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FIGHTING CHEMISTRY WITH CHEMISTRY: NEW ANTIDOTES AGAINST NERVE AGENT AND PESTICIDE INTOXICATION

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Abstract

Highly toxic nerve agents such as sarin, VX and tabun are known for their use in chemical warfare, assassinations and terror attacks.^[1] Not dissimilar in their chemical structure to nerve agents, pesticides as well account for a large number of annual fatalities worldwide.^[2] They work by covalently inhibiting an enzyme called acetylcholinesterase (AChE), an important player in neuronal signalling. The inhibition of said enzyme leads to neural overstimulation and ultimately, death.^[3] To rinse the nerve agent and reactivate the enzyme, oxime antidotes are commonly applied alongside symptomatic treatments.^[4] The current drugs, however, have several drawbacks, as they possess but poor blood-brain-barrier penetration and are often specific to a certain type of nerve agent.^[5] Hence, a fast treatment upon nerve agent exposure is of the essence.

In our group, we aim to develop molecules which are not only able to penetrate the bloodbrainbarrier, but work sufficiently fast on a broad spectrum of nerve agents. Therefore, we and our collaboration partner, the Swedish Defence Research Agency (FOI), combine expertise within computational chemistry, biochemistry and organic chemistry. We evaluate possible new antidotes with simulations and synthesise a library of these molecules in the laboratory. FOI aids us through the entire process with their knowledge of nerve agent inhibition and provides us with the opportunity to assess the reactivation properties of our new compounds on nerve agent inhibited AChE. We also want to delve deeper into the actual reactivation mechanism and explore it with physicochemical NMR methods to aid us in our development of new antidotes.

Keywords: Chemistry, Medicinal Chemistry, Organic Chemistry, Pharmaceuticals, Drug Development, Acetylcholinesterase, Nerve Agents, Covalent Drugs, Oxime Reactivators

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SOCIAL INNOVATION FOR ENVIRONMENTAL SUSTAINABILITY: A BUSINESS MODEL LENS

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Abstract

Environmental problems have become increasingly more severe and have led to pressing issues like climate change and loss of biodiversity. These ecological crisis can, in part, be attributed to an increasing population which has led to an increase in human activities like production, consumption, and farming. Greener technologies, conscious consumers, CSR initiatives, in addition to other market driven solutions have been insufficient in addressing these problems. In an attempt to focus on solutions that are largely not market driven, this dissertation looks upon social innovations as a promising alternative. Social innovations are defined by the EU Commission ^[1] as: "...new solutions that simultaneously meet a social need and lead to new or improved capabilities and relationships and better use of assets and resources. In other words, social innovations are good for society and enhance society's capacity to act."

The concept of social innovation is closely related to sustainable development ^[2], but there has been a lack of focus on environmental sustainability issues and the relationship between human activities and our planet ^[3]. As such, research on social innovation has primarily focused on social sustainability issues, but in this dissertation focus is placed on how social innovation can address problems relating to environmental sustainability. We recognize that environmental sustainability should be prioritized, because humanity is dependent on the natural environment, which encompasses society and the economy ^[4], meaning that without a livable natural environment, there is no functioning society or economy.

The first overarching research question this dissertation seeks to address is *how can social innovations for environmental sustainability be conceptualized?* This first research question relates to having a sustainability perspective that assumes that environmental sustainability should be prioritized above all else, and thus seeks to answer the question of how social innovations could be developed to align with the principles of strong sustainability. Strong sustainability assumes that natural capital or nature resources, cannot be substituted for by manmade capital or new technologies and that we need to value caring for our planet before we consider addressing other sustainability aspects ^[5].

Not only is there little research on how social innovations can address environmental issues, but yet there is also a dearth of research, and practical knowledge, on how social innovations can be financially sustainable in the long-run. This leads to the second research question which is: *how can social innovations capture value in order to sustain themselves in the long-term?* Our second research question stems from different characteristics of social innovation. For example, due to social innovations primary motivation of seeking to benefit society as a whole while addressing pressing societal issues (social and environmental sustainability), economic sustainability is generally not a priority. Oftentimes, the products or services offered by social innovations are not being sold like tradition products and services in the sense that there is not always a clear buyer.

Further, in the context of this dissertation, social innovations that are driven primarily, if not solely, by an environmental purpose are attempting to benefit the natural environment. Thus, social innovations struggle to capture the value that they create. As a result, there is a lack of knowledge about sustainable business models for social innovations. As a result, the second research question and second purpose is to discover sustainable business models for social innovations with a focus on how to capture value.

Primarily, qualitative research methods will be used to collect data. Data will be collected in cooperation with the collaborating partner of this dissertation, Coompanion Västerbotten, a business development consultancy organization who works with helping develop social innovations. Our collaboration is within a project called Arena Social Innovation which has the purpose of promoting a social innovation network. Together, we seek to develop existing and potential social innovations in addition to expanding

the knowledge about the social innovation concept. Primarily, qualitative interviews will be conducted to discover more information about the processes of how social innovations develop, run, and maintain their organizations.

In all, four articles will be written. The first article will be a systematic literature review with the purpose of understanding how environmental sustainability is discussed in the existing social innovation literature. Next, the second article will focus on the research question of how to conceptualize social innovation for strong sustainability and will use some qualitative case studies. Thereafter, the third article will use qualitative case studies to identify sustainable business models for social innovations. Lastly, the fourth and final article will use qualitative case studies to explore how social innovations develop within an ecosystems for social innovations.

Keywords: Social innovation, environmental sustainability, business models.

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MAKING VEGETABLES “COOL”: IMPROVING THE EATING HABITS OF WALES’ YOUNGER GENERATION

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Abstract

Background: The literature revealed that poor consumption of fresh produce is rife amongst adolescents. For example, only 52% of children in Wales consume vegetables daily ^[1]. This may be attributed to the increased autonomy and freedom of choice experienced during adolescence ^[2]. Upon starting secondary school, individuals are vulnerable to making choices based on those in “cool” social groups that they aspire to belong. Adolescents may seek ‘belongingness, stimulation, loyalty, devotion, empathy and resonance’ from their fellow peers rather than their family ^[3]. Individuals may conform to pervasive social norms concerning their food choice and intake; however, these implicit codes of conduct may lead to sustained behavioural change if an individual’s behaviour changes ^[4].

The aim of this research is to develop a detailed insight into young adolescents’ (aged 11 to 13 years old) behaviour concerning vegetables through experimental research.

Methodology: An ongoing Contextual Review consists of the relevant literature and contextual research. The research project is taking a triangulated approach, involving amalgamating multiple research methods in order to provide a more holistic approach to addressing the research questions ^[5]. Quantitative data will be collected from school canteen purchases made using cashless fob systems or biometric data. The majority of the research will be qualitative and three schools were recruited. At present, the Catering Manager interviews have been done and school-based observations were completed over two non-consecutive school days for Key Stage Three pupils at each school. Currently, Focus Groups are being carried out at each school: (1) adolescents in year 7 and 8; (2) parents; and, (3) catering staff. After this, ethnographic observations of six families will take place. This will involve immersing oneself in the participant’s life whilst observing and informally interviewing them ^[6].

Results and Discussion: Research is ongoing, but thus far, thematic analysis has indicated four themes: convenience, parents, peers and cost. The school-based observations revealed that adolescents are in a rush and choose items that are convenient and quick to consume. Cost and price constraints emerged as a key influencing factor in all of the focus groups to date. Perhaps the most surprising finding up to now has been that adolescents believe their parents influence their choices more so than their peer group. It will be interesting to continue to explore this finding in future focus groups together with the ethnographic observations.

Research Impact and Outcome: The insights and novel findings derived from the research stage will be used to work in collaboration with an industry partner – Puffin Produce – to design and develop innovative branding and merchandising practices. The ultimate aim of the PhD project is to develop a new and innovative mass-manufactured vegetable-based product that will be targeted towards the younger generation in Wales, or perhaps ‘cross the border’ into the English market.

Keywords: Qualitative, adolescents, vegetables, food, Wales, eating, new product development, convenience, schools, ethnography, observations, focus groups, social norms, cool.

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A REALIST EVALUATION OF COMMUNITY (HEALTH) DEVELOPMENT PROJECTS IN WALES

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Abstract

A realist evaluation of geographically distinct community (health) development projects: what works in Wales, for whom, how, why, and in what circumstances?

Community development for health and wellbeing is back in fashion across Wales. Renewed interest in governance at the community level, building local resilience and empowering people to make the most of their wellbeing assets is influencing a wide range of projects. The Well-Being of Future Generations (Wales) Act (2015)^[1] provides a further impetus to this through requiring all public bodies to work together to make an impact upon sustainable development by driving them, through better collaboration and joint action, to build wellbeing within communities.

However, this very faddism brings inherent problems as the history of community development is vast, draws from many disciplines and ideologies yet these are often hidden in implementation^[2]. The result is that projects borrow approaches uncritically and consequently in application in local circumstances the initiatives don't quite 'fit'.

Each community development trend has brought theories, values and principles, even toolkits, but on the whole these suggest **what** works not **how** projects work, **for which** communities, and in which specific types of circumstance (**contexts**) the **mechanisms** operating within projects will 'fire' to make an impact and produce wellbeing **outcomes**^[3].

Using realist evaluation methodologies^[4] this research attempts to 'unpack the black box' of community health development.

Realist methodology is a theory driven approach to programme evaluation and is suited to this study as it helps to penetrate the complexities of interventions, unpacking what is really working in such projects to enable a more granular learning to be applied and uniquely reconstructed in other contexts. Often communities look at programmes and interventions successful elsewhere and try to replicate them within in their own different local contexts but with limited results. This research provides them with the tools to build their own success not merely patents to copy.

Phase 1 has explored with community stakeholders what is working in practice, what myriad theories of change are driving the actors and actions in these projects and how the two are related.

Concept mapping was undertaken alongside stakeholder workshops in four place-based community projects (Isolation/Loneliness in Anglesey, Youth Sheds in Denbigh, The Holway Housing Estate, and Wrexham Homelessness). Soft systems methodology^[5] was used to facilitate stakeholders to express through rich pictures "what makes a good community (health) development project?"

In realist research this stage aims to develop candidate theories, or 'context- mechanism – outcome' (CMO) configurations^[2]. Four initial propositions emerged from the first phase to test further in a realist review:

1. Appreciate and build **identity** between members of a community
2. Develop individual and community **coherence**
3. Provide physical and personal **space**
4. Reframing from '*what is wrong*' to '*what is strong*'

These four emerging propositions will now be further developed into CMO configurations and a purposive search for and appraisal of the evidence to support them will be undertaken in Phase2 of the research.

Keywords: Community Development, health, wellbeing, realist evaluation, context, mechanism, outcomes.

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AN 'OMICS APPROACH TO QUANTIFY CHANGES IN MICROBIAL FUNCTION IN RESPONSE TO CHANGING NITROGEN SUPPLY AND EXTREME DROUGHT

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Abstract

Climate change is expected to increase the frequency and severity of droughts in the UK. Soil health is likely to be negatively impacted by these extreme events. It is therefore important to understand the impact of drought on soil functioning and the delivery of soil-related ecosystem services. This study aimed to assess the resilience and change in physiological status of the microbial community under extreme conditions using novel biological analysis techniques – complex lipidomics and untargeted primary metabolomics as well as identify changes in microbial community structure using phospholipid fatty acid (PLFA) profiling. Samples were collected during an extreme drought event and post-drought from a grassland site with two grass species AberNiche *Festulolium* and AberEcho with contrasting rooting strategies and at two nitrogen (N) loading rates (0 and 300 kg N ha⁻¹ yr⁻¹). Control plots were irrigated throughout the drought at a rate of 50 l m⁻² week⁻¹. PLFA results showed there was a distinct shift in microbial community between drought and post-drought conditions, primarily driven by N loading ($p = 0.001$) and water deficit ($p = 0.022$). Complex lipid analysis identified 1246 compounds and untargeted primary metabolomic analysis identified 440 compounds. Both complex lipid and primary untargeted metabolomic data showed a number of compounds with the potential to act as biomarkers for drought conditions. Additionally, triacylglycerols (TAGs), often used as storage in lipid droplets (LDs) in eukaryotes were found in greater concentrations during drought conditions. Recovery of the lipidome and metabolome to control levels post-drought was rapid. Considerable changes in primary metabolomic and lipidomic concentrations shown in this study are likely to be directly related to the ability of the microbial and plant community to function under stress. Our findings therefore demonstrate the potential for these novel microbial indicators of soil health and function. As well as the need to further understand the biological stress response of LDs and TAG metabolism.

Keywords: Complex lipids, primary metabolomics, PLFA, soil quality, climate change.

DEVELOPMENT OF A NOVEL FASCIOLA HEPATICA FEC KIT

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Abstract

Liver fluke costs the global agricultural sector £3 billion/year in production losses, treatment costs and carcass condemnations^[1], and current diagnostic methods available to farmers are complex, expensive, time-consuming and involve a vet or research laboratory.

My project seeks to develop a pen-side kit for farmers to use to make a rapid diagnosis of active liver fluke infection in their livestock. The test will help inform treatment decisions, be economically beneficial and improve farm animal health and welfare. Beyond this, vets and animal health specialists could use the kit to provide a robust diagnostic service for their customers. My plan is to:

- Optimise a current technique to work for detecting liver fluke by developing a protocol taking the 'best-bits' from current methods
- Validate the technique in the lab by using known infection status samples to determine the accuracy of the test and then trial it on participating farms
- Monitor in-flock prevalence of disease throughout the grazing season and develop a control strategy for farmers

The impact of this project is farmers (and vets) will have a new tool they can use to monitor and improve the health of their animals, reducing parasitic infections, use less drugs and farm more economically efficiently.

Keywords: Faecal egg counting, liver fluke, farm animal health, diagnostics.

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TOWARDS THE REALISATION OF POLYMER OPALS AS NEXT GENERATION FUNCTIONAL MATERIALS

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Abstract

Polymer opal (PO) thin films, arrays of core-shell (CIS) particles (fig. 1), exhibit structural colour. This iridescent phenomenon appears throughout nature in butterflies (fig. 2), birds, and berries. Structural colour is caused by constructive Bragg diffraction^[1,3] from ordered structures described by a periodic refractive index function^[3] - it is angle dependent, strain tuneable, and more saturated than pigments and dyes. With particle diameters of 100-400nm^[4] POs can be engineered to facilitate UV, visible, and infrared reflection^[3]. As a result, POs show promise as optical coatings and filters.

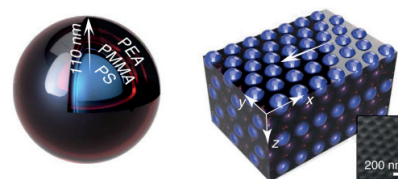


Figure 1: Polymer opal nanoparticles form highly ordered hcp structures^[1]

POs can be manufactured from a range of materials. They primarily comprise of polystyrene (PS) cores with a polyethyl-acrylate (PEA) shell, cross-linked by a polymethyl-methacrylate (PMMA) interlayer^[5] (fig. 1). This is achieved using emulsion polymerisation (EP), where polymer chains are grown within protective micelles. However, the variation in process replicability has been a barrier to large scale production. One challenge to process development is the lack of understanding around the creation of particle growth sites. Preliminary research suggests growth sites have an 'active lifetime' during which particle growth can occur. Understanding growth behaviour will aid process optimisation, and allow for the synthesis of particle sizes for specialised PO applications.

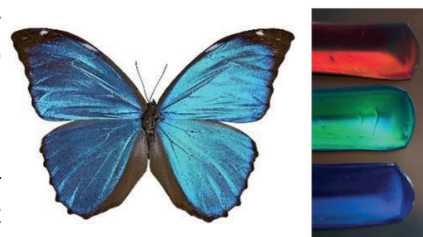


Figure 2: Structural colour from a morpho butterfly^[2] and various polymer opals^[3]

Once the PO particles have been manufactured, they are melted and extruded into ribbons^[1]. These are laminated and subsequently processed around heated rollers to form thin films. This bending induced oscillatory shear (BIOS) orders the films^[5]; beginning at the edges, and penetrating into the structure with further processing. POs are known to equilibrate at maximum order with 40 BIOS passes, which has been observed with scanning electron microscopy. Increased structural order intensifies structural colour and an almost 100% increase in the saturation of colour from POs between 1 and 40 BIOS passes has been observed.

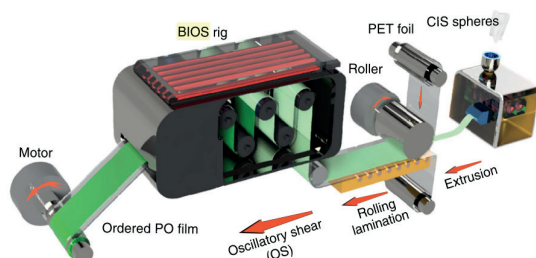


Figure 3: BIOS processing using heated rollers, resulting in ordered PO thin films^[1]

Further measurements are aimed at fully characterising the light scattering behaviour of POs, with particular focus on transmission, colour hue, and saturation. This will be achieved by performing bi-directional light scattering goniophotometry, polarised light ellipsometry, and hemispherical scattering measurements through the use of an integrating sphere.

It is envisioned that from this research POs will be engineered to achieve industry specific goals; such as through use as solar cell coatings as a mechanism of improving efficiency and photostability. This requires refinement of EP; finesse of the BIOS process; and characterisation of PO light scattering. The use of metals and inorganics such as silica within polymer shells is also a promising avenue of further research^[5]. Spherical POs are the first step towards the development of fully scalable methods and principles applicable to more complex architectures

on a scale that has been mechanically prohibitive. It is hoped once this is achieved, POs will be attractive to industry and find application as a versatile technology.

Keywords: polymer, structural colour, ordering, structural assembly, emulsion polymerisation, thin film interference

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CLASSROOM TO CAMBODIA: RESILIENCE ON OVERSEAS EXPEDITIONS

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Abstract

Introduction: Substantial literature exists supporting the benefits of resilience for optimal human functioning (Masten & Wright, 2010), with settings such as expeditions shown to provide an environment where resilience can be developed (e.g., Ewert & Yoshino, 2011; Stott et al., 2013). However current literature on the definition of resilience is beset with inconsistencies (cf. Bryan et al., 2017), with resilience measures that are either inadequate, or only emphasize certain parts of what resilience means (cf., Bryan et al., 2017; Windle, 2011). Further, although expedition research has shown there are psychological benefits to them (e.g., Mutz & Müller, 2016; Neill & Dias, 2001), results regarding resilience outcomes from expeditions are mixed (Skehill, 2001), and often contain methodological limitations such as; a lack of control group, being snapshot in nature, only examining one expedition, and employing inadequate measures (cf., McElligott et al., 2012; Mutz & Müller, 2016).

Aims of research programme: To overcome limitations of the research literature related to resilience and expeditions, and, based on the needs of the company partner (Outlook Expeditions), we developed a resilience model encompassing the mechanisms of resilience and domains of functioning. Specifically, we view resilience as a process of being pro-active and reactive (cf., Fletcher & Sarkar, 2016) and thus that resilient individuals can anticipate, plan for, manage, and then bounce-back from challenges (Alliger et al., 2015; Chen et al., 2015). We then used this model to develop and subsequently test a resilience scale, and then we will go on to design an intervention for use with overseas expedition teams to prepare young people for an expedition, as well as enhance the psychological benefits they gain from the expedition.

Method for scale development: From the literature, we created a large pool of potential items. After following a rigorous process to assess validity and reduce it (cf. McEwan et al., 2018; Smith et al., 2008) we ended with 20-items to use across five domains (making a 100-item measure) on a four-factor model of resilience processes (i.e., anticipate, minimize, manage, and mend). Domains were separated by instructional vignettes into general, physical, social, cognitive, and emotional contexts (e.g., Cassidy, 2016). We recruited 181 High School students ($M_{\text{age}} = 16.8$ years, $SD = .74$ years) on their final preparation day before leaving for an expedition. To explore the factorial validity of the scale, a Bayesian approach to structural equation modelling (BSEM) was employed.

Results: BSEM showed excellent fit for the four factors across each five domains after being reduced to a 13-item model within each domain (65-items in total). Associations between subscales were generally as expected.

Discussion: We have preliminary evidence for acceptable psychometric properties of the Resilience Process Scale (RPS) model. Current research is testing these results with other samples. Furthermore, a resilience training intervention based on the Bangor model of resilience is being piloted during expedition training weekends, prior to the students going on expedition.

Keywords: Bayesian structural equation modelling, Outdoors, Psychology, Resilience, Wellbeing

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SERVICE USERS' EXPERIENCES OF ACCESSING MENTAL HEALTH SERVICES

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Abstract

Research by Lever and Geurts (2016) found that 79% of individuals with Autism Spectrum Disorder (ASD) met the criteria for a psychiatric disorder at least once in their lives. This evidence suggests that a large proportion of individuals with ASD will experience mental health difficulties and may subsequently require support from mental health services at some point.

Recent research conducted by Camm-Crosbie et al. (2018) suggested that service users with co-existing ASD and mental health disorder felt that professionals had a poor knowledge of ASD and needed better training in ASD. Additionally, it was argued that lacking understanding/knowledge in professionals could act as a barrier to a service user accessing the most appropriate treatment/support^[1].

This study has three aims: (1) to explore the needs of service users with co-existing ASD and mental health disorder, (2) to establish whether Adult Mental Health Services in Cwm Taf University Health Board (CTUHB) fulfil these identified needs, and (3) to evaluate the knowledge and understanding of ASD amongst staff working within Adult Mental Health Services in CTUHB.

This project consists of 2 phases and has a mixed methods design. Phase 1 involves the undertaking of focus groups/individual interviews (either online or face-to-face) with service users with co-existing ASD and mental health disorder to identify the needs of service users. Phase 2 firstly involves the distribution of a questionnaire to staff working within Adult Mental Health Services to measure knowledge and understanding of ASD. There will later be an opportunity for ten members of staff to take part in a follow-up focus group to explore staff perceptions of their knowledge of ASD in relation to the service user feedback from Phase 1.

The needs of service users with co-existing ASD and mental health disorder will be identified, and whether these needs are being met by CTUHB will be determined. Staff knowledge of ASD will also be established. Based on the above findings, recommendations for CTUHB's Mental Health Service will be developed and presented.

Keywords: Autism Spectrum Disorder, Mental Health, Mental Health Services, Neurodevelopmental Disorders, Co-existing Conditions, Adults, Focus Groups, Individual Interviews, Questionnaire.

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ALTERNATIVE SYNTHESIS OF AJOENE IN CONTINUOUS FLOW

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Abstract

Garlic and its extracts have shown to possess a range of biological properties. Ajoene is a compound that can be obtained from garlic and has been linked to the prevention of stroke, coronary thrombosis and atherosclerosis. Despite its medicinal utility, there are only two reported syntheses of ajoene. The first by E. Block et. al. where ajoene is obtained via a thermal rearrangement from allicin^[1]. Due to the nature of the rearrangement, ajoene is obtained as one component in a mixture of other rearrangement products. Since the route is not selective for the desired product, purification is challenging. The second method to obtain ajoene is a chemical synthesis reported by F. Silva et. al. in 2018^[2]. Although selective for the desired product, the batch synthetic route utilises selenium to install the terminal allyl functionality. Thus, there are concerns of both toxicity, low atom economy and high waste. This work presents the possibility of an alternative route that is selective for ajoene that starts from readily available and inexpensive starting materials. The alternative synthesis eliminates the use of selenium and thus, presents higher efficiency and atom economy. The batch synthesis has been proven and is currently being translated into a continuous flow system. Continuous flow offers advantages such as that volatile intermediates are contained within tubing, mixing efficiency is significantly increased, and reaction times can be greatly reduced.

Keywords: Innovation, technology, research projects.

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DEFINING VALUE AND VALUE-BASED HEALTHCARE

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Abstract

Background

There are increasing incidences of cancer occurring within Wales, as such considerable focus has been on providing excellent care within the cancer care setting to improve outcomes of those affected [3]. To achieve this, current healthcare policy has encouraged a movement from the purely volume-based approach of the past, to that of a value-based approach. There is a plethora of literature on the various definitions and arguments concerning the concept of Value-based Healthcare. However, there is a lack of critical exploration into the different definitions, the factors that influence these, and thus a true consensus around Value-based Healthcare. A crucial aspect in achieving this is ensuring that patient and citizens values are considered in the value assessment of 'value'. Therefore, this PhD is to be conducted in partnership with Velindre NHS Trust to explore Value-based Healthcare in terms of their development of more sustainable methods of patient education/information conveyance to ensure they are based upon patient and citizens values.

Aim and Objectives

The overall aim of the PhD is to develop an evaluative criteria for future education and activation programmes based on patient and citizens values, so as to uphold the practicing of value-based care and thus achieve quality healthcare. However, this abstract is focused on the projects first set of objectives which are to compare definitions of value and Value-based Healthcare held by stakeholders in Velindre NHS Trust, to establish how they came to hold their perspective and to establish their awareness of alternative definitions of these principles.

Proposed Methods

A purposive sample of stakeholders throughout clinical and non-clinical areas in Velindre NHS Trust will be gathered. Semi-structured interviews, that will be audio-recorded, will be conducted and the resultant data will be analysed via Nowell et al., (2017) thematic analysis approach.

Expected Outcomes

This study will facilitate the establishing of a working definition of value in the cancer care setting and serve to identify communication difficulties that could arise when value and Value-based Healthcare are discussed in further studies within the PhD. It will inform the shaping and refining of subsequent studies within the PhD and facilitate the development of a robust evaluative criteria for education sessions in Velindre NHS Trust. As a result, this will support Velindre NHS Trust in establishing more sustainable methods of education/information conveyance that are co-produced with patients and citizens and are, as such, in line with Prudent Healthcare (2015).

Keywords: Value, Value-based Healthcare, patient education, patient activation.

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BIOREFINING OF STEEL MANUFACTURING CO-PRODUCTION GASES

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Abstract

Steel manufacturing is a greenhouse gas (GHG) intensive industry with Port Talbot steelworks contributing to over 15 % of Wales' total GHG emissions. Steel is a necessary material for continued global economic development. In 2015, government officials across 195 countries adopted the first legally binding global climate deal in the Paris agreement to manage increasing global temperatures and emissions. Aims included holding the increase in the global average temperature to below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C. On 08th October 2018 the IPCC released a report predicting global temperatures would reach the crucial threshold of 1.5 °C by as early as 2030. Should this be prevented, GHG emissions from industrial processes, transport and energy production need to be drastically reduced or recovered.

The aim of this research was to develop technology for the continuous conversion of surplus industrial carbon dioxide and carbon monoxide to chemicals to produce bioplastics, chemicals and coatings. Sewage sludge from wastewater treatment plants contains bacteria with the ability to grow on carbon dioxide and carbon monoxide and convert the gases to acetic acid, a useful building block chemical. Sludge from an anaerobic digestion plant in South Wales was used to inoculate 1 L reactors with 200 mL working volume to test whether the bacteria could directly convert industrial off-gas streams. Results showed the bacteria were robust and resistant to contaminants and varying conditions. The process was then optimised and scaled up to 150 L pilot scale plant situated on TATA steelworks and fed directly from the blast furnace gas. Should the process be successful it will permanently trap the carbon, therefore reducing the global warming potential and emissions of the steel industry.

The production of acetic acid is a process that has previously been overlooked in favour of ethanol production due to the difficulty of extracting the acetic acid from nutrient rich streams at low concentrations. A combined membrane technique using PTFE membranes and electro dialysis (ED) has been developed and is currently being tested on working bioreactors. The membrane process could offer in situ extraction of organic acids coupled to bioreactors, which has not yet been achieved on an industrial scale.

Keywords: Greenhouse gas, carbon dioxide, industry, acetic acid, steel manufacturing, sustainability, global warming.

DATA-DRIVEN BIKE FITTING

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Abstract

As cycling is gaining popularity rapidly worldwide, research in this sport on pro cyclists, as well as amateur cyclists, is very important. Your position on the bike is crucial to ride injury free and in an efficient manner. A lot of people saw the potential and started to conduct bike fits. These are specific services offered by a wide range of professionals, such as kinesiologists, sport scientists, general practitioners, etc. to adjust the configuration of the bike to your individual needs. There are many bike fitters, and from our experience we found that they often focus on other aspects of the cycling movement. This might be due to their different backgrounds, experience levels or personal beliefs.

To solve the expert subjectivity problem, and to improve the overall fitting process, we started a research project to develop a methodology to perform automatic bike fitting based on novel data-driven decision-making processes. The data is provided by the Bioracer Motion motion capture system, which consists of two arrays of three high-speed infrared cameras which capture positional data of the active infrared markers on the cyclists' body.

The dataset consists of over 350 annotated data points, each data point is a recording of 15 seconds of the cycling movement. Novel machine learning techniques are used on this dataset to construct a prediction algorithm for new data. Preliminary experiments^[1] have showed the feasibility of our proposed methodology and provided the needed evidence that an automatic bike fitting system is possible.

We conduct this research project in cooperation with Bioracer Motion and with the support of VLAIO. This company is founded by Raymond Vanstraelen (founder Bioracer), Pieter Mertens (general practitioner and former pro cyclist) and Jeroen Dierckx (former head software engineer at Telenet). Together they developed the Bioracer Motion system because there was no other system on the market that could measure what they wanted to measure. Their focus in bike fitting has always been on symmetry and stability, this originated from the ideas of Raymond, who was the first bike fitter that used video as an analysis tool 30 years ago.

With 10,000 bike fits, Raymond is one of the most experienced bike fitters around the world. We can proudly say that we have the most advanced tool to do cycling movement analysis. But still, the tool is only as good as the bike fitter working with it. Therefore, our main focus is to educate the people within the cycling community about bike fitting and the possible consequences. Our goal is that all bike fitters who use the Bioracer Motion system advice the same optimal cycling position for an individual. This research project will provide Bioracer Motion with an automated virtual bike fit assistant to advice the bike fitter and even do stand-alone bike fits when no expert is available. In the end the system should be available to bike shops so when their client buys a new bike, they also get a bike fit to get the most out of their cycling training.

Keywords: Bike fitting, cycling, innovation, motion capture, infrared, data science, machine learning.

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THE IMPACT OF LOADING RATIO, COLUMBIC EFFICIENCY AND TEMPERATURE ON AMMONIA REMOVAL AND RECOVERY FROM SOUR WATER

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Abstract

In recent years (bio)electrochemical systems emerged as a more energy attractive alternative to recover total ammonia nitrogen (TAN) from wastewaters, mostly urine and digestate^[1]. These waste streams typically contain up to 5 g TAN/L. For this technology, to actually make an impact on the currently disrupted nitrogen cycle, developing a technology for a more concentrated point source of ammonia could be more interesting. In this paper we propose to use sour water (15 g TAN/L), generated during the gasification of coal as a potentially interesting ammonia point source. We propose to update the currently existing Ammonia Kreislauf Wäsche (ASK) process, which currently recovers sulphur and removes ammonia^[2]. By adding an electrochemical cell (EC) in combination with membrane stripping technology, the energy and steam demand of this process can be reduced, as well as the recovery instead of removal of ammonia is established. The performance of this type of systems depends on several parameters, such as current density, TAN loading, pH and Temperature. The interaction between these different factors needs to be understood in order to achieve maximum efficiency at minimal energy input levels. A technical installation, consisting of an EC (projected surface area 0.04 m²) coupled to a membrane stripping unit, was operated at current densities from 100 to 500 A/m², loading rates varied from 70 g to 240 g TAN/m² h and temperature ranged from 25 to 90 °C. Preliminary tests have shown that a loading rate of 70 g TAN/m² h required the smallest amount of energy per kg of Nitrogen that was removed.

Keywords: Nitrogen recovery, sour water stripping, membrane stripping, coal-gasification, process development

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INTELLIGENCE ENABLED FACTORIES OF THE FUTURE

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Abstract

What: Developing methods, applications, use-cases and research towards equipping the manufacturing industry with intelligence enabled tools to assist the design process, improve the working conditions, increase the yield of the assembly. Intelligence enabling consist of deriving models of some process in the factory or product lifecycle. Combining the models and available data into a seamless integrated framework, and use the ensemble to optimize the whole and improve the selected key performance indicators. The optimization itself can be done with classic optimization routines or data-driven, machine learning approaches.

Why: Manufacturing industry faces stringent consumer requirements of mass customization demands. To remain profitable, unit costs need to be low even when lot sizes shrink. This trend is observed in the whole industry. To remain profitable, manufacturing leaders are looking for ways to incorporate and solidly new, emerging digital technology in as much industrial processes as possible. The goal is to reduce lead times, costs, inefficiencies, defects,... in environments that are becoming increasingly dynamic as demand fluctuates and consumer trends shift.

How: Most companies active in manufacturing have a digital innovation plan, usually denoted as "Industry 4.0" to incorporate digital technology into their factory. Yet, many are struggling on implementation aspects such as: what manufacturing data should be logged? How can it be made accessible? What insights can be gained from them? Also information barriers exist: what technology is out there and what can be (re-)used? To tackle these questions, at Ghent university we collaborate intensely with the Flanders Make organisation which brings together the common industrial needs of manufacturing companies with university researchers.

When: We are working with some big companies such as Atlas Copco, Siemens, Case New Holland as well as Flemish small and medium-sized enterprises in fundamental research projects lasting four years, as well as two year projects with the goal to apply scientific findings directly into added value for companies. In the project "Product and Assembly Co-design (PACo)", launched in September 2018, we are working on jointly optimization of product and assembly design with human-machine interaction.

Keywords: Industry 4.0, Manufacturing, Modelling, Optimization.

PREPARATION OF ESTERS BY HOMOGENOUS AND HETEROGENEOUS CATALYSTS

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Abstract

Many research groups looking for a new kind of renewable fuel, which could replace the fossil fuel. Biodiesel (mixture of methyl esters of higher fatty acids) is one of alternative fuel to petroleum diesel and can be the solution to increasing world fuel consumption. Biodiesel is non-toxic, biodegradable, and sulphur-free fuel. It can be prepared from triacylglycerides, which are contained in vegetable oil, animal fats or waste cooking oils, by transesterification with alcohol (methanol, ethanol and butanol). Transesterification is a reversible reaction, therefore, the excess of alcohol is used to shift reaction towards the products and it has to be stopped after reaction time^[1]. The transesterification is usually catalysed by a homogeneous catalysts, because these catalyst are relatively cheap and high efficiency, but they are not possible to reuse. Moreover, they react with oil and acids and forms soaps, which decrease the yield of esters, make the separation difficult and also consume the catalyst. The homogeneous catalyst cannot be separated from the reaction mixture and has to be removed by washing off^[2]. The reusable types of catalysts such as heterogeneous catalysts are studied today. These catalysts can be separated from reaction mixture by filtration. Between heterogeneous catalysts belong mixed oxides such as Ca-Al, Ca-Zr, Mg-Fe, etc.^[3].

My research is focused on the study of alkali homogeneous (KOH) and heterogeneous (Mg-Fe mixed oxides) catalyst in the transesterification of rapeseed oil, especially. The transesterification was carried out in a batch reactor in our laboratory and also in a fixed bed reactor in company Unipetrol Centre for Research and Education (Litvínov-Záluží), which we compare. The transesterification was carried out with three types of alcohols in batch reactor (methanol, ethanol and butanol) and with methanol in fixed-bed reactor. The main aim is prepare esters, which fill the European norm EN 14214, especially esters with low content of fatty acids. The transesterification had to be stopped by neutralization of the catalyst after the reaction time. One possibility is stopped by weak acid gaseous CO₂, which is not able to convert soaps (formed by side reaction) to fatty acids. However, the prepared methyl ester does not fill the norm (water and potassium content is above the norm)^[4]. Other possibility is used inorganic acid (for example H₃PO₄) and if the acid is added until pH felt down approximately 2-3, then fatty acids are formed from soap. The formed fatty acids can be neutralized by Ca(OH)₂. The formed calcium soaps are separated by centrifugation^[5]. If the acid is added accurately then the fatty acids are not formed and the acid number remains almost zero. Moreover the obtained methyl ester fills the norm EN 14214^[6].

Other part of my work is focused on heterogeneous catalysts. A several types of mixed oxides, with various types of metals and of synthesis, were used as heterogeneous catalyst for transesterification. All synthesized materials were characterized by several techniques such as XRD, thermogravimetric analysis, specific surface area and SEM. The relation between structure/composition and activity/selectivity/stability will be studied in the model reactions.

Keywords: biodiesel, transesterification, homogenous catalyst, heterogeneous catalyst

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AN URBAN CONSOLIDATION CENTER AS A SOLUTION TO THE LONG-TERM CITY LOGISTICS PROBLEMS IN THE CZECH REPUBLIC CITIES

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Abstract

Nowadays the impact of logistics activities in the cities is closely followed in many European cities as well as in the Czech Republic. Freight transport in cities affects nearly all aspect of residents' life. The negative impact of freight transport in cities caused mainly by the growing demand of end-customers, not only affects ecological situation in the cities, but also social and economic. The previous studies and authors' experience indicate poor knowledge of problems generated by freight transport in cities. Along with well-known ecological problems such as air pollution, noise, vibrations and climate changes, there are also social problems like congestion and an increased risk of traffic accidents. Economic situation in cities could also be affected by unsustainable freight transport, for example, it could be higher funds that local authorities need to spend on road transport and road maintenance, higher logistical costs that end-customers pay or economic competitiveness of urban areas that could be damaged due to the uncontrollable traffic situation in this area. Negative externalities mentioned above are difficult to identify and calculate, as local authorities very often do not have the information about numbers of freight cars, which are circulating in each city every day. As a result, with the e-commerce growth, the end-customers require their order to be delivered as soon as possible and force the transport companies to provide inefficient delivery. Because of above a lot of trucks from different transport companies circulating in cities every day and more important, the key indicator for truck loading is the number of stops not the load factor. The problems mentioned before is mostly the reason of a high interest in the city logistics methods. City logistics can be characterized as a complex system aims to achieve a sustainable way of arranging transportation activities in cities. Unfortunately, current studies are focused on the effective last mile delivery, however, the most common solutions like vehicles using alternative fuels or the electric vehicles for supplying the cities are not enough anymore. There is a need to focus on the total number of vehicles in cities as well as sufficient use of loading space of these vehicles. It is very important to use different measures of city logistics, but sustainable development could be achieved just by creating a synergy effect of those. An urban consolidation center (UCC) could be a great example of it. UCC can be identified as a consolidation center in the city or close to the area, it will be serving. The main purpose of UCC is reducing part deliveries with unappropriated low loaded trucks into an urban center. Under the condition of using UCC, it is possible to reduce the number of vehicles need for supplying the city, use more environmental-friendly vehicles and provide additional services for the receivers. That is the reason why, so high attention is being paid to UCC in cities all over the world. At the current moment, there are different publications about examples of UCC in different cities, but a big part of attempts of providing functional UCC fails. This article aims to provide an analysis of critical criteria, the fulfillment of which is necessary to build and operate an UCC in the Czech Republic. As the Czech Republic does not have the experience with UCC in any city yet, the analysis will be provided from the foreign experience. Also, the article aims to identify and describe the most important areas, that need to be concerned before the UCC is implementing.

Keywords: city logistics, urban consolidation center, sustainability, analysis.

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SELECTIVE OXIDATION OF METHANE TO METHANOL OVER BINUCLEAR SPECIES IN ZEOLITES

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Abstract

Zeolites represent the largest group of heterogeneous catalysts apply for fluid catalytic cracking, selective catalytic reduction of hydrocarbons, and for NO_x abatement. Recently, it was shown that iron-exchanged zeolites (*BEA and ZSM-5) effectively stabilized active oxygen from N₂O, which can be further used for oxidation of methane to methanol^[1]. Our previous results supported by DFT calculation reveal that binuclear Fe species in ferrierite (FER) are responsible for easier splitting of N₂O and stabilization of active oxygen (Fig. 1)^[2, 3]. The aim of this work was targeted at preparation of the binuclear Me (Me = Co, Ni, Mn) centers in FER and FTIR analysis of their redox properties in selective oxidation of CH₄ originating from N₂O.

Fully ion exchanged FER (Me/Al 0.33) guarantees the highest concentration of binuclear species^[4]. Co-, Ni-, and Mn-FER (FER, Si/Al 8.6, Tosoh Comp.) with the highest loading of binuclear species were prepared using ion exchange (Co-FER) or impregnation (Ni- or Mn-FER) method^[5]. Chemical analysis confirmed that Me/Al ratio of prepared Me-FER exceed 0.3. Redox behaviour of Me-FER was monitored by in-situ FTIR spectroscopy. FTIR spectra were recorded after i) evacuation at 450 °C, ii) oxidation by N₂O at 200 °C, and iii) methane interaction at 200 °C with previously N₂O oxidized samples.

FTIR spectra of dehydrated samples exhibited the band at around 920 cm⁻¹, which confirms the location of Me(II) in binuclear species. Interaction of Me-FER with N₂O, resulting in the shift of the band characterizing Me(II) from 920 to 870 cm⁻¹, which indicated oxidation of Me(II) to [Me(III)-O]²⁺ and formation of active oxygen form on the Me cation. The interaction of N₂O oxidized Me-FER with CH₄ shift the band from 870 to 920 cm⁻¹, which confirms the complete reduction of the [Me(III)-O]²⁺ species by CH₄. FTIR spectra after interaction with CH₄ reveals the presence of the additional bands at 2960, 2853, and 2920 cm⁻¹ attributed to formate, methanol and methoxy, respectively.

FTIR in-situ studies confirmed that binuclear transition metal species (Mn, Ni and Co) stabilized in FER split of N₂O and stabilized active oxygen from, which can oxidize methane to oxygen containing organic products.

Keywords: zeolite, ferrierite, binuclear species, nickel, cobalt, manganese, methanol, catalysis.

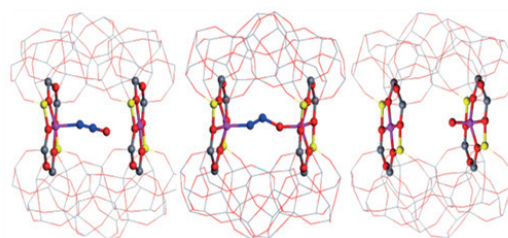


Fig. 1. N₂O splitting over binuclear Fe centres in FER.

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SYNTHESIS OF THE PROPARGYL ALCOHOL CONNECTION PRESENT IN ALFAPROSTOL Ω -CHAIN

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Abstract

Prostaglandins are a group of lipid mediators with multiple pharmaceutical and veterinary applications. Their synthesis includes a complex multi-step pathway with over 20 steps and high associated production costs.

Cayman Pharma s.r.o., located in Neratovice, Czech Republic, is specialized in the synthesis of Prostaglandins Active Pharmaceutical Ingredients (API) for the last 30 years. Currently, Cayman Pharma represents an important source of API for the treatment of glaucoma, erectile dysfunction, and pulmonary hypertension as well as API used in veterinary field as luteolytic agents.

The collaboration between the Institute of Organic and Technology of Pardubice University and Cayman Pharma s.r.o. started in 2012 and aims the study of improved strategies for the synthesis of prostaglandin analogues. Alfaprostol (Fig. 1) is a nonhalogenated synthetic PGF_{2 α} methyl ester analogue with veterinary application as luteolytic agent.^[1]

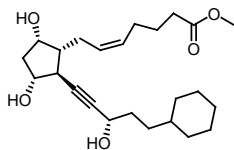


Fig.1: Alfaprostol

Current efforts are being targeted for the development of a new synthetic approach for the propargyl alcohol connection present in alfaprostol molecule. Literature described two main methodologies for the preparation of optically active propargylic alcohols, namely: asymmetric reduction of a propargyl ketone or the asymmetric alkylation of a carbonyl group.^[2] In this context, both methodologies have been considered and applied to target alfaprostol.

Stille coupling has been successfully used to afford propargyl ketone susceptible of asymmetric reduction.^[3] Presently we are focusing our effort on the direct preparation of propargyl alcohol with appropriate stereoselectivity using Corey lactone derivatives and 3-cyclohexylpropanal as starting materials.

Keywords: Prostaglandins, Propargyl alcohol, Asymmetric Reduction, Stereoselective Alkylation

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DEVELOPMENT OF A HEXANE AND HEPTANE (COMMERCIAL GRADE) PURIFICATION PROCESS

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Abstract

Hexane and heptane are solvents obtained through fractional distillation of petroleum with utility in the food, pharmaceutical and polymer industries ^[1]. Currently the methods to purify these solvents (to remove their aromatic and olefinic impurities) either don't meet the increasing demands of the market or do so by employing the use of toxic and expensive extraction agents, heavy metal catalysts and with high energy demands. For this reason, the aim of this work is to develop a novel, sustainable and environmentally friendlier process to achieve this purification so that the company to remain competitive in these markets.

In this work the solution proposed is the use of ionic liquids as extraction solvents. Ionic liquids are salts composed by large organic cations and organic/inorganic anions which are liquid below 100 °C and are perceived as green solvents. They have negligible vapour pressure, high chemical and thermal stability and can be designed for the intended separation. Furthermore, there have been studies that showed good promise for the use of ionic liquids in this separation, even when compared with the traditional processes ^[2]. It is also proposed to employ these solvents in a membrane contactor unit as this will allow for a more compact unit with operational flexibility, a large area for a reduced volume which will result in a significantly smaller solvent to feed ratio, and easy scale-up.

Since there is a large array of possible cation/anion combinations, up to 10⁶ different ionic liquids can be synthesized ^[3], the experimental characterization of these solvents stands unfeasible. Thus, the use of correlations, models and equations of state that allow the selection of those with the highest potential stands crucial. For this reason, the COSMO-RS method was employed as it allows to predict the thermophysical properties and behaviour of pure fluids and mixtures without any previous knowledge of the compounds' properties or interaction parameters, which are not fully defined for all the possible combinations. In this work, the screening of the ILs using COSMO-RS allowed to qualitatively identify the ionic liquids with the most promising separation capacity. Some promising liquids were then evaluated experimentally, which allowed to validate the method and access the impact of the cations/anions in the separation.

The next steps will consist of an evaluation of thermophysical properties like viscosity and density as they are detrimental for the application of the ionic liquids in a liquid-liquid membrane contactors unit. Further along, the choice of material for the membrane contactors will also be studied and experiments will be performed with real sampling.

Keywords: Aliphatic purification, Ionic Liquids, Membrane Contactors, Petrochemistry.

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FRACTIONATION OF MONOMERS DERIVED FROM THE LIGNIN OXIDATIVE DEPOLYMERIZATION LIQUOR USING AQUEOUS BIPHASIC SYSTEMS

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Abstract

Lignin, one of the main structural components of all woody plants, plays a significant role in the current industry framework. It is available at large-scale from the pulping liquor produced by the pulp and paper industry, representing a potential renewable resource. Nowadays, pulp and paper mills largely burn this liquor in an integrated process to produce electric and thermal energy, consequently recovering the inorganic chemical content. Although this combustion is still a valuable contribution to reduce fossil fuels consumption, lignin offers perspectives for higher added-valued applications and could be converted into several profitable commodities, a key factor for creating economically feasible biorefinery processes. This is an opportunity to transform conventional pulp and paper mills into integrated forest biorefineries that not only produce pulp and paper but also new biochemicals or biomaterials, in compliance with the recommendations for sustainable development required for the forest industry.

In this framework, oxidative processes for lignin conversion to phenolic compounds are widely recognized ^[1]. As such, in this work we propose to determine efficient ways to separate a synthetic, representative mixture of lignin's oxidative depolymerization liquor, composed of five aromatic monomer compounds: vanillin, vanillic acid, syringaldehyde, acetovanillone, and p-hydroxybenzaldehyde. This was accomplished using three types of aqueous biphasic systems (ABSs), namely polymer-polymer-electrolyte, polymer-salt and co-polymer-salt ^[2]. The identification of the partition coefficients of the different monomers in the ABSs were determined and the most performant systems selected.

Keywords: Oxidative Depolymerization, Aqueous Biphasic Systems, Ionic Liquids, Electrolytes.

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