actor-critic algorithm was applied to train the RL agent. This algorithm adapted the warm-starting policy during interaction with a simulated process to yield the improved control policy. All policies instantiated during training have an inherent safety mechanism called the soft active region which ensures that the RL agent selects actions according to PI control if excessive feedback error is accumulated. The adapted policy can be easily visualised which makes the RL controller interpretable. Hence, the work contributes to the industrial adoption of RL technology in the process industries.

Fractionation of 1-alcohol and n-alkane systems via supercritical CO2

AM Brown, Prof CE Schwarz & Ms N Motang

Detergent range alcohols (C8-20) that are often found in cleaning and personal care products present a large market. When commercially producing these alcohols via the oxygenation of alkanes, alkane-alcohol mixtures are formed in product streams. The desired alcohols must be separated from the alkane-alcohol mixtures. However, overlapping melting and boiling points eliminate more traditional separation processes such as distillation and crystallization. Azeotropic distillation is currently employed in industry to separate the alkane-alcohol mixtures but has many drawbacks. Supercritical fluid fractionation (SFF) is proposed as an alternative separation technique. SFF processes are operated above the critical point of the selected solvent and thus complex phase behaviour may arise in the system. This complex phase behaviour must be understood to explain results obtained from SFF processes and to develop accurate thermodynamic models and subsequently appropriate simulated process models. The process models are valuable since experimental data collection is costly. This study aims to experimentally investigate the effect of complex phase behaviour found in mixtures of supercritical CO_2 and detergent range 1-alcohols and n-alkanes on the performance of SFF and to subsequently evaluate the prediction capabilities of a process model within commercial process simulating software. Thus, the SFF of two multicomponent systems known to exhibit complex phase behaviour were examined, namely the CO_2 + 1-dodecanol + n-hexadecane system and the CO_2 + 1-dodecanol + n-tetradecane system. Experimental and literature pilot plant data over a wide range of conditions were used to model the separation process in Aspen Plus®.

A comparison of experimental and parameterisation uncertainties in the thermodynamic modelling of 1-alcohol and 1-alkane systems

N Buitendach, Ms DL de Klerk & Prof CE Schwarz

The thermodynamic modelling of industrially relevant 1-alcohol + 1-alkane systems using the Non-Random Two-Liquid (NRTL) model involves several uncertainties. Binary interaction parameters (BIPs) are regressed using experimental phase equilibrium data which are associated with uncertainties. These uncertainties are required to be reported with the published data. Numerous studies have demonstrated the effect of these uncertainties on predicting thermodynamic behaviour. This has been achieved using uncertainty quantification techniques, amongst which Monte Carlo Simulation (MCS) is a popular approach. The reporting of uncertainties associated with process design outputs is encouraged for better safety factor quantification. When regressing the model parameters, additional uncertainties arise through the choice of objective function, optimization algorithm and initial guesses (called the regression elements). These elements should remain constant in the MCS approach to independently demonstrate the effect of experimental uncertainty propagated to the BIPs. However, these elements may influence the experimental uncertainty analysis outcomes. This work aims to compare the influence of experimental data uncertainty to that associated with the regression of model parameters for the thermodynamic modelling of isobaric (low pressure) 1-alcohol + 1-alkane phase equilibrium data using the NRTL model. Such a comparison is currently overlooked in literature. Systems with different boiling point temperature ranges are investigated. Furthermore, three common combinations of temperature (in)dependent parameters (TDPs) are evaluated to increase the model flexibility. For the regression uncertainties, the effect of the choice of objective function and model parameter initial guesses on the thermodynamic modelling are investigated. This work shows that the experimental uncertainty propagation is specific to the system, and the objective function. Furthermore, all types of uncertainties depend on the combination of TPDs being regressed. It is thus recommended that engineers perform a thorough investigation on the effect of thermodynamic modelling uncertainties to gain better insight on the uncertainty propagated to the model parameters.

Spectroscopic measurement of associating and solvating binary mixtures for the determination of monomer fraction data towards thermodynamic model improvement

AE Burgess, Prof AJ Burger & Dr JT Cripwell

Recent global initiatives aim to transition to more sustainable processes, with a focus on enhancing energy efficiency and adopting cleaner alternatives such as green solvents and biodiesels in sectors such as petrochemicals, pharmaceuticals, and bioprocessing. However, hydrogen bonding phenomena in these chemicals pose a longstanding challenge for thermodynamic modelling and process design. The monomer fraction, a thermophysical property indicative of the extent of hydrogen bonding, is commonly measured using Fourier Transform Infrared (FTIR) spectroscopy. Surprisingly, its practical application in testing thermodynamic models remains underexplored, partly due to limited data and discrepancies in measurement techniques. This research investigates an alternative method for generating monomer fraction data and its applicability in testing thermodynamic modelling performance. Specifically, spectroscopic measurements of monomer fractions in binary systems containing ethanol and short-chain esters are conducted using FTIR spectroscopy coupled with Multivariate Curve Resolution through Alternating Least Squares (MCR-ALS) regression, a chemometric technique rooted in sound machine learning principles. The newly derived monomer fraction data will be used to assess thermodynamic models based on Statistical Associating Fluid Theory (SAFT). This study addresses the gap in utilizing monomer fraction data practically and contributes to the development of more accurate thermodynamic models, aiding the transition to a circular economy while enhancing the sustainability of processes in the aforementioned sectors.

The interdependencies of food and water within the water-energy-food nexus for the City of Cape Town

V Hofmann, Prof Görgens &Prof NJ Goosen

From climate change to increasing urbanisation, the city of Cape Town is facing numerous challenges in managing its water and food resources. Traditionally, issues in different sectors have been addressed individually, without honouring the complex interactions between them. This thesis presents a qualitative and quantitative system dynamics model designed to explore the intricate connections between water and food systems in Cape Town. The research addresses the urgent need for sustainable planning strategies to ensure the city's resilience in the face of water scarcity and food security threats. The model is part of a larger research effort to simulate the water-energy-food nexus (WEF nexus) for the city of Cape Town. It incorporates key variables, such as population growth, climate change impacts, agricultural practices, water supply infrastructure, and policy interventions. It utilizes system dynamics techniques to simulate feedback loops, delays, and nonlinearities that characterize the water-food nexus in an urban environment. The results of the model reveal complex interactions between water and food systems, highlighting vulnerabilities and potential leverage points for intervention. Including the city's plans for future policies and investments, different scenarios are developed. By assessing these scenarios, this research offers insights into policy strategies that can enhance Cape Town's capacity to sustainably manage its water and food resources. While a model cannot be used as a tool to predict the future, the findings about the benefits and trade-offs of different interventions from this research can be used to guide stakeholders and inform policies.

Techno-economic analysis of biorefinery scenarios for scFOS, ethanol, tryptophan, erythritol and collagen production from sugarcane

M Klaver, DR AM Petersen, Prof J Louw & Prof Görgens

The sugarcane industry is under threat due to low international prices and oversupply of sucrose markets. In an effort to alleviate this economic strain, this study explored the economic and environmental sustainability of five potential products derived from sugarcane-based feedstocks: short-chain fructooligosaccharides (scFOS), ethanol, tryptophan, erythritol, and collagen. Nine biorefinery scenarios were investigated, including small-scale facilities that are decentralized and large-scale facilities that are annexed to an existing sugar mill. The small-scale implementation of biorefinery scenarios for production of scFOS alone and scFOS with bio-ethanol were economically feasible. However, the large-scale production scenario of scFOS and/or ethanol provided better economics than small-scale facilities, despite a cheaper feedstock and the selection of simplified process technologies. However, small-scale production was the preferred investment option for scFOS-only production in a biorefinery, due to appropriate production rates for the size of the global market, to avoid oversupply. Furthermore, from the GHG analysis results, the large-scale scenarios consistently exhibited lower equivalent CO2 emissions per unit product compared to their small-scale counterparts. Large-scale production of scFOS and/or ethanol in annexed biorefineries were compared to similar scenarios producing tryptophan, erythritol or collagen. Tryptophan demonstrated the highest profitability, with an MSP that was 59.7% of its market price. Despite this, the large-scale production of collagen was deemed more economically viable due to the avoidance of market oversupply. The large-scale production of erythritol was unfruitful due to the low market price and high operational costs associated with this scenario. Moreover, the GHG analysis showed all scenarios to have low emissions. Among all the large-scale scenarios, only the production of ethanol and collagen were deemed viable market opportunities due to their favourable profitability and low market contribution. Despite the positive economic results of the other scenarios, their high market contribution (over 45%) led to their disqualification, as it would negatively affect product market prices

Optimizing a method for leaching PGMs from simulated spent auto-catalyst material using ozone & hydrochloric acid

MA Knight, MR AP van Wyk, Prof GA Akdogan & Prof SM Bradshaw

Automotive catalysts are a required component in internal combustion vehicles and use the PGMs Pt, Pd, and Rh to catalyse the conversion of harmful gases into more environmentally benign ones. The demand for these PGMs in the auto-cat sector exceeds that for both jewellery and industrial uses. Hydrometallurgy reports high extraction rates for these PGMs but generally uses aggressive oxidants such as $Cl_2(g)$. The aim of this research was to optimize a PGM extraction leaching process from simulated spent auto-catalyst material using a HCl lixiviant and $O_3(g)$ as a safer and less corrosive oxidant. Simulation of milled spent auto-cat material was conducted by combining PGM-oxide and synthetic cordierite powders and subjecting them to a formic acid prereduction. Conducting three-phase leaches, the ozone mass flow ($\dot{m}_{O_3}$), initial acid concentration ($[HCl]_0$), and temperature (T) were varied using a Box-Behnken experimental design. The achieved maximum extraction percentages for Pt, Pd, and Rh were 88.6%, 85.0%, and 41.5% at $\dot{m}_{O_3}$ and $[HCl]_0$ values of 5.01 g/h and 5.0 M; and T values of 30oC for Pt and Pd, and 90oC for Rh. Statistical analyses indicated optimum conditions of 5 g/h, 5 M, and 90oC when maximizing the overall PGM extraction. Further optimum conditions were established by minimizing Rh extraction and the dissolution of impurities (namely Si, Al, and Mg) through the increase and decrease of the $[HCl]_0$ and T ranges, respectively. Conditions in the second leach practically facilitated max extractions of 2.89%, 2.59%, 2.79%, and 4.10% for Rh, Si, Al, and Mg, while Pt and Pd extraction percentages at these conditions were approximately 64%. Therefore, the extraction of impurities was successfully minimized while a majority proportion of Rh remained in solid form for hypothetical downstream reclamation.

State estimation and model-based fault detection in a submerged arc furnace

I Kristensen, Prof SM Bradshaw & Prof TM Louw

Model-based state estimators are a group of mathematical techniques that combine process model knowledge and noisy plant measurements to provide accurate and timely state estimates. The aim of this project was to perform model-based fault detection using state estimation in a complex chemical unit operation and compare the model-based method to a data-driven method under plant-model mismatch. To validate the use of state estimators and corroborate the findings of the fault detection, a system observability and fault detectability analyses were first conducted. The performance nonlinear state estimators, namely the extended Kalman filter (EKF), the unscented Kalman filter (UKF), the particle filter (PF), and the moving horizon estimator (MHE), were assessed. Model-based fault detection using state estimation was employed and compared to data-driven fault detection using PCA under plant-model mismatch. A submerged arc furnace (SAF) for platinum group metal smelting was used as a case study to apply these techniques. The state observability analysis found the SAF system to be locally observable and the measured states to have a higher degree of observability than the unmeasured states. The fault detectability analysis identified all faults investigated to be structurally detectable. The EKF and UKF displayed good estimation accuracy and fast computation times. The computational requirements of the MHE proved to be its greatest limitation. The PF, showing superior estimation accuracy, and the EKF, being the most popular and simplest algorithm, were selected to be used in model-based fault detection. Lastly, this study found that the model-based fault detection using the PF outperformed the EKF and the data-driven method. However, this method showed exceptionally poor robustness to plant-model mismatch. The investigation then demonstrated that residual evaluation of the PF and EKF residuals in a reduced-dimensional space using PCA improved the classification performance of the method in the presence of plant-model mismatch.

The use of spent pulping liquors as binders for chromite pellets

H le Roux, Dr L Tyhoda, Prof TM Louw & Prof JF Görgens

Keywords: Chromite, Pelletisation, Pulping liquors, Strength tests

Chromite fines must be agglomerated before being smelted in submerged arc furnaces to prevent disruptions and damage to equipment. Bentonite is the most commonly used binder for fines agglomeration in the ferrochrome industry; however, fluctuations in its availability has led to the investigation of alternative binders. Spent pulping liquors are under-utilised resources that are predominantly combusted for energy and/or pulping chemicals recovery but have shown binding potential for coal and iron ore fines. Four spent pulping liquors, i.e., sodium lignosulphonate, magnesium lignosulphonate, Kraft liquor and soda liquor, were therefore investigated as binders for the agglomeration of chromite fines into pellets, for the industrial Outokumpu and Premus processes. The green impact strengths of the resulting pellets were found to increase with an increase in binder mass percentage, with all four pulping liquors outperforming bentonite. For the indurated compressive strength test, Outokumpu pellets were oxidatively sintered at 1 200 °C, while Premus pellets were indurated in an inert atmosphere at 700 °C. For the Outokumpu pellets, all the pulping liquors produced pellets with similar or higher strengths than the control pellets made with 0.8 % bentonite. For the Premus pellets, all of the pulping liquors outperformed bentonite but had similar performances to each other. The fluxing ability of the sodium and calcium components in the pulping liquors was found to potentially be responsible for the differences in the sintered strengths of the Outokumpu pellets made with different pulping liquors. Both the inorganic and organic components of the pulping liquors were required to produce Kraft liquor Outokumpu pellets with sufficiently high strengths. Lime was not found to be a suitable additive when tested with sodium lignosulphonate and Kraft liquor for Outokumpu pellets. Overall, the pelletisation of chromite fines with spent pulping liquors was found to be technically feasible and thus suitable for further application to industrial processes.

The impact of thermal treatment on comminution performance of blue mussel (Mytilus edulis) and South African abalone (Haliotis midae) shell waste

T Lesofe, Mr AP van Wyk & Prof NJ Goosen

Keywords: Shell waste, Calcium carbonate, Comminution, Energy reduction, Roasting

Mussel and abalone cannery industries generate large amounts of waste shells. Most waste shells are being discarded into landfills and public water bodies resulting in pollution. Mussel and abalone shells contain up to 98% $CaCO_3$, which can substitute conventional mined limestone. However, the nacreous layer of the shells makes size reduction of difficult. Since comminution circuits are energy intensive, the study focuses on developing a processing strategy to improve the comminution performance of mussel and abalone shell waste into industrially ready calcium carbonate. Mussel and abalone shells were roasted in a retort kiln at roasting temperatures ranging from 300 °C to 480 °C for roasting times ranging from 10 minutes to 45 minutes. The roasted shells were then ball milled for times ranging from 10 minutes to 40 minutes and the best operating conditions were selected. For mussel shells, the best operating conditions were at a roasting temperature of 400 °C, roasting time of 25 minutes, and milling time of 30 minutes. For abalone shells, the best operating conditions were at a roasting temperature of 400 °C, roasting time of 30 minutes, and milling time of 30 minutes. A comparison of mussel and abalone shells showed that untreated abalone shells were harder to mill than mussel shells. Thermal pre-treatment was found to improve the comminution performance of both abalone and mussel shells.

Metathesis of unsaturated fatty acid ethyl esters for production of value-added surfactants and chemical intermediates.

C Lourens, Prof M Tadie & Prof NJ Goosen

Olefin metathesis is a powerful chemical reaction providing new avenues for producing essential chemicals. In the context of shifting focus towards sustainability and renewable resources, there is a growing demand for value-added surfactants and chemical intermediates sourced from renewable materials like natural oils and fats. This study explores self-metathesis of a mixture of unsaturated fatty acid esters derived from sunflower oil as an alternative method for producing value-added surfactants and chemical intermediates. Metathesis of this unrefined mixture was compared to that with a higher purity ethyl oleate feedstock. The product distribution from metathesis of these feedstocks revealed a range of unsaturated ethyl esters, internal alkenes and unsaturated diethyl diesters. The study investigated the effect of temperature, time and catalyst loading on metathesis efficiency, with varying results for the two feedstocks. The sunflower-based feedstock required higher catalyst loadings, possibly due to impurities in the feedstock, deactivating the catalyst. Organic solvent nanofiltration effectively removed the Grubbs 2nd generation catalyst from the reaction mixtures and allowed for partial product fractionation. However, complete fractionation was hindered by compound-membrane interactions and the proximity of the molecular weights of the products. Foaming tests suggested potential surfactant properties in the metathesis reaction mixtures, although critical micelle concentrations could not be determined for these mixtures due to low water solubility. Comparison of the surfactant efficiencies of the reaction mixtures to the feedstocks, indicated that the surfactant potential of the feedstocks were upgraded through metathesis. In summary, this study demonstrated that metathesis of sunflower oil-derived ethyl esters offers a promising pathway for producing a mixture of products (C12-C18 alkenes, C16-C21 ethyl esters and C18-C24 diethyl diesters) with surfactant properties. Further product fractionation could be useful in increasing the industrial value of the metathesis products. This pathway facilitates production of value-added surfactants and important chemical intermediates, contributing to a more sustainable and diverse chemical industry.

Process development for the valorisation of industrial kelp waste

R Mampana, Prof RWM Pott & Prof NJ Goosen

Keywords: Ecklonia maxima, Molecular weight, Oligosaccharides, Sequential hydrolysis, Solubilisation yield

Seaweed processing is one of the fastest-growing biomass-based industries, producing products for various applications, including: textiles, food, medical, agricultural, and pharmaceutical industries, amongst others. The products are derived from three groups of seaweeds (brown, green and red) using various extraction and beneficiation methods (such as organic solvent extraction, acid / alkaline hydrolysis, enzymatic, microwave, or ultrasound-assisted extraction). However, the industry faces the challenge of low biomass usage, resulting in a considerable amount of feed material being discarded as waste. Therefore, this project proposes chemical hydrolysis methods for the valorisation of industrial kelp waste (brown seaweed specie, Ecklonia maxima). The study outlines suitable methods for producing an oligosaccharides-rich product with potential agricultural application. The aim was achieved through sequential hydrolysis, using both acid and alkaline hydrolysis (each conducted for 3 h at 70 C), aided by the addition of hydrogen peroxide. Using this approach, a high degree of solubilisation of waste biomass was demonstrated. Most approaches resulted in good hydrolysis, however, two gave the highest degrees of solubilisation. For the first, 85.9 % overall solubilisation was achieved using 0.3 M ascorbic acid and 0.3 M H_2O_2, for the initial acid step, followed by 0.5 M KOH and 0.1 M H_2O_2, for the alkaline step. For the second set of conditions, 85.5 % was achieved using 0.5 M KOH and 0.1 M H_2O_2 for the alkaline step followed by 0.5 M nitric acid for the acid step. The production of oligosaccharides during these hydrolysis steps was analysed using size exclusion chromatography. Sequential hydrolysis resulted in considerable hydrolysis of high molecular weight fractions (e.g., 700 – 1 020 kDa) down to lower molecular weight constituents: 16.0 – 57.5 kDa and even smaller fractions. The highest extent of hydrolysis was achieved by first acidifying the kelp waste using 0.3 M ascorbic acid and 0.3 M H_2O_2 followed by 0.5 M KOH and 0.1 M H_2O_2. This approach yielded a high concentration of a 16.0 kDa fraction, along with 1.6 and 0.8 kDa fractions – the literature identifies these small molecular weight oligosaccharides as having high bioactivity. Nevertheless, to evaluate the potential application of the oligosaccharide fractions in-depth, further work is required to identify and characterise the hydrolysis products.

Investigating options for reducing the environmental impact of hydrometallurgical lithium-ion battery recycling plants using life cycle assessment

RF Maritz, Prof GA Akdogan & Prof C Dorfling

Lithium-ion batteries (LIBs) have become commonplace for everyday use in consumer electronics and have gained considerable popularity recently for usage in industrial applications such as electric vehicles and stationary storage systems. The continuously increasing demand for LIBs results in a fast-growing end-of-life (EOL) LIB waste stream containing valuable metals such as lithium, cobalt, nickel, and manganese. LIBs have traditionally been recycled through means of pyrometallurgical methods, but due to the lithium in the batteries being lost to the slag phase and given the fact that severe lithium shortages have been forecasted for 2030, industry focus has shifted towards alternative process technologies such as hydrometallurgical processes.

The aim of this study was thus to perform a life cycle assessment (LCA) to compare the environmental impact of different hydrometallurgical processes for the recovery of metals from EOL LIBs to help determine the selection of the most sustainable process technologies. This study considered the use of 3 lixiviants (hydrochloric-, sulphuric-, and citric acid) alongside the use of 3 flowsheet options (sequential metal precipitation, mixed metal precipitation, and hybrid sequential precipitation - solvent extraction systems). The study considered a mixed feed of LiCoO2, LiFePO4, and NMC111 batteries. The reference flow for the LCA was chosen to be 1 kWh of EOL LIBs fed to recycling, and because the process forms multiple products, the avoided burden method was applied.

The potential environmental impacts of mineral acid-based processes were found to generally be lower than that of organic acid-based processes by 18 to 61 percentage points. Furthermore, mixed metal precipitation provided the greatest environmental benefit of the flowsheet options considered by 46 to 117 percentage points when compared to the closest competing processes using similar lixiviants. Finally, the LCA system was subjected to extensive uncertainty and scenario analyses which served to confirm the trends already observed.

Quality improvement of liquid fuels derived from waste tire pyrolysis.

M Masha, Prof JF Görgens & Prof CE Schwarz

The liquid product from waste tire pyrolysis (TDO) fails to meet quality standards prescribed by regulations for specific fuel applications. This failure can be due to low flash points, high sulphur content, and high densities and viscosities, amongst others. It is imperative to produce fuels from TDO that can meet regulations, because TDO can potentially be a substitute for fossil fuels. Using tires for pyrolysis can also reduce the piled-up waste tires that are associated with multiple environmental concerns. The solution to using TDO as a fuel substitute would involve separating the components that contribute to the poor-quality characteristics from the fuel components. This study aimed to optimize the fractional condensation of tire pyrolysis vapors in 3 condensers in series to separate TDO by condensation temperature into heavy (>190 °C), medium (130 – 190 °C) and light fraction (<150 °C) thus dividing the components by boiling point between the 3 condensers. Components with low boiling temperatures have low flash points, densities and viscosities, while majority of TDO sulphur is thiophene derivatives (boiling point > 220 °C). The primary focus of the optimization was on sulphur content, boiling point, flash point, density and viscosity. The system was expected to isolate most of the sulphur content to the heavy fraction. The other fuel properties were expected to be approximately similar to those of petroleum derived fuels in same boiling temperature range. The heavy, medium and light fractions should correspond to marine bunker oil, diesel and naphtha respectively. Oxidative desulphurization (ODS) was conducted on each fraction to further reduce the sulphur content of the fuel fractions. ODS converts the sulphur containing compounds in the fuel into sulfones. The oxidized sulphur compounds become more polar than the oil phase and can be extracted using a polar solvent. Peracetic acid was used as an oxidizing agent while acetonitrile and DMF were used as solvents.

Assessing water-energy nexus dynamics for sustainable resource management in Cape Town: a system dynamics approach

T Ndlela, Ms I de Kock & Prof NJ Goosen

This study explores the crucial connection between urban energy and water resources, aiming at bringing solutions to the day-zero water crisis in Cape Town and the load shedding throughout South Africa. The approach to the study is developing a model to simulate the intricate relationship between energy and water. The findings emphasize essential strategies for preventing future shortages by showing the need to augment electricity supply and water alongside behavioural changes that reduce waste. This work contributes to Cape Town's vision of becoming a resource-resilient city by recognizing the pivotal role of sustainable water resource management. The model is tailored to this industry's unique challenges and employs system dynamics due to its capacity to capture sustainability-related complexities. The water scenarios tested include water conservation and water demand management (WC&WDM), exploring groundwater, increasing wastewater reuse and climate change. After undergoing rigorous scenario testing, the model shows promising results. It projects that with a combination of the scenarios, there will be a balance between water supply and demand by 2035 which indicates significant progress in sustainable management of this resource. If Cape Town takes immediate action and makes strategic investments, it can meet its water requirements adequately. The study also examines energy scenarios that involve a 650 MW backup system and the integration of independent energy producers. These interventions enhance energy supply, reduce the risk of shortages, and promote a diversified and resilient energy network. This aligns with global trends towards decentralized and renewable energy systems, positioning Cape Town as a forward-thinking sustainable city. These measures not only ensure reliable energy supplies for growth but also foster an environment conducive to economic development and innovation while ultimately contributing to environmental sustainability.

Process simulation and technoeconomic assessment of recombinant enzymes used in the production of mRNA vaccines

H Nyikadzawanda, Prof JF Görgens & Prof SL Tai

Keywords: Bioprocess simulation, Recombinant enzymes, mRNA vaccines, Techno-economic evaluation, South African vaccine industry

In the dynamic field of medical science, mRNA-based vaccines have proven their efficacy, notably during the global SARS-CoV-2 pandemic. In Africa, where less than 1% of vaccines are locally produced, this technology offers a path to vaccine self-sufficiency. Yet, a critical challenge remains – the heavy reliance on imported recombinant enzymes RNase inhibitor protein, restriction endonucleases, inorganic pyrophosphatase, T7 RNA polymerase, deoxyribonuclease I, vaccinia capping enzyme, and 2-O-methyltransferase), constituting approximately 80% of the production cost for mRNA vaccines. This project employs a quantitative approach, employing SuperPro Designer (Intelligen, USA) simulator software for process design, modelling, optimization, technoeconomic assessment, and production scheduling of each recombinant enzyme, as well as the simultaneous production of all recombinant enzymes in a single facility. Data collection involves a thorough review of existing literature, patents, and industry reports, as well as data generated by Stellenbosch University's SAMVAC project. The study aims to address the knowledge gap by assessing process development and the economic feasibility of producing recombinant enzymes for mRNA vaccines in South Africa, ultimately establishing a local supply chain throughout the African continent. The research addresses economic indicators (CAPEX, OPEX, NPV, IRR, and ROI), production operations at manufacturing scales, scheduling, sensitivity analysis on critical parameters (production titer, yield recovery, bioreactor scale), and multiproduction of all seven enzymes in a single facility. The outcomes of this project will guide policy decisions and encourage investment in vaccine production in Africa.

A techno-economic evaluation of decentralized direct potable reuse

JI Ross & Prof VL Pillay

Keywords: Direct potable reuse, Decentralised water treatment, Membrane filtration, Electrodeionisation, NPV analysis

The potable reclamation of wastewater has garnered interest as a viable means to ensure future water security. Large scale water and wastewater treatment facilities in South Africa however are rapidly degrading, mismanaged and do not meet green or blue drop standards. Hence, this research explores the water treatment unit operations that may be feasible for use in a small-scale direct potable reuse (DPR) treatment system. Various unit operations were used to treat secondary effluent discharge from Stellenbosch wastewater treatment plant (WWTP) in bench scale laboratory investigations with an aim of producing potable water that complies with SANS 241 drinking water standards. This study of technical feasibility was complimented by a brief economic analysis so that an ideal treatment train may be proposed. The select unit operations for such a treatment train have been optimized in terms of both economic and technical feasibility for small scale water reclamation in decentralized settings.

Extending the s-SAFT-γ Mie equation of state to nonaqueous alkanolamine-based carbon capture systems

A Schulze-Hulbe, Prof AJ Burger & Dr JT Cripwell

Alkanolamine-based post-combustion carbon capture (PCC) is a mature technology for removing carbon dioxide from fossil fuel combustion effluent gases. However, high energy costs remain a key obstacle to large-scale implementation of PCC. A promising route to reduce these energy costs is to replace the typical aqueous process fluid with a nonaqueous alternative. However, given the sheer range of available organic components, experimental investigation to identify a suitable water alternative is challenging. A cost-effective proxy to experimental measurement is provided by advanced thermodynamic modelling tools like the Statistical Associating Fluid Theory (SAFT) equations of state (EoSs). Further, SAFT EoSs that utilise the group-contribution framework can provide property predictions for mixtures for which little or no data exist, as is the case for a wide range of nonaqueous alkanolamine-based process fluids. To this end, the aim of this work was to extend the s-SAFT-γ Mie group-contribution EoS toward a description of nonaqueous alkanolamine-based carbon capture fluids. This presents the first instance in which a group-contribution SAFT EoS was extended to these nonaqueous systems. However, there is no set procedure for parameterising group-contribution thermodynamic models. Pertinently, a lack of guidance regarding model parameterisation poses a barrier to the successful implementation of advanced thermodynamic models in industrial settings. Therefore, a secondary aim of this work was to provide an example of how group-contribution SAFT models can be parameterised consistently and systematically for nonaqueous alkanolamine-based carbon capture systems. s-SAFT-γ Mie was found to provide a robust description of nonaqueous alkanolamine-based carbon capture systems: The model could qualitatively predict changes in temperature, liquid phase composition as well as the chain length of the organic water alternative. s-SAFT-γ Mie's predictive capabilities render it suitable for use in screening more promising nonaqueous carbon capture formulations from less promising ones, highlighting its value to carbon capture researchers.

Decontamination strategies and enzyme dosages for ethanol production from food waste

J van Rooyen, Prof JF Görgens & Prof E van Rensburg

Innovative solutions are required to deal with an ever-increasing energy demand and generation of organic waste. Processes where energy or useful chemicals can be produced from waste will be support a circular economy and a sustainable future. Ethanol production from biomass, such as maize or sugar cane, is a mature technology. However, ethanol production from food waste (FW) is a far more challenging, given variable feed composition and microbial contamination. The aim of this research was to produce ethanol from food waste by evaluating (i) different types of food wastes typically found at commercial food waste processors, (ii) different decontamination strategies, and (iii) different yeast strains, an advanced yeast Saccharomyces cerevisiae ER T12 and S. cerevisiae Ethanol Red. Ethanol fermentation using pre- and post-consumer FW were conducted in shake flasks at 30°C for 72 hours. Thermal sterilisation proved effective for post-consumer FW at a low liquefaction temperature of 55 °C with a significant ($p < 0.05$) increase in ethanol yield of 77.79% compared to 67.29% for fermentation without sterilisation. At low liquefaction temperature of 55 °C for pre-consumer FW the ethanol yield increased substantially from 48.2% for the negative control to 92.19% when applying thermal sterilisation, however this was attributed to the preference for high gelatinisation temperatures of pre-consumer FW. Substantial decreases in enzyme dosages were achieved by using a consolidated bioprocessing (CBP) yeast S. cerevisiae ER T12 without affecting on the ethanol yield of 80.87% ± 1.40 and productivity 1.51 g/L/h compared to 82.56% ± 2.81 and 1.54 g/L/h when using S. cerevisiae strain Ethanol red as benchmark. Although sterilisation proved to be an effective decontamination method, it remains energy intensive that could affect the financial feasibility of the process. Using the CBP yeast can substantially decrease operational costs due to the reduced requirements for commercial enzymes, which is key to developing a sustainable FW fermentation process.

The recycling of end-of-life lithium-ion batteries in South Africa: reverse logistics and material flow analysis

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Keywords: Material flow analysis, Reverse logistics, Lithium-ion battery recycling, Circular economy, Network optimisation

The increasing demand for lithium-ion batteries (LIBs) in South Africa (SA) raises concerns over their disposal and recycling once they reach end-of-life (EOL). There are currently no LIB waste processing facilities in SA and no specific legislation to mandate their collection and recycling. There is thus an urgent need for sustainable recycling routes for EOL LIBs in SA. Given this, the aims of this study are to: (1) develop and optimise an environmentally sustainable (carbon emission minimisation) and economically viable reverse logistics network (RLN) for the recycling of EOL LIBs, and (2) perform a material flow analysis (MFA) to track the flows and fates of materials resulting from their recycling. RLNs for integrated EOL LIBs and e-waste recycling were modelled using anyLogistix® supply chain software, which considered the following stages: waste material collection, pre-processing, hydrometallurgical processing, and end-product distribution. RLNs were modelled and optimised for the period of 2023 to 2033 and considered scenario variations in the hydrometallurgical processing route (inorganic vs. organic acid), product types, and process facility configurations. Three primary MFAs were performed: an MFA over the entire RLN boundary, an MFA over the processing boundary, and an elemental flow analysis (EFA) over the processing boundary. An RLN consisting of 212 waste collection centres, 9 dismantling facilities and a single, centralised scaled-up hydrometallurgical process plant utilising an inorganic acid-based approach was found to be the optimal RLN configuration, yielding a net present value (NPV) of 485 million South African Rand (ZAR). From an MFA perspective, the viability of the RLN is heavily dependent on the EOL LIBs collection rate, conveying the urgent need for regulatory action. Inorganic acid-based processes are preferred to organic processes from a waste treatment, saleable product, and metal of interest (MOI) recovery perspective. Organic acid-based processes are preferred from a reagent consumption perspective.

The comparison of pre-treatment methods for cellulosic nanofibril production from sugarcane bagasse

C Warwick & Prof JF Görgens

Lignocellulosic biomass (LCB) is the most abundantly available, renewable biopolymer. LCB can be found in the primary cell walls of most plants and is readily available as a commercial feedstock from agricultural industry waste. Sugarcane bagasse (SCB) is an available agricultural industry waste comprised of LCB. LCB is mainly comprised of cellulose, hemicellulose, and lignin. It has favourable properties that make it useful for energy (biofuel) and non-energy (material) production. Cellulose has mechanical and physical properties that can be suitable for producing various materials. For SCB to be used for the production of value-added materials, it must be pre-treated to extract cellulose, hemicellulose, and lignin from the recalcitrant LCB. Pre-treatment methods are categorized into physical, chemical, biological, and their combinations. This study compares different pre-treatment methods for the production cellulose nanofibrils (CNF) (For industrial purposes). This will be achieved through physical pre-treatment by the use of a supermasscolloider and the combination of physical and chemical pre-treatment (physiochemical) by use of steam explosion, organosolv and alkali pre-treatment. The extracted CNF-rich pulp will be characterized by its CNF yield, CNF fibril length, diameter, viscosity, composition (cellulose, hemicellulose, and lignin content), thermal stability, and lastly its crystallinity index. This will be done by using methods such as centrifugation, transmission electron microscopy (TEM), NREL fibre analysis, thermogravimetric analysis (TGA), and X-ray diffraction, respectively. These measurements we screened the quality of CNF produced from the different methods.

The purification and characterisation of fucoidan from the South African seaweed Ecklonia maxima

G Wilkinson, Prof NJ Goosen & Mr Z Mapholi

Fucoidan is a term that groups a family of fucose-rich sulphated polysaccharides that display biological properties such as anticancer, anticoagulant, and antioxidant. This polysaccharide can be found in brown seaweeds such as Ecklonia maxima, an underexplored species endemic in South Africa. However, their inherent heterogeneity and the co-extraction of contaminants whilst trying to extract fucoidan has led to the difficulty in isolating fucoidan in a pure form that would allow for an accurate understanding of its structure-activity relationship. This project aims to determine the chemical structure of fucoidan extracted and purified from the South African kelp, Ecklonia maxima. To date, an improved methylene blue assay for the specific quantification of fucoidan has been developed. Fucoidan could be specifically determined at pH 1 without the interference of alginate and other seaweed extract contaminants. Quantification of fucoidan at pH 7 (buffer and water) and 11 led to interference from alginate and gallic acid. Furthermore, it was concluded that an intact fucoidan is required for a colour change to occur, ensuring no free sulphates are measured during quantification. A mixture design was conducted to test the required concentrations of contaminants for interference to occur. Further, toluidine blue O has been successfully immobilised to ReliZyme beads for the purification of fucoidan. Upon placing them in fucoidan solutions, fucoidan concentrations decreased over time demonstrating the successful adsorption of fucoidan onto the resin.

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