# 3<sup>rd</sup> FERIA

The European Conference on Fuel and Energy Research and its Applications

## **Acknowledgements**

We are grateful to our sponsors for their support of this conference













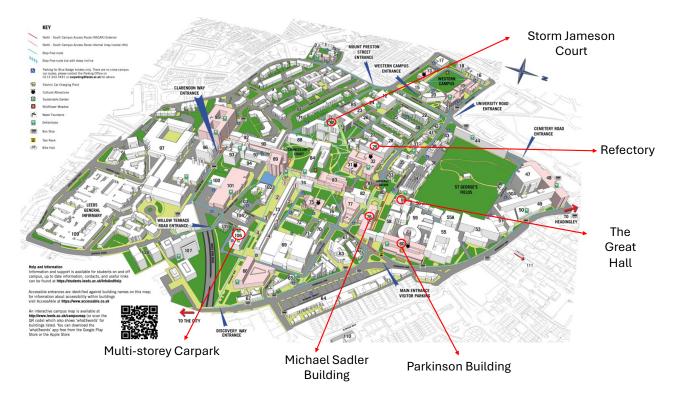
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## **Information for Delegates**

### Travel and finding your way around

The map below shows the map of the University of Leeds Campus with the important venues marked



### **Parking**

Delegates can park their cars in the multi storey car park marked on the map above on a first come first serve basis. A discounted parking rate of £7.00 per day can be achieved by using the car parking code **889891**. On arrival the delegate will need to enter the code at the, payment machine located on the first floor of the multi-storey, they will be asked to input how many days car parking is required then payment will be requested. They will be able to come and go throughout this period without incurring any additional costs.

## **Accommodation at Storm Jameson Court**

- Check in from 14:00 on the day of arrival
- Check out before 10:00 on the day of departure
- 24-hour reception service
- Fully accessible via accessible lifts
- Spacious lounge area ideal for networking and socialising
- Guest games room
- Outdoor seating area
- Complimentary use of the onsite sports centre, with a swimming pool, sauna, steam room, large fitness suite and additional sports facilities
- Complimentary wi-fi throughout
- Access to the Refectory located just 100 metres away, where Breakfast will be served
- Access to explore the University's historic, 100-acre campus, featuring impressive architecture, fountains, tree-lined walkways and gardens

## Travelling to and from the City Centre

By Bus – Leeds City Centre is well accessible from the University of Leeds with most buses going to the city centre. The timetable for the buses can be found at <a href="https://www.wymetro.com/buses/">https://www.wymetro.com/buses/</a>

## **Information for Delegates**

By Taxi – There is a taxi rank outside the Parkinson Building and the journey into the city centre would take approximately 7 to 10 mins. Uber also operates in Leeds.

By Walking – The Leeds city centre is approximately 20 minutes walk from the University of Leeds.

### **Luggage Storage and Cloakroom**

An unsecured storage facility will be available at The Michael Sadler Building on Friday, and more details can be found at the reception desk. Items are left here at your own risk.

### **Emergency Procedures**

The emergency procedures vary between rooms and buildings. The fire alarm is tested in Michael Sadler on Friday morning before 9am. The alarm will sound for around 30 seconds. In the event of a real fire alarm member of the University team will ensure that all persons have left the building and made their way to the assembly point. The assembly point is the pavement outside of Baines Wing & Great Hall. The lifts in this building are not fire lifts and should not be used in the case of an emergency. Refuge points are located at the outer stairwells. A General Emergency Evacuation Plan will be provided to you upon arrival.

## **Security and Interruption**

Please note that conference badges <u>must</u> be worn at all times (access may be denied if not worn). Both the use of mobile phones, recording, nor photography is permitted during the conference presentations, and permission should be sought from presenters if you wish to photograph their posters.

### **Smoking**

No smoking is permitted within the building, and smokers should go outside the building to smoke.

#### **Internet Access**

The information for accessing wifi will be via a QR code or SMS system. The details for this will be available at the FERIA reception desk on arrival.

#### **Badges**

Black Full attendees (all days, both dinners)

• Navy Blue One day attendees and Clean Energy Science Lecture attendees

Green Conference Organising Committee and Helpers

• Red Exhibition Trade Staff

Please return all badges (pouches and lanyards) to the registration desk before you leave the conference as they will be reused.

### **Conference Dinner**

The conference dinner will be held at Great Hall which is situated on the University of Leeds Campus, starting with a welcome drink at 7 pm on Thursday, 11th September. Please wear your badge to the dinner.

### **Site Visits**

On Thursday 11th September 2025, there will be an opportunity for conference delegates to register for one of three industrial site visits on a first come first serve basis. Safety boots will be required for some of these tours but you might be required to bring your own for others. Please read carefully which one The site visits will be as follows:

## Veolia Recycling and Energy Recovery Facility in Leeds: (maximum 30 spaces)

This tour will start at 14.00 and will last for approximately two hours. All PPE will be provided for this site. Please note that there will be a large number of steps on tour, visitors must wear trousers/ long sleeves, sensible flat soled, closed toe shoes (not trainers). Safety boots can be provided by the site if required. All other PPE will be provided by the site. No Photography/ mobile phone use allowed.

## **Information for Delegates**

## Enfinium EfW Ferrybridge. (maximum 20 spaces)

This tour will start at 14.30 and will last for approximately one and a half hours. Please note that there will be a large number of steps on tour, visitors must wear trousers/ long sleeves, sensible flat soled, closed toe shoes (not trainers). All other PPE will be provided by the site.

## Blue Phoenix Ash Recycling Facility, (maximum 30 spaces)

This tour will start at 14.30 and will last for approximately one and a half hours. Safety boots will be required for this site and you will need to bring your own safety boots. All other PPE will be provided by the site.

Registration for the site visits can be done at:

https://www.tickettailor.com/events/thefuelandenergyresearchforum1/1693175

## Introduction

### **Background**

The Fuel and Energy Research Forum has been created to bring together all those with interests in fuel and energy research, particularly biomass, waste and fossil fuels and to promote and integrate these interests in the UK and worldwide. These research areas are increasingly important as low and zero carbon- fuels continue to play a key role in the energy mix of today. These fuels provide a widely- distributed, secure and reliable source of energy that is relatively easy to obtain. Clean carbon- fuel technology is the order of the day, with particular attention being paid to carbon capture and storage in view of global warming and carbon dioxide emissions from carbon-based usage.

### Introduction

This 3rd FERIA Conference, the Successor to a long series of Forum Conferences going back to 1996 at Loughborough University, builds on the success of the previous fourteen biennial Conferences, is to be held at the University of Leeds..

### **Scope and Purpose**

The purpose of this Conference is to bring together academic researchers and participants from industry and anyone that is interested in the applications of fuel and energy research.

### **Proceedings**

All authors of accepted abstracts are invited to submit a full paper for possible inclusion in a Virtual Special Issue of FUEL to be published on the Elsevier website. The papers submitted must be prepared strictly in accordance with the Guide for Authors and must be submitted electronically via <a href="https://www.sciencedirect.com/journal/fuel">https://www.sciencedirect.com/journal/fuel</a>. When submitting your manuscript please select the correct portal for article type "VSI: 3rd FERIA 2025". The portal for submission to the VSI in FUEL will be open from the 1st October 2025. All papers submitted to the VSI will be subject to the normal peer review requirements for the journal

#### Venue

Home to just under 800, 000 people, including more than 63, 000 students at the 3 main Universities, Leeds is situated centrally in the North of England on the edge of the Yorkshire Dales. Leeds grew to become one of the largest cities in the UK following the boom of the industrial revolution and today, whilst retaining a rich industrial heritage Leeds can also be regarded as a cultural centre and the financial capital of the North. It is the only English city outside London with its own opera house, repertory theatre, and ballet companies and Leeds Art Gallery has one of the UK's best collections of contemporary British art. The city is also home to the national collection of arms and armour at the Royal Armouries. Leeds is also known as a favoured location for shoppers and with five miles of shopping streets and one of the country's largest pedestrianised zones. The city also has an excellent nightlife scene, with many restaurants and independent bars, and is widely regarded as one of the UK's best cities for dining out. This bustling and vibrant city provides an excellent base for the conference and a showcase for the North of England, Leeds also has a long sporting heritage including one of the oldest Association Football clubs in England, (Leeds United, EFL Championship League), Rugby League, (Leeds Rhinos, Super League), Rugby Union, (Leeds Tykes, National League 1), and Yorkshire County Cricket Club, the most successful cricket team in England. It is a rich, diverse, multicultural city which is proud of its reputation for being one of the friendliest and safest major cities in the UK

Leeds is a particularly well- chosen location for this 3rd FERIA Conference as energy research is a core activity at the University of Leeds. It is home to the University's Energy Leeds which encompasses many institutes and research themes across the University, including, Energy Transition and Net Zero, School of Chemical and Process Engineering, Institute for Thermo fluids, School of Mechanical Engineering, Cities, Infrastructure and Energy, School of Civil Engineering, Water, Public Health and Environmental Engineering, School of Civil Engineering, Preistley Centre for Climate Futures, Institute for Transport Studies, Institute of Communication and Power Networks, School of Electronic and Electrical Engineering, Sustainability Research Institute, Agri-Energy systems. Global Food and Environment Institute, Geosolutions Leeds, Policy Leeds, where the research within these centres all fit well with the themes of the Conference.

# Committee

## **Conference Organising Committee**

Prof Bill Nimmo	Conference Chairman	University of Sheffield
Dr David McCaffrey	Conference Finance Officer	McEnergy Consultancy
Dr Bijal Gudka	Conference Committee Secretary and Conference Manager	Gudka Energy Consulting
Mrs Jill Nimmo	Assistant Conference Manager	
Dr Andrew Goddard	Sponsorship Officer	Freeland Horticulture Ltd
Dr Carolina Font-Paima	Publicity Officer	University of Hull
Prof Jenny Jones	Main Local Organiser	University of Leeds
Dr Andrew Ross	Conference Programme Group and Local Organiser	University of Leeds
Dr Junfeng Yang	Local Organiser	University of Leeds
Prof Meihong Wang	Head of Conference Programme Group	University of Sheffield
Prof Ed Lester	Conference Programme Group	University of Nottingham
Dr Meisam Babaie	Conference Programme Group and Local Organiser	University of Leeds
Dr Will Quick	Industrial Representative	Uniper Technologies Ltd

# Outline Programme Wednesday, 10<sup>th</sup> September

## Wednesday 10th September 2025

08.00 Arrival and registration (Refectory)

Opening Session: Rupert Beckett Lecture Theatre, Michael Sadler Building, 09.00–10.50

- 09.00 *Opening address:* Prof Bill Nimmo, 3<sup>rd</sup> FERIA Conference Chairman.
- 09.05 **Welcome address**: Prof Catherine Noakes, Professor of Environmental Engineering for Buildings, The University of Leeds
- 09.10 *Plenary presentation:* David Parkin, Director at Progressive Energy Ltd
- 09.50 Keynote presentation 1: Conversion of Woody Biomass Waste (African invasive plants and hardwoods) to Hydrogen-rich Syngas and Briquettes
   Prof Micheal Daramola, University of Pretoria, South Africa
- 10:20 Keynote presentation 2: Optimal Control of Solvent-based Carbon Capture Process Integrated with Coal-fired Power plant

Prof Xiao Wu, Southeast University, China

- 16.30 **Poster Session 1**: The Refectory
- The 6<sup>th</sup> Clean Energy Science Lecture: Rupert Beckett Lecture Theatre, Michael Sadler Building
   Biomass versus Coal: Some of the challenges and prospects"
   Professor. Jenny Jones, Past EPSRC Advanced Research Fellow and a Professor in Sustainable Energy at the University of Leeds.
- 18.30 **Poster Session 2 and Poster Reception and Buffet Dinner**: The Refectory

	Session 1A Bio-Char – Rupert Beckett Lecture Theatre	Session 1B Hydrogen/Ammonia – LG15	Session 1C OPTIMAL – LG19
	Session Chair – Dr Will Quick	Session Chair – Dr Carolina Font-Palma	Session Chair – Prof Meihong Wang
11.20	Evolution of Biochar Structure and Porosity with Temperature and its Impact on Metal Adsorption Nura Garba, University of Nottingham, UK	Potential of the Co-Products of Blue, Green, and Turquoise Hydrogen – A Process System Analysis Usman Ali, <sup>1</sup> Net Zero Industry Innovation Centre, Teesside University, UK	Simulation, Process Analysis and Performance Assessment of Solvent Based Carbon Capture for Refinery Mohammed Alshemali, University of Sheffield, UK
11.40	Techno-Economic and Sustainability Assessment of Lignocellulosic Biomass Conversion to Biofuel Ali Alazzawi, University of Leeds, UK	Hydrogen: the Practical Way to Decarbonise Heat by 2040 Gordon Andrews, University of Leeds, UK.	Modelling\Simulation and analysis of CO <sub>2</sub> Capture with Chemical Absorption for CCGT Power Plants Using Rotating Packed Beds with Mixed Solvent Idris Jibrin, University of Sheffield, UK.
12.00	A practical approach to determine self-heating tendencies in biomass stored in bulk quantities Baldeep Kaur, The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, UK	Efficient Low Carbon Ammonia Production through Combined Biomass Gasification, Nitrogen Self-Sufficiency, and Waste Heat Recovery Kazeem Mohammed, (EBRI), Aston University, UK	Study of Optimal Operation of Ethylene Plant Integrated with Carbon Capture Through Artificial Intelligent based date-driven modelling and Optimisation  Jin Ma, University of Sheffield, UK
12.20	The potential of hydrothermal carbonisation as a pre- treatment for thermochemical and biochemical conversion  Andy Ross, University of Leeds, UK	Planning Industrial Hydrogen Demand through Optimisation Modelling  Matthew Lovelady, University of Hull, UK.	Modelling\simulation, optimisation and performance assessment of large-scale rotating packed bed (RPB)-based post combustion carbon capture (PCC) process using concentrated MEA for large scale combined cycle gas turbine (CCGT) power plant  Abiodun Tolulope Okeleye, University of Sheffield, UK
12.40	Morphological Analysis of Biomass wood Pellets Using Scanning Techniques Veronika Savchenko, University of Nottingham, UK	Carbon Negative Biochar and Hydrogen Production via Integrated Pyrolysis – Chemical Looping Combustion (PyCLC) Fatih Gulec, University of Nottingham, UK	Hybrid modelling\simulation and techno-economic performance assessment of direct air capture integrated with post-combustion capture using different solvents for ethylene plant Yao Zhang, University of Sheffield, UK
13.00	Lunch	<u>l</u>	1

	Session 2A Biomass/Waste 1 – Rupert Beckett Lecture Theatre	Session 2B Gasification/Pyrolysis – LG15	Session 2C Emissions – LG19			
	Session Chair – Toluleke E Akinola	Session Chair – Dr Andrew Ross	Session Chair – Dr Will Quick			
14.00	Opportunities and Challenges in Process Intensified CO <sub>2</sub> capture from Biomass (BECCS)  Muhamad Akram, University of Sheffield, UK.	Pyrolysis gas and biochar generation for five woods Gordon Andrews, University of Leeds, UK	European Power Sector emissions: Are we sure Gas is better than Coal? Stewart Bradley, Uniper Technologies Ltd, UK.			
14.20	Multi-Objective Optimisation of Waste-to-Resource Management for Small-Island Developing States Keeran Ward, University of Leeds, UK.	Improving combustion and gasification performance of refuse derived fuel using torrefaction  James Banks, Cardiff University, UK	Influence of Model Butyl-based Biofuel Blending with HVO Biodiesel on Engine Performance and Emissions Katterin.S. Hernández-Domínguez, University of Leeds, UK			
14.40	Resource Assessment of Water Hyacinth in India and it's Bioenergy Potential Ryan Longley, University of Leeds, UK	Pyrolysis/non-thermal Plasma/catalysis of Waste Plastics for the Production of Liquid Fuels and Chemicals Jayden (Jie) Gu, University of Leeds, UK	Application of ammonia water in a Venturi tube Serhii Horianoi, Thermal Energy Technology Institute, Ukraine			
15.00	Characterisation of chars produced from washed and thermochemically pretreated wood biomass – an intermediate biofuel for hydrogen production Michael O Doromola, University of Pretoria, South Africa	Gasification of Whisky Distillery Waste for Distillery Heat Gordon Andews, University of Leeds, UK	Optimizing Ship Engine Performance and Emissions Under Transient Operating Conditions Richard J Brown, International Laboratory for Air quality and Health, Australia			
15.20	Utilising electrochemical hydrogenation for the mild upgrading of Pinewood and Wheat straw bio-oils Cesar Catizane, Cranfield University, UK	Direct Chemical Looping Gasification of Biochar/Biomass: A Pathway to Efficient Syngas Production  Maryam Awode, University of Nottingham, UK	Economic Assessment for Chemical Recycling from Mixed Plastic Samaila Hassana, Newcastle University, UK			
15.40	Tea/Coffee Break					
16.30	Poster Session 1: Refectory					
17.30	The 6 <sup>th</sup> Clean Energy Science Lecture: Rupert Beckett Lecture Theatre					
18.30	Poster Session 2 and Poster Reception and Buffet D	Poster Session 2 and Poster Reception and Buffet Dinner: Refectory				
		END OF DAY 1				

**Outline Programme** 

*Thursday 11<sup>th</sup> Se*ptember

09.00	Opening Session – Rupert Beckett Lecture Theatr	е	•			
09.05	Keynote presentation 3: Integrated CO₂ capture and utilisation (ICCU) using solid dual functional materials  Professor Chunfei Wu, Queen's University, Belfast, UK					
09.35		Keynote presentation 4: Comprehensive Energy Utilization of Fluoride-salt-cooled High-temperature Small Modular Nuclear Reactor Associate Professor Quanbin Zhao, Xi'an Jiatong University, China				
	Session 3A CCUS 1 – Rupert Beckett Lecture Theatre  Session 3B Energy Storage – LG15  Session 3C Combustion Processes 1 – L					
	Session Chair – Dr Olajide Otitoju	Session Chair – Prof Xiao Wu	Session Chair – Dr Junfeng Yang			
10.10	Comparison of Micro- and Meso-Pore Analysis Techniques to Understand Carbon Capturing Capability of Plant Derived Biochar Baldeep Kaur, The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, UK	Hybrid State of Charge Estimation for Lithium-Ion Batteries Using Kalman Filters and AI: Enhancing Accuracy and Sustainability  Mansur Mustapha, University of Salford, UK.	IMPULSE® Cleaning and its Applications in the Power Industry Thomas Ball, RJM International, UK			
10.30	Comparing the Performance of MOFs and Amines as Carbon Capture Technologies through Life-Cycle Assessment Nicholas Landon, University of Nottingham, UK	Fabric Waste Derived Carbon-Based Electrode Materials for Energy Storage Applications Emine Yagmur, University of Nottingham, UK	Investigation into Hydrogen Pre-ignition Induced by a Single Oil Droplet Olayinka Ramnou, University of Leeds, UK			
10.50	The Difficulties of Modelling the Manufacture of Carbon Capture Technologies for Life Cycle Assessment Nicholas Landon, University of Nottingham, UK	ТВС	Torrefaction of spelt husks to increase its fuel properties Abubakar Halidu, Newcastle University, UK			
11.10	Tea/Coffee Break	1	1			

	Session 4A Anaerobic Digestion- Rupert Beckett Lecture Theatre	Session 4B CCUS 2 – LG15	Session 4C Biomass/Waste 2 – LG19	
	Session Chair – Prof Bill Nimmo	Session Chair – Prof Ed Lester	Session Chair – Prof Jenny Jones	
11.40	A comparison of pre-treatment approaches for enhancing the biogas yield from water hyacinth Betul Esen, University of Leeds, UK	Making Waste Carbon Negative: Integrating Carbon Capture with EfW's Sinéad Goodall, Suez Recycling and Recovery UK.	Evaluating the Effectiveness of Spraying PVA Glue with Water to Supress and Bind Biomass Wood Pellet Dust  Veronika Savchenko, University of Nottingham, UK	
12.00	Integration of biohydrogen production from food waste into existing anaerobic digestion systems: samples pretreatment and process stability Cythia Okoro Shekwaga, University of Leeds, UK	Mechanisms of using NaCl-CaCl <sub>2</sub> molten solar salts in enhancing the integrated CO <sub>2</sub> capture and utilization via reverse water gas shift (ICCU-RWGS) process with CaO alone  Xiatong Zhao. Queens University Belfast, UK	Comparative Analysis of Low- and High-Impact Forces on the Disintegration of Wood Pellets  Veronika Savchenko, University of Nottingham, UK	
12.20	Generation of Biogas from Continuous Anaerobic Codigestion of Agro-waste and Chicken Droppings Esther Babatunde, University of Johannesburg, South Africa	Can Carbon-Based Materials from Waste Fabrics Provide a Sustainable Solution for CO <sub>2</sub> Capture?  Emine Yagmur, University of Nottingham, UK	Pre-Treatment of Municipal Solid Waste using dry, saturated steam in rotating autoclaves to present a homogenous, high percent biomass product for sustainable, solid, liquid, and gaseous biofuels Tom Wilson, Wilson Biochemical Ltd, UK	
12.40	TBC	Integrated CO <sub>2</sub> capture and utilisation (ICCU) using CaO based dual functional materials for syngas production Chunfei Wu, Queens University Belfast, UK	Energy, Exergy, Economic and Environmental Analysis of an Integrated Coal-Biomass Gasification Fuel Cell System for Low-Carbon Energy generation and Methanol production  Xiao Wu, Southeast University, China	
13.00	Lunch	<u> </u>		
14.00	Industrial Site Visits			
19.00	Conference Dinner – The Great Hall			

Outline Programme Friday, 12<sup>th</sup> September

9.00	Opening Session				
09.05	Keynote presentation 5: Integration of direct air captu Dr Eni Oko, Newcastle University, UK	re and green hydrogen for sustainable fuel production			
	Session 5A China-Clean Energy Research – Rupert Beckett Lecture Theatre	Session 5B CATALYSE - LG15	Session 5C Combustion Processes 2 – LG19		
	Session Chair – Dr Chunfei Wu	Session Chair – Dr Eni Oko	Session Chair – Dr Andrew Goddard		
09.35	Experimental study on hydrogen production by methanol reforming under multiple conditions: temperature gradient regulation and product selectivity optimisation  Runzei Feng, Xi'an Jiaotong University, China	Air Capture and Piperazine-based Post-combustion	Low NOx Burners for Hydrogen: Why the NOx can be lower than for Natural Gas Gordon Andrews, University of Leeds, UK		
09.55	Unravelling Atomic-Scale Mechanisms and Parameter Synergies in Coal Supercritical Water Gasification: A ReaxFF Molecular Dynamics Study Ruiqui Mu, Xi'an Jiaotong University, China	Solar-driven direct air capture and CO <sub>2</sub> utilisation for syngas production using CH <sub>4</sub> -fluidised solar calcination  Yide Han, University of Sheffield, UK	Neural ODE Method for NH <sub>3</sub> /H <sub>2</sub> Combustion Chemistry Acceleration Kai Hong Luo, University College London, UK		
10.15	Performance Analysis of a Coal-Biomass Co-fired Boiler Based on Numerical Simulation Xiao Wu, Southeast University, China	Adsorption Breakthrough Study of CO <sub>2</sub> /CH <sub>4</sub> Separation in a Vacuum Pressure Swing Adsorption using Water-based Aluminium Fumarate Metal Organic Framework (MOF) Michael O Daramola, University of Pretoria, SA	Selective catalytic reduction systems for ammonia combustion in heavy duty engines-a modelling study Madhumitha Rajendran, University of Sheffield, UK		
10.35	Mass flowrate measurement of gas-liquid two-phase CO <sub>2</sub> flow under CCS conditions Caiying Sun, <sup>1</sup> Inner Mongolia University of Science & Technology, China	Application of Response Surface Methodology (RSM) to the Synthesis of Chitosan Applicable in Post-Combustion CO <sub>2</sub> Capture  Michael O Daramola, University of Pretoria, SA	Experimental investigation of NOx, NO emissions in combustion vessel Rawan Alkandari, University of Leeds, UK		
10.55	An improved NSD optical flow method for dynamic feature extraction and combustion state identification of burner flames  Sixu Pu, Southeast University, China.	Pilot Plant Study of MCFC with Co-production of Hydrogen: CO <sub>2</sub> Management and Achieving Negative Emissions Luma Sh. Al-Saadi, University of Leeds, UK	TBC		
11.15	Tea/Coffee Break	<u> </u>	<u> </u>		

Outline Programme Friday, 12<sup>th</sup> September

	Session 6A Net Zero Research – Rupert Beckett Lecture Theatre	Session 6B Green Processes -LG19	Session 6C Fuels and New Fuels – LG19			
	Session Chair – Dr Andy Ross	Session Chair – Prof Meihong Wang	Session Chair – Prof Bill Nimmo			
11.45	Navigating the Path to Net Zero Emission: Biofuels Development in Indonesia Ferry Fathoni, University of Leeds, UK	Manufacturing of green carbon for the iron and steel industry: Industrial Scale trials.  Jenny Jones, University of Leeds, UK	A Portable Dilution System for the Generation of Synthetic Biomethane Reference Materials Oliver Williams, National Physical Laboratory, UK			
12.05	Modelling tools to assess low-carbon hydrogen routes to reach net zero Carolina Font-Palma, University of Hull, UK	Opportunities to facilitate the decarbonisation of steelmaking through the recovery of process dust arisings from the steel industry Julian Steer, Cardiff University, UK	Green Solvent-Assisted Catalytic Hydrodeoxygenation of Bio-oil to Engine-Ready Drop-in Fuel Jude Onwudili, Aston University, UK			
12.25	Scale-up of a Fluidised Bed Reactor for Sorption- Enhanced Steam Methane Reforming using CPFD Simulation Chinonyelum Udemu, University of Hull, UK	Ammonia decomposition on Ru-CeO₂ layers for hydrogen production – A DFT Study Nomcebo P Motsa, University of Pretoria, SA	Solvent-Assisted Esterification: A Cost-Effective Strategy for Bio-oil Upgrading to Engine-Ready Drop-in Fuel Himanshu Patel, Aston University, UK			
12.45	Green Methanol Production from FCC Unit Flue Gas in Basrah Refinery: A Circular Economy Approach Nadeen Al-Janabi, Reem F. Badr, Ministry of Oil, Iraq.	TBC	TBC			
13.05	Award Presentations					
13.15	Closing Address – Prof Bill Nimmo, Conference Chairman					
13.25	Lunch					
	END OF CONFERENCE					

## **Poster Catalogue**

1. Upgrading of Biogas using Ex-situ Biochar Immobilised Bioreactor Approaches Munira Alateeqi, University of Leeds, UK

2. A Comparison of the Baseline Thermal Characteristics and Composition of Hydrochar and Pyrochar from Faecal Sludge and Water Hyacinth

Flora Chitalu, University of Leeds

3. Increasing Fuel Flexibility of converted biomass boilers.

Bijal Gudka, University of Leeds, UK

- **4.** Hydrothermal Liquefaction of Water Hyacinth and its comparison to different Invasive Aquatic Plants *Karim Ismail, University of Leeds, UK*
- 5. Comparison of Micro- and Meso-Pore Analysis Techniques to Understand Carbon Capturing Capability of Plant Derived Biochar.

Baldeeep Kaur, The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich. UK

6. Supercritical water liquefaction of waste plastics to produce oil high value fuels and chemicals.

Maria Mathew, University of Leeds, UK

7. Efficient Low Carbon Ammonia Production through Combined Biomass Gasification, Nitrogen Self-Sufficiency, and Waste Heat Recovery.

Isaac Okereke, Aston University, UK

- 8. Selective catalytic reduction systems for ammonia combustion in heavy duty engines-a modelling study. *Madhumitha Rajendran, University of Sheffield, UK*
- 9. Characterisation of Invasive Aquatic plants in India and their potential conversion by aquatic digestion.

  Andy Ross, University of Leeds, UK
- 10. Fundamental studies of lifted and attached jet hydrogen flames in cross-flow.

Chengpei Wu, University of Leeds, UK

11. Fabric Waste Derived Carbon-Based Electrode Materials for Energy Storage Applications.

Emine Yagmur, Ankara University, Turkey

12. Size Distribution Measurement of Pneumatically Conveyed Pulverised Fuel in a Square-Shaped Pipe through Acoustic Emission Detection and Electrostatic Sensing.

Yong Yan, Beihang University.

13. Co-processing Sargassum with Lignocellulosic Biomass by Hydrothermal Carbonisation: Impacts on Hydrochar Quality.

Sangeetha Piriya Ramasamy, University of Leeds, UK

14. Using carbonate-based nanofluids in an integrated heat pump-thermal energy storage system for providing sustainable domestic heating.

Aashir Zaheer, University of Leeds, UK

15. Structure-Performance -Environment Mapping of Cu-based Catalysts for Green Methanol Synthesis.

Xiaodong Liu, University of Sheffield, UK

16. Production and Optimisation of Oxygenated Biofuel Blend Components via the Butanolysis of Different Lignocellulosic Biomass feedstocks

Andy Ross, University of Leeds, UK.

17. A kinetic and mechanistic study of on-purpose renewable propane production via butyric acid hydrothermal decarboxylation over Pt/C.

Seyed Emad , Aston University, UK

# Session 1A. Bio-Char Wednesday, 10<sup>th</sup> September

Forename	Surname	Job Title	Organisation	Email
Aashir	Zaheer	PhD student	University of Leeds	pm20az@leeds.ac.uk
Abiodun	Okeleye	PhD Student	University of Sheffield	atokeleye1@sheffield.ac.uk
Ali	Alazzawi	PhD Student	University of Leeds	pmaaala@leeds.ac.uk
Andrew	Goddard	R&D Manager	Freeland Horticulture Ltd	andrew@freelandhorticulture.co.uk
Andrew	Ross	Associate Professor	University of Leeds	a.b.ross@leeds.ac.uk
Atul	Sharma	Consultant Engineer	Wolfson Centre for Bulk Solids Handling Technology	Atul.sharma@gre.ac.uk
Baldeep	Kaur	Senior Consultant Engineer	Wolfson Centre for Bulk Solids Handling Technology	b.kaur@gre.ac.uk
Betul	Esen	PhD student	University of Leeds	ml19be@leeds.ac.uk
Bijal	Gudka	Conference Manager	Gudka Energy Consulting	bijal@gudka-energy.co.uk
Bill	Nimmo	Professor	University of Sheffield	w.nimmo@sheffield.ac.uk
Bron	Steadman	Product Manager	Sci-Med Ltd	bronwen.steadman@scimed.co.uk
Caiying	Sun	Professor	Inner Mongolia University of Science & Technology	suncaiying2006@163.com
Carolina	Font-Palma	Senior Lecturer	University of Hull	c.font-palma@hull.ac.uk
Cesar	Catizane	Research Fellow	Cranfield University	Cesar.catizane@cranfield.ac.uk
Chengpei	Wu	PhD Student	University of Leeds	ml18c25w@leeds.ac.uk
Chinonyelum	Udemu	Researcher	University of Hull	c.udemu@hull.ac.uk
Chunfei	Wu	Professor	Queens University Belfast	c.wu@qub.ac.uk
Dan	Clarke	Product Manager	Sci-Med Ltd	dan.clarke@scimed.co.uk
Darren	Machen	Product Manager	Sci-Med Ltd	darren.machen@scimed.co.uk
David	McCaffrey	FERF Executive Committee Member	The Fuel and Energy Research Forum	mail@tferf.org
David	Parkin	Director (	Progressive Energy	david.parkin@progressive-energy.com
Edward	Lester	Professor	University of Nottingham	Edward.lester@nottingham.ac.uk
Emine	Yagmur	Researcher	University of Nottingham	Emine.Yagmur@nottingham.ac.uk
Eni	Oko	Senior Lecturer	Newcastle University	eni.oko@newcastle.ac.uk
Esther	Babatunde	Postdoctoral Research Fellow	University of Johannesburg	ebabatunde@uj.ac.za
Fatih	Gulec	Assistant Professor	University of Nottingham	Fatih.Gulec1@nottingham.ac.uk
Ferry	Fathoni	PhD student	University of Leeds	gyff@leeds.ac.uk
Flora	Chitalu	PhD Student	University of Leeds	pmfkc@leeds.ac.uk
Gordon	Andrews	Professor of Combustion Engineering	University of Leeds	profgeandrews@hotmail.com
Himanshu	Patel	Research Fellow	Aston University	j.onwudili@aston.ac.uk

Session 1A. Bio-Char Wednesday, 10<sup>th</sup> September

Session 1A. Bio-Char Wednesday, 10 September				
Forename	Surname	Job Title	Organisation	Email
Idris	Jibrin	PhD Student	University of Sheffield	ljibrin1@sheffield.ac.uk
James	Banks	PhD Student	Cardiff University	BanksJE@cardiff.ac.uk
Jenny	Jones	Emeritus Professor	University of Leeds	fuejmj@leeds.ac.uk
Jie	Gu	PhD Student	University of Leeds	pmjgu@leeds.ac.uk
Jill	Nimmo	Assistant Conference Manager		jillnimmo15@gmail.com
Jude	Onwudili	Professor	Aston University	j.onwudili@aston.ac.uk
Julian	Steer	Research Fellow	Cardiff University	SteerJ1@cardiff.ac.uk
Junfeng	Yang	Associate Professor	University of Leeds	J.Yang@leeds.ac.uk
Junjie	Yan	Vice Principal	Xi'an Jiaotong University	yanjj@xjtu.edu.cn
Kai	Luo	Chair of Energy Systems	University College London	k.luo@ucl.ac.uk
Karim	Ismail	PhD Student (Student Helper)	University of Leeds	Pm17ki@leeds.ac.uk
Katterin	Hernández	PhD Student	University of Leeds	pmkshd@leeds.ac.uk
Kazeem	Mohammed	Postdoctoral Researcher	Aston University	k.mohammed5@aston.ac.uk
Keeran	Ward	Lecturer	University of Leeds	k.r.ward@leeds.ac.uk
Lingxiao	Chen	PhD student	Southeast University	230249557@seu.edu.cn
Luma	Al-saadi	Research Fellow	University of Leeds	Fzzb134@leeds.ac.uk
Madhumitha	Rajendran	PhD Student	University of Sheffield	Mrajendran1@sheffield.ac.uk
Maeve	McLaughlin	Product Manager	Sci-Med Ltd	maeve.mclaughlin@scimed.co.uk
Mansur	Mustapha	PhD Student	University of Salford	m.l.mustapha@edu.salford.ac.uk
Maria	Matthew	PhD student	University of Leeds	pmmmat@leeds.ac.uk
Maryam	Awode	PhD Student	University of Nottingham	Maryam.awode@nottingham.ac.uk
Matthew	Lovelady	PhD Student	University of Hull	m.j.lovelady-2018@hull.ac.uk
Meihong	Wang	Professor of Energy Systems Engineering	University of Sheffield	meihong.wang@sheffield.ac.uk
Meisam	Babaei	Lecturer	University of Leeds	m.babaie@leeds.ac.uk
Michael	Daramola	Professor	University of Pretoria	Michael.Daramola@up.ac.za
Mohammed	Alshemali	PhD Student	University of Sheffield	M@al-shemali.com
Musa	Idi	PhD student	Newcastle University	m.idi2@newcastle.ac.uk
Nicholas	Landon	EngD Research Student	University of Nottingham	eaynpl@nottingham.ac.uk
Nicholas	Tann	PhD Student	University of Sheffield	ntann1@sheffield.ac.uk
Nomcebo	Motsa	PhD student	University of Pretoria	nomcebo.motsa@up.ac.za
Nura	Garba	PhD Student	University of Nottingham	nura.garba@nottingham.ac.uk
Olajide	Otitoju	Post-Doctoral Research Associate	University of Sheffield	o.otitoju@sheffield .ac.uk
Olayinka	Ramonu	PhD Student	University of Leeds	mnojr@leeds.ac.uk
Oliver	Williams	Higher Scientist	National Physical Laboratory	oliver.williams@npl.co.uk

Session 1A. Bio-Char Wednesday, 10<sup>th</sup> September

Session TA. Bio-Chai Wednesday, 10° September				
Forename	Surname	Job Title	Organisation	Email
Quanbin	Zhao	Vice director of Thermal Energy Power and Control Engineering Institute	Xi'an Jiaotong University	zhaoquanbin122@xjtu.edu.cn
Rawan	Alkandari	PhD student	University of Leeds	mnria@leeds.ac.uk
Richard	Brown	Professor of Mechanical Engineering	Queensland University of Technology	richard.brown@qut.edu.au
Ruiqi	Mu	PhD student	Xi'an Jiaotong University	mrq1998@stu.xjtu.edu.cn
Runze	Feng	PhD student	Xi'an Jiaotong University	3123103039@stu.xjtu.edu.cn
Ryan	Longley	PhD Student	University of Leeds	Ed12r3l@leeds.ac.uk
Sa	Li	PhD student	Southeast University	230239376@seu.edu.cn/lisa@seu.edu.cn
Samaila	Hassan	PhD student	Newcastle University	s.hassan6@ncl.ac.uk
Serhii	Horianoi	Junior Research Associate	Thermal Energy Technology Institute, NAS of Ukraine	horianoisv@gmail.com
Seyed Emad	Hashemnezhad	PhD student	Aston University	220258773@aston.ac.uk
Shengyuan	Huang	PhD Student	University of Sheffield	shuang55@sheffield.ac.uk
Simon	Corrigan	Sales Engineer	Signal Group	Simon.corrigan@signal-group.com
Sixu	Pu	PhD Student	Southeast University	psx_666@163.com
Stewart	Bradley	Low Carbon Services	Uniper Technologies Ltd	stewart.bradley"uniper.energy
Thomas	Ball	Lead Process Engineer	RJM International	tball@rjm-international.com
Toluleke	Akinola	Post-Doctoral Research Associate	University of Sheffield	t.e.akinola@sheffield .ac.uk
Tom	Wilson	Managing Director	Wilson Bio-Chemicals Ltd	rebecca.addy@wilsonbio-chemical.co.uk
Trudy	Beeley	Head of Engineering	RJM International	tbeeley@rjm-international.com
Usman	Ali	Research Fellow	Net Zero Industry Innovation Centre	U.Ali@tees.ac.uk
Veronika	Savchenko	EngD Research Student	University of Nottingham	Veronika.savchenko@nottingham.ac.uk
Will	Quick	Low Carbon Services	Uniper Technologies Ltd	will.quick@uniper.energy
Xiao	Wu	Professor	Southeast University	wux@seu.edu.cn
Xiaodong	Liu	PhD Student	University of Sheffield	xliu245@sheffield.ac.uk
Xiaotong	Zhao	PhD student	Queens University Belfast	Xzhao27@qub.ac.uk
Xingxing	Zeng	PhD Student	Beihang University	zeng970121@163.com
Yide	Han	PhD Student	University of Sheffield	yhan33@sheffield.ac.uk
Yong	Yan	Professor	Beihang University	yongyan@buaa.edu.cn

# Conversion of Woody Biomass Waste (African invasive plants and hardwoods) to Hydrogen-rich Syngas and Briquettes

Michael O. Daramola

Sustainable Energy and Environment Research Group (SEERG), Department of Chemical Engineering, Faculty of Engineering, Built Environment and Information Technology (EBIT), University of Pretoria, Hatfield 0028, Pretoria, South Africa.

The increasing world's population has created the need for more sustainable timbre buildings for shelter and increased agricultural activities. These activities have led to a large production of woody biomass waste. Regrettably, these woody biomass wastes are indiscriminately disposed of by open-burning, thereby creating adverse environmental effects burnt as a means of waste disposal. Additionally, to mitigate climate change due to CO2 emission, demand for clean energy sources has significantly increased. Therefore, research efforts on valorizing wood-waste into clean energy sources are on the rise. However, the scramble for clean energy, resulting from non-renewable fossil-fuels and its adverse environmental effect, paves the way for thermochemical conversion of wood-waste into clean energy and value-added products. Despite other social impediments, bio-energy technologies, though promising, still have many scientific hurdles and knowledge gaps for efficient implementation. Therefore, this paper highlights some results of studies undertaken in this area in my research group, specifically research efforts on converting woody biomass waste into hydrogen-rich syngas, nanocomposite briquettes, and biobased chemicals using thermochemical methods or biological methods. Interestingly, our results reveal that pretreatment (e.g. torrefaction and solvolysis) of woody biomass wastes is important in improving their fuel quality. Furthermore, nanocomposite briquettes obtained from wood biomass are a potential biofuel for industrial and household applications and conversion of invasive plants (e.g. African mesquite and Bugweed) and African hardwoods into hydrogen-rich syngas via pyrogasification is promising. Kinetic studies carried out on these woody biomass wastes also underscore that kinetic study can be instrumental in modelling the devolatilization process as well as designing an optimized reactor suitable for pyrolysis of wood waste to energy sources.

**Keywords:** Woody biomass wastes; African invasive plants; Pyrogasification; Pyrolysis; Briquettes; Syngas

# Optimal Control of Solvent-based Carbon Capture Process Integrated with Coal-fired Power plant

## Xiao Wu

National Engineering Research Center of Power Generation Control and Safety, School of Energy and Environment, Southeast University. Nanjing, China.

The use of carbon capture technology is important for the decarbonisation of coal-fired power plants. Although many efforts have been made on solvent development, process upgrade of carbon capture system, less attention has been paid on control. Control system offers a number of attractive feature for the operation of carbon capture process, such as adaptation to frequent flue gas fluctuations of upstream power plants and the demand for downstream CO2 products; offering additional flexibility for the power plants.

This presentation will start with an introduction to the operating challenges of solvent-based carbon capture system integrated with coal-fired power plant, followed by motivations of this research. The main part will be our research on control-oriented modelling, coordinated scheduling and dynamic control of carbon capture system. How to improve the flexibility of carbon capture system will also be discussed. Then the topic will be extended to our current research efforts to intelligent modelling and control of carbon capture systems. Finally, we present a control engineering practice on 500,000 t/a carbon capture project in National Energy Group Taizhou Power Plant, China (The largest power plant carbon capture project in Asia; and the largest power plant carbon capture project currently in operation in the world).

*Keywords:* Solvent-based carbon capture, Coal-fired power plant, Modelling, Optimal control, Scheduling, Flexible operation.

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# Evolution of Biochar Structure and Porosity with Temperature and its Impact on Metal Adsorption

\*Nura Garba a, b, Wei Li a, Lee Stevens a, Clement Uguna a, Will Meredith a, Colin E. Snape a

An in-depth characterisation study using techniques including X-ray photoelectron spectroscopy (XPS) to probe heteroatom functionality, and BET surface area measurements, has been conducted on biochars prepared over the production temperature range of 400-700°C from woody biomass and anaerobic digestate (AD). Further, hydropyrolysis to quantify the fraction of stable polyaromatic carbon (SPAC) was used to predict the long-term environmental stability of the biochars. This study aims to understand how the trade-off between surface area, stability and heteroatom functional groups affects metal adsorption, with Cu and Zn being used as examples. Although biochar yields on a mass basis decreased with production temperature, yields on a carbon basis remained relatively constant, *ca.* 50% for AD biochar produced from 550-700°C. As expected, the atomic H/C ratio decreased with temperature and was *ca.* 0.3 at 650 and 700°C corresponding to a biochar with predicted high stability, as confirmed by the SPAC content being close to 90%. Below 600°C, the atomic H/C ratio increased to >0.5 with much higher SPAC values. XPS confirmed decreasing concentrations of O and N surface functional groups with increasing temperature, where the O 1s band indicated a shift away from double bonds (carbonyl, carboxyl) to single bonds (phenols and furans) with increasing temperature. BET surface area increased with temperature from typically 100 m²/g at 400°C to 180 m²/q at 600°C and above.

Biochar adsorption potential for Cu and Zn was studied at different pHs, contact times and solution concentrations, with a pH of 8 found to be optimal. The levels of Cu and Zn removal were considerably higher at 600°C compared to 400 and 500°C. This indicates that any loss in heteroatom functional groups involved in complexing Cu and Zn is more than offset by the increase in surface area for the biochar investigated.

Keywords: Adsorption, Anaerobic Digestate, Biochar, Woody Biomass, Surface area

Acknowledgement: This work is supported by the Petroleum Technology Development Fund (PTDF), Nigeria and the Department of Chemical and Environmental Engineering, University of Nottingham, United Kingdom

<sup>&</sup>lt;sup>a</sup> University of Nottingham, Faculty of Engineering, Department of Chemical and Environmental Engineering, NG7 2RD, United Kingdom

<sup>&</sup>lt;sup>b</sup> Department of Environmental and Resources Management, Usmanu Danfodiyo University, P.M.B 2346, Sokoto, Nigeria

## Techno-Economic and Sustainability Assessment of Lignocellulosic Biomass Conversion to Biofuel

Ali Alazzawi<sup>1</sup>, Valerie Dupont<sup>1</sup>, Christian Michelbach<sup>1</sup>, Mohamad Anas Nahil<sup>1</sup>, Andy B. Ross<sup>1</sup>, Alison Tomlin<sup>1</sup>, Christian Michelbach<sup>1</sup>

<sup>1</sup> School of Chemical and Process Engineering, University of Leeds, Leeds, United Kingdom, LS2 9JT

Ethyl levulinate (EL) is a candidate for potential biofuel blending applications. Producing lignocellulosic-derived ethyl levulinates is considered a sustainable alternative to conventional fossil fuels due to potential reductions in CO<sub>2</sub> footprint. This study evaluates the feasibility of producing a rich ethyl fuel blend via an acid-catalysed ethanolysis process from lignocellulosic biomass (in this case, corncob) by developing a robust technoeconomic analysis and carbon footprint analysis based on process modelling.

**Techno-economic analysis**: Aspen Plus is used to conduct a comprehensive steady-state simulation of the process, covering key stages such as reaction, neutralisation, purification of the products, and recycling of the unreacted ethanol. Integration was performed for the Aspen Plus thermodynamic property database, methods, mass and end energy balances, and phase equilibrium data. The economic performance is analysed using the Aspen Process Economic Analyzer. Several scenarios were investigated using a variety of approaches for the provision of heating and cooling utilities in order to evaluate energy and cost requirements through the proposed lifetime of the plant.

**Energy optimisation and waste valorisation:** Biorefineries are an energy-intensive industry that requires tremendous cooling and heating utilities. This study uses different technologies and techniques to tackle high energy demands, such as valorising waste heat integration approaches and alternative efficient separation technologies. Aspen Energy Analyser software is used to create the heat exchanger network for the process to ensure maximum heat exchange and the lowest capital cost.

**Electrification**: This study also aims to assess the impact of process electrification by replacing fossil energy-dependent heating utilities with electrically heated hot oil and developing a novel heat pump configuration for the process steps that consume the most energy. The heat pump configuration is optimised using thermodynamic and process modelling. This transition aims to enhance energy efficiency, lower carbon emissions, and increase process sustainability.

**Carbon footprint analysis:** This will be performed using the SimaPro software for the different plant design scenarios to quantify environmental metrics such as greenhouse gas emissions. The software is used in conjunction with a comprehensive life cycle inventory database to allow the practitioner to estimate the carbon footprint of the different process steps using methods that comply with ISO 14040 standards.

This research gives essential insight into the energy requirements, costs, and carbon footprint of an example biorefinery, which produces biofuel blends and all expected byproducts from lignocellulosic waste. It also identifies the key process parameters, such as operation conditions, energy optimisation parameters, process scaling up, and the sustainability impacts of transitions towards the electrification of liquid fuel production.

Keywords: biofuel, lignocellulosic biomass, techno-economic analysis, life cycle assessment, ethanolysis

Acknowledgement: The work was conducted as part of project EPSRC/SFI grant (EP/T033088/1), Tailored Production and Utilisation of Sustainable Low-Cost Lignocellulosic Advanced Biofuel Blends as Diesel and Petrol Substitutes: SusLABB—a PhD scholarship from CNOOC and the Ministry of Iraqi Oil support Ali Alazzawi.

# A practical approach to determine self-heating tendencies in biomass stored in bulk quantities

\*Baldeep Kaur<sup>1</sup>, Venkata Sai Chinmayi Puppala<sup>2</sup>, Atul Sharma<sup>1</sup>, Michael Bradley<sup>1</sup>

<sup>1</sup> The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, Chatham Maritime, Kent, UK, <sup>2</sup> School of Engineering, University of Greenwich, Chatham Maritime, Kent, UK.

Biomass is one of the key contributors to renewable energy production in the UK and Europe, and its use is growing rapidly worldwide. However, large biomass stores regularly experience fires due to self-heating, leading to significant financial losses (often £millions per event), pollution and risks to life. Such types of fires are more common than anticipated and experience shows that plant owners need to consider this problem on the basis of when it will happen, rather than if.

Ventilation is a commonly used technique in the USA, intended to reduce the reactivity in freshly manufactured pellets; there is a common belief that it may help to reduce the reactants present, the common belief being that ventilation will increase the speed of reaction and therefore the rate of self-heating. However, UK and European storage and handling facilities do not ventilate the biomass pellet fuel. Clearly, given these contrary views there are good reasons to explore the role and effectiveness of ventilation to minimise self-heating in biomass pellets.

Past experiences in developing various tests for characterising bulk solids have demonstrated that testing and prediction of behaviour based on chemistry and nominal physical specifications (e.g. particle size) fails to accurately represent behaviour of particles in a bulk form. This is because of the near-infinite variations in physical form including particle shape, fines content, durability, surface texture, homogeneity, wood species, ageing etc., all of which affect the behaviour, but that cannot be entirely captured by basic chemical analysis. Thus, any reliable measurement must involve testing small samples of the actual bulk solid in its real form as present in the system, including effects of particle breakage, segregation, environmental effects etc. This research examines the effect of pellet ageing on availability of reactive substances, the markers during off-gassing to indicate ageing, measures to remove reactants and explore the availability of reactants.

**Off-gassing**: Experimental work focused on measuring the trend of gases released during the ageing process of biomass samples during storage under controlled environmental conditions. The aim was to develop a quick laboratory-based method for off-gassing analysis using small quantities of representative biomass samples. These measurements can be conducted simultaneously on multiple samples and accelerated by the elevated temperature and relative humidity conditions. Interestingly, this approach can be applied to range of biomass and waste materials to understand the relationship between the ageing, environmental conditions, off-gassing and self-heating.

Keywords: biomass, biomass storage and handling; self-heating.

Acknowledgement: Authors acknowledge the support of technical staff at The Wolfson Centre, masters research student Mr. Khaleed Miah at the University of Greenwich.

# The potential of hydrothermal carbonisation as a pre-treatment for thermochemical and biochemical conversion

Andy Ross, Aaron Brown, Aidan Smith, Isabel Smith, Shaaz Umar

School of Chemical and Process Engineering, University of Leeds

Hydrothermal carbonisation (HTC) involves the processing of biomass and biowastes in hot compressed water at temperatures ranging between 150 -250°C. The resulting products include a solid carbonaceous product called hydrochar, a process water containing soluble organics and inorganics and a gaseous product containing mainly CO<sub>2</sub>. HTC overcomes many of the drawbacks of biomass fuels such as low bulk density, high moisture, low calorific value, milling issues and ash problems and can be used as a pre-treatment for further thermochemical conversion. The most investigated approaches include the use of hydrochar as a solid fuel in combustion however there is also potential for integration with gasification, pyrolysis and liquefaction approaches.

HTC is ideal for processing wet wastes with high and nutrient content such as aquatic plants and algae, manure, digestate and food waste. Its behaviour however is very feedstock dependent. The hydrochar and process water composition are heavily influenced by feedstock composition (e.g. biochemical composition and ash content), reaction conditions (temperature, time and solid loading) and process design. A case study investigating the HTC of aquatic plants such as water hyacinth and macroalgae will illustrate the effect of process conditions on product properties and their potential for integration with different thermochemical and biochemical conversion approaches. The behaviour of the hydrochar as a solid fuel in combustion and gasification are reviewed together with more novel approaches for stabilisation and liquefaction of hydrochar using pyrolysis and liquefaction. Hydrochar behaves similar to coal during combustion and demineralisation of alkali metals can improve ash behaviour however this is feedstock dependent. Gasification of hydrochar affect H<sub>2</sub>/CO ratio, reduce tars and unlock difficult to process feedstocks. The stabilisation of hydrochars by pyrolysis and activation can produce highly porous materials and liquefaction approaches can produce biocrude intermediates that can be further upgraded to SAF.

Integration with biochemical processes such as anaerobic digestion and dark fermentation can produce biomethane and bio-hydrogen which can contribute to energy recovery while dealing with the process waters. Generally lower temperature processes are less inhibitory towards biochemical conversion however once again, there is feedstock dependency. The benefits of hydrothermal pretreatment is that it improves the performance of the feedstock in the secondary conversion approach, e.g. increased energy density, improved handing et; it unlocks difficult to process biomass and wastes, potentially allowing utilisation of novel underutilised resources; it has the potential for multiple uses, e.g. power generation, biofuels and bioproducts.

## Morphological Analysis of Biomass wood Pellets Using Scanning Techniques

Savchenko, V.a, Lester, E.a, Güleç F.a, Williams, O.a

<sup>a</sup>Faculty of Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, UK

Dust formation from biomass pellets continues to be an operation issue for bioenergy plants. Understanding the structural characteristics of biomass pellets is critical to optimizing their processing, transportation and reducing dust generation during handling. In this study, biomass pellets were broken down in a ball mill (without balls) for varying times and speeds to replicated high impact conditions seen in transportation systems. Subsequently, the product was sieved into size fractions, with the pellets remaining in the top size (> 4.75 mm) being separated out from the broken down pellets in the smaller size fractions.

To gain an understanding of the morphological changes in pellets both before and after the milling process, a detailed scanning technique was employed. The analysis aimed to elucidate the mechanisms of pellet breakdown and their relationship to the structural composition of the pellets. High-resolution imaging was conducted using an EPSON scanner with an open lid for 3 batches of a commonly used biomass pellet in large scale bioenergy systems, one commercially available pellet (Balcas energy wood pellets), and one torrefied "black" pellet.

The resulting scans (images) were processed using Axio Vision SE64 for segmentation and binary analysis, providing data on parameters such as area, diameter, Feret minimum and maximum, fiber length, Feret ratio, and perimeter. These measurements were converted to millimetres and tabulated for comprehensive analysis. Key findings highlight changes in surface morphology, including the formation of cracks and fissures, which serve as points of weakness during milling. This study underscores the value of using simple scanning techniques in characterizing biomass pellets breakdown.

Keywords: scan techniques, biomass pellets, breakdown, milling, images, morphological changes.

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## Potential of the Co-Products of Blue, Green, and Turquoise Hydrogen – A Process System Analysis

\*Usman Ali<sup>1</sup>, Mahdi Amanipour<sup>2</sup>, Andrew Smallbone<sup>2</sup>, Kumar Patchigolla<sup>1</sup>, Kin Wai Cheah<sup>1</sup>, Nashwan Dawood<sup>1</sup>

> <sup>1</sup> Net Zero Industry Innovation Centre, Teesside University, Middlesbrough UK, <sup>2</sup> Department of Engineering, Durham University, Durham, UK

Global energy sector is shifting towards cleaner and sustainable energy sources to tackle the climate change. Hydrogen is considered as an important energy vector for decarbonization and achieving the net zero goal. In a year from 2022 to 2023, the global hydrogen production has increased by about 2.5 %, with 63 % being produced from natural gas without carbon capture. Further, the global water electrolysis potential has reached to 1.4 GW. The present research is part of Research England Hydrogen Innovation Project (REHIP) with key objective to identify and characterise the main co-products from blue, green, and turquoise hydrogen pathways, map out the potential end-users for such co-products and valorise these through technoeconomic evaluation. Blue hydrogen is produced when reforming of the natural gas is done with carbon capture resulting in  $CO_2$  as a co-product while  $O_2$  is produced as a co-product when green hydrogen is generated through water electrolysis. In turquoise hydrogen production scheme, the pyrolysis of the methane is achieved which results in solid carbon in parallel to the hydrogen. In addition, the excess heat is generated in different hydrogen production routes which must be utilized in the neighboring industry. Therefore, the present research addresses the fundamental question, "how these co-products can reduce the local hydrogen production cost inside an industrial cluster?"

For blue hydrogen, steam methane and auto thermal reforming are considered while for the green hydrogen alkaline and proton exchange membrane electrolysis are modelled and for turquoise hydrogen production scheme the catalytic and thermal pyrolysis of methane were investigated. The modelling and simulation of the different hydrogen production schemes are realized in Aspen Plus as to characterize the main co-products from the blue, green, and turquoise hydrogen production routes. Due to the order of magnitude of the commercial facility, the reliable and predictive process simulations are necessary to successfully employ these technologies. The hydrogen capacity of 200 MMSCFD is considered to resemble the commercial-scale hydrogen production. The hydrogen purity is fixed at a mole fraction of 99.90 % while the co-products purity is based on the ISO standards. The CO<sub>2</sub> capture rate for the blue hydrogen is 95 %. It is observed that the blue, green, and turquoise hydrogen results in 32 %, 40 % and 45 % of the excess heat, respectively. The capture and use of the excess heat presents a significant opportunity for the synergy with major industrial processes. The modelling will result in evaluation of the amount and quality of the coproducts along with GJ's of the residual heat generated. Further, the captured CO<sub>2</sub> from the blue hydrogen can be utilized for pipeline, storage, enhanced oil recovery, liquefaction, food, beverage, and medical purposes. Purified oxygen from the green hydrogen brings opportunities around oxy-flames and reactions along with medical use. Further, the solid carbon from the turquoise hydrogen production scheme can be utilized to strengthen the rubber in tires, act as pigment, filler, and insulating applications. The project evaluated the potential of the co-products and their opportunities for their use when these co-products will be available in abundance.

Keywords: Blue hydrogen, green hydrogen, turquoise hydrogen, process simulation

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Hydrogen: the Practical Way to Decarbonise Heat by 2040

\*Gordon Andrews<sup>1,2</sup>, Ramon Quinonez<sup>2</sup>, Francis Olanrewaju<sup>2</sup>, Steve Smith<sup>2</sup>

<sup>1</sup> Leeds University, Leeds, UK, <sup>2</sup> Clean Burner Systems (CBS), Ltd. UK.

The UK Government has announced that it is to scrap the 2035 ban on gas boilers in its new house building standards, which enables the repurposing of the gas grid to hydrogen and the conversion of existing and new boilers, fires and cookers to hydrogen. This decision was inevitable following the failure to install sufficient heat pumps, as new houses could not be left without adequate heating. The requirement for heat pump installations was 600,000 per year by 2028, which for the 30M dwellings in the UK would take 50 years to decarbonise domestic heat, when only 25 years is available. At the 2024 heat pump installation rate it would take 500 years to decarbonise heat. The reasons for the public's resistance to heat pumps will be discussed in the paper. The lack of local electricity supplies for new housing developments with heat pumps, has forced the continued installation of gas boilers to enable the house building target to be achieved.

The only practical solution to decarbonise heat in less than 25 years is repurposing the gas grid for hydrogen, which at the current gas boiler renewal rate of 1.6M per year with 0.25M gas fires, would take 14 years to decarbonise heat in the 25M homes connected to the gas grid. The new plants to manufacture hydrogen could also be built in the same timescale and thus domestic heat decarbonisation could be achieved by 2040. All new boilers, fires and cookers need to be hydrogen ready and the required developments were funded in the Governments Hy4Heat programme and the authors were awarded four Hy4Heat contracts.

The UK should have been pioneers in hydrogen for heat, but Germany has now already made the decision and allocated the funds to convert its gas grid to hydrogen. The UK gas industry similarly needs to be authorised to repurpose the gas grid for hydrogen. It is technically and financially feasible to do this in 15 years, as gas grid fuel switching was completed in 12 years, 50 years ago. The cost will fall on consumers at about £100 per year. The hydrogen appliance cost and appearance would be little different to current appliances. So, this is a practical solution to the decarbonisation of domestic heat and the hydrogen gas grid could also be used to decarbonise industrial process heat and electricity from gas turbines.

The UK Government's definition of clean electricity in 2030 allows 5% of electricity to come from the continued use of natural gas in the existing 50 gas turbine (GT) electricity generators (32 GW), when wind and solar are low. This converts to 4.8  $g_{CO2}/MJ_{elec}$  compared with 30.9  $g_{CO2}/MJ_{elec}$  in 2023. A heat pump using grid electricity would have 2  $g_{CO2}/MJ_{heat}$  in 2030 compared with 11  $g_{CO2}/MJ_{heatc}$  in 2023. Currently up to 60% of electricity is generated from natural gas fired GTs on days when renewables are low, so the gas grid needs to continue to exist in 2030. The conversion of GTs to hydrogen is established technology and so repurposing the gas grid for hydrogen would solve the problem of supplying zero carbon electricity and heat.

Hydrogen, with CCS, can be manufactured from NG at  $<5~g_{CO2}/MJ_{heat}$  and  $<1~g_{CO2}/MJ_{heat}$  for pyrolysis of NG to hydrogen and carbon, which exists on a commercial scale. Taking carbon out of the fuel, rather than out of the exhaust, is a more efficient process. Hydrogen by electrolysis in 2030 using grid electricity would be 7  $g_{CO2}/MJ_{heat}$  but 44  $g_{CO2}/MJ_{heat}$  in 2023. So electrolysis based hydrogen is only as low as NG based hydrogen if the 5% of electricity from NG can be achieved in 2030, until then NG is a lower carbon source of hydrogen. The paper will also address the factual errors in the vociferous campaign to persuade the Government to abandon hydrogen.

Keywords: Hydrogen, heat, decarbonisation, heat pumps, energy policy.

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## Planning Industrial Hydrogen Demand through Optimisation Modelling

\*Matthew Lovelady, Carolina Font-Palma

School of Engineering, University of Hull, HU6 7RX, Hull, UK

As more UK hydrogen projects are evolving through industrial clusters, a localised hydrogen economy is starting to form. To assist in the growth of this hydrogen economy, a number of optimisation models have been developed to derisk the implementation of these technologies in the long-term scale working up to 2050 targets. However, few optimisation models are looking at short term (up to 5 years) investment decisions for enabling industries and hydrogen providers a route of open communication to work towards these optimisation projections. Creating a 'chicken and egg' problem of unmatched hydrogen production and industries not utilising the clean fuel.

The aim of this project is to enable both the hydrogen suppliers and energy-intensive industries committed to decarbonise by fuel switching to hydrogen, an easier path of communication and informing the hydrogen suppliers the appropriate investments to keep up with demand through an optimisation model focusing on a period up to 5 years of current infrastructure.

Two sister models are being developed to enable a business case to quickly calculate their annual cost of hydrogen and to inform the hydrogen producers of the best method of increasing the supply to match demand with the minimal effect to the hydrogen cost. Both these sister models will draw from and update a database containing the current infrastructure, demand, cost and emissions of the current hydrogen supply chain. The fist model will calculate the annual cost of hydrogen for a business based on their annual energy demand and current infrastructure in the hydrogen supply chain. If the cost is accepted as part of the business case, the new load will be added to the database and the model will calculate if the current hydrogen production has the flexibility to accommodate the new demand. If this new demand is not met with the current production infrastructure, an error will display in the database. This will communicate to the hydrogen suppliers that new investments are required to meet the increased demand. The sister model utilises the evolutionary algorithm to recommend the best investment to reach the new demand. The evolutionary algorithm will use different capacities of blue/green hydrogen production, storage and renewable energy production capacities as decision variables. These decision variables will mimic reproduction, mutation, recombination, and extinction, with each iteration. Once the demand is met with the smallest effect on the cost of hydrogen will be saved in the data base as the recommended infrastructure to implement. To maintain the government targets for emissions, constraints are used.

From these results, the hydrogen suppliers will be able to construct new infrastructure knowing there will be a buyer for the new capacity. Additionally, by prioritising the output to the costing of hydrogen, the overall effect of the new infrastructure will reduce the change in quoted hydrogen cost to the industry whose requested the increase in new capacity.

Keywords: Hydrogen, Industry, Evolutionary algorithm

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# Carbon Negative Biochar and Hydrogen Production via Integrated Pyrolysis – Chemical Looping Combustion (PyCLC)

Maryam Awode<sup>1</sup>, Thomas Poulson<sup>1</sup>, Begum Tokay<sup>2</sup>, Colin E. Snape<sup>1</sup>, \*Fatih Güleς<sup>1,2</sup>

<sup>1</sup>Low Carbon Energy and Resources Technologies Research Group, Faculty of Engineering, University of Nottingham, Nottingham NG7 2TU, United Kingdom.

To limit global temperature rise to  $1.5^{\circ}$ C, the Royal Society's models estimate that GGR must reach 230 GtC by 2100, necessitating scalable, long-term CO<sub>2</sub> sequestration. Biochar, a stable form of carbon storage, could contribute significantly to the UK's GGR target of 20-40 MtC per year by 2050. However, conventional biochar production faces challenges, such as limited feedstock availability and CO<sub>2</sub> emissions from production. Similarly, while hydrogen is a clean energy source critical to the UK's Net Zero strategy, most hydrogen today is produced from fossil fuels via steam methane reforming (SMR), which produces significant CO<sub>2</sub>. This study explores an innovative pyrolysis-based process for simultaneous biochar and hydrogen production, coupled with chemical looping combustion for heat generation. This novel approach offers a carbon-negative pathway to sustainable biochar and hydrogen production. The objective is to simultaneously produce biochar for CO<sub>2</sub> sequestration and green H<sub>2</sub> as a clean energy source, with an auto thermal process leveraging bioenergy with CO<sub>2</sub> capture and storage (BECCS).

In this study, two types of waste biomass—Irish Sawdust Whitewood (WW) and Used Coffee Grounds (CG)—were utilised as feedstocks for biochar production in Py-CLC concept. The pyrolysis and integrated combustion reactions were investigated under a non-isothermal process, where the temperature was gradually increased from room temperature to a target range of 450-750 °C. The experiments were conducted in a fixed-bed reactor configuration, using a Fe<sub>2</sub>O<sub>3</sub>-to-biomass ratio of 1.0-1.4 under an inert atmosphere. Following each reaction, the resulting biochars were collected and analysed for  $CO_2$  adsorption capacity using thermogravimetric analysis (TGA) to assess their potential as solid sorbents for carbon capture applications. Furthermore, the reduced metal oxides were collected to identify the reduction mechanisms of  $Fe_2O_3$  to  $Fe_3O_4/FeO$  through the advanced combustion of volatiles.

This research is a proof of concept of the potential advancement in the pyrolysis process for efficient and simultaneous biochar (14-20 wt.% of biochar yield) and hydrogen production, coupled with the generation of heat through CLC. This integrated process not only serves as an alternative route for sustainable and carbon-negative biochar and hydrogen production but also positions itself as a cost-effective solution in the landscape of CO<sub>2</sub> capture technologies. Since the biochars produced from WW and CG in the Py-CLC concept demonstrated CO<sub>2</sub> adsorption capacity of 60-180 mg CO<sub>2</sub>/g (6-18%).

Keywords: BECCS, Chemical Looping Combustion, CO<sub>2</sub> capture, Green H<sub>2</sub> production.

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<sup>&</sup>lt;sup>2</sup>Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, United Kingdom.

## Simulation, Process Analysis and Performance Assessment of Solvent-Based Carbon Capture for Refinery

Mohammed Alshemali1 Toluleke Akinola<sup>1</sup> \*Meihong Wang<sup>1</sup>

<sup>1</sup> School of Chemical, Materials and Biological Engineering, University of Sheffield, Sheffield, UK.

While significant research efforts have been directed toward CO<sub>2</sub> mitigation in the power generation sector, the petroleum refinery industry remains an underexplored yet substantial contributor to global CO<sub>2</sub> emissions. Contributing approximately 4% of the total global CO<sub>2</sub> emissions, making them the third-largest stationary source of CO<sub>2</sub> emissions worldwide (IPCC, 2005; Lei et al., 2021). This presentation concerns solvent-based post-combustion capture technology for the refinery through process simulation, specifically focusing on post-combustion CO<sub>2</sub> capture with chemical absorption for the refinery's fluid catalytic cracking (FCC) unit. It will provide a cost-effective and energy-efficient carbon capture process model for FCC through simulation using Aspen Plus® software. To achieve this, the study follows a structured methodology covering four major stages: process modelling and validation, scaling-up, process optimisation, and performance assessment.

**Process modelling and validation:** Develop a carbon capture process model using (30%MEA vs 40% PZ and validate with pilot-scale experimental data from the literature. The pilot plant at the University of Kaiserslautern (Mangalapally and Hasse, 2011) is chosen to validate the MEA process model, while data from the pilot plant located at the University of Texas at Austin (reported by (Plaza and Rochelle, 2011) and (Wagener and Hamilton, 2011) is chosen to validate the PZ process model.

**Scale-up:** The model scale-up is a key step for the process model simulation, aiming to redesign the size of the capture plant model to match the requirements of the flue gas from the FCC unit. The model of the CO2 capture process at the pilot scale will be scaled up based on chemical engineering principles about estimating column diameter and pressure drop through a generalised pressure drop correlation (GPDC) given by (Sinnott, 2005).

**Process Optimization:** The process model parameters will be optimised to enhance capture efficiency for real world applications. First, the main key performance evaluation matrix (e.g., energy consumption, capture level, and cost) is identified. This is followed by sensitivity analysis to determine which variables are more sensitive to this particular performance matrix. Then, the objective function for optimisation is set up.

**Performance Assessment:** To assess the carbon capture plant performance, a comprehensive technoeconomic analysis (TEA) will be conducted. The findings from this analysis are expected to help decision making in industrial applications, providing valuable insights for policymakers and industry leaders.

Keywords: carbon capture, petroleum refineries, post - combustion capture, process simulation, techno-economic analysis, fluid catalytic cracking unit .

Acknowledgement: The first author is supported by Kuwait Institute for Scientific Research (KISR). The authors would like to thank the financial support of the EU RISE project OPTIMAL (Ref: Grant Agreement No: 101007963)

# Modelling\Simulation and analysis of CO<sub>2</sub> Capture with Chemical Absorption for CCGT Power Plants Using Rotating Packed Beds with Mixed Solvent

Idris Jibrin, Toluleke E Akinola, Olajide Otitoju, Meihong Wang\*

School of Chemical, Materials, and Biological Engineering, The University of Sheffield, S1 3JD

The increasing urgency to mitigate CO2 emissions has led to significant research into solvent-based post-combustion carbon capture (PCC) technologies. Conventional packed bed technology, while widely used, poses major challenges such as high energy consumption of power plant energy production, large equipment footprints, and substantial operational costs. Rotating Packed Beds (RPBs) have emerged as a promising alternative due to their enhanced mass transfer efficiency and reduced equipment size. However, limited studies have explored the potential of solvent mixture systems in RPB-based PCC, despite their promising advantages in improving capture efficiency and reducing energy demands. Solvent such as Monoethanolamine (MEA) are energy intensive, thermal degradation, high volatility, corrosion, limited CO2 capture capacity and environmental concerns.

The aim of this study is to investigate the viability and the performance blend of Piperazine(PZ)/sodium hydroxide (NaOH) vs glycerol/MEA in RPB. PZ/NaOH can improve absorption kinetics while reducing regeneration energy compared to amine solvents such as MEA. Similarly, due to the volatile nature of MEA solvent and degradation, glycerol/MEA blend can lower solvent volatility and degradation, extending operational lifespan and reducing solvent losses. The novelty of this research lies in the innovative solvent mixture (PZ/NaOH) and glycerol/MEA and their performance using RPB remain unexplored in the existing literature.

The research methodology will involves developing a rate-based model in Aspen Custom Modeller and Aspen Plus to simulate CO<sub>2</sub> absorption in RPB using a blend mixture of PZ/NaOH and glycerol/MEA. To achieve fast kinetic, alkalinity boost, viscosity control and CO<sub>2</sub> capture capacity. Solvent concentrations 5-15wt% PZ, 2-5 wt.% NaOH, 5-10wt% and 20-30wt% MEA, will be investigated. The models will be validated against experimental data, and a techno-economic analysis (TEA) will assess scalability for industrial applications. Potential challenges, such as solvent stability under RPB conditions, will also be explored. This research could significantly advance the development of energy-efficient and cost-effective CO<sub>2</sub> capture systems, contributing to global climate change mitigation efforts.

## Keywords:

Carbon capture, rotating packed beds, process intensification, hybrid solvents, process modeling, techno-economic assessment.

Acknowledgement: The authors would like to thank the financial support of the EU RISE project OPTIMAL (Grant Agreement No: 101007963).

## Study of Optimal Operation of Ethylene Plant Integrated with Carbon Capture Through Artificial Intelligent based date-driven modelling and Optimisation

Jin Ma<sup>1,2</sup>, Shengyuan Huang<sup>1</sup>, Yao Zhang<sup>1</sup>, \*Meihong Wang<sup>1,2</sup>, Wenli Du<sup>2</sup>, Feng Qian<sup>2</sup>

<sup>1</sup> School of Chemical, Materials and Biological Engineering, The University of Sheffield, Sheffield S1 3JD, United Kingdom

<sup>2</sup> Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, School of Information Science and Engineering, East China University of Science and Technology, Shanghai 200237, China

In the context of global climate change, reducing carbon emissions from industrial processes has emerged as a crucial research priority. Steam cracking-based ethylene production plants, emitting approximately 1-2 ton of  $CO_2$  per ton of ethylene produced, are energy-intensive with significant carbon emissions, making carbon emissions reduction urgent. Among various carbon emissions reduction methods, solvent-based post-combustion carbon capture technology has become the most promising approach for decarbonisation of ethylene production processes, due to its maturity and reliability. However, its performance is highly dependent on the characteristics of flue gas generated by ethylene plant, which is affected by the operating variables such as excess air coefficient.

To achieve low-cost decarbonization in ethylene production processes, this paper proposes an operational optimisation framework for the heat integrated system. This system combines thermal cracking furnace and the carbon capture process with flue gas heat recovery. Based on this system, artificial intelligence-based optimisation is adopted to optimal cracking furnace operating conditions, so as to minimize energy consumption and CO<sub>2</sub> capture cost of the system while maintaining cracking efficiency. A surrogate model for the combustion process of thermal cracking furnace was constructed using a model order reduction approach, while the steam drum and the convection section of the cracking furnace was developed using gradient boosting regression trees. Additionally, a data-driven model of the carbon capture process with flue gas heat recovery was established using physics-informed neural networks.

Three scenarios were investigated: Case 1, an ethylene plant with carbon capture but no heat integration; Case 2, an ethylene plant with carbon capture and heat integration; and Case 3, an ethylene plant with carbon capture, heat integration, and operational optimization. The analysis reveals that, relative to Case 1, Case 2 reduces energy consumption and CO<sub>2</sub> capture costs by 37.7% and 36.7%, respectively, whereas Case 3 achieves reductions of 42.6% and 48.7%, respectively. These results highlight the importance of high temperature and high CO<sub>2</sub> and water vapor concentration of flue gas in reducing the energy requirement and capture cost, providing valuable insights of ethylene production toward carbon neutrality

Keywords: carbon capture, ethylene plant, heat integration, artificial intelligent, modelling and optimisation

Acknowledgement: The UK authors would like to thank the financial support of the EU RISE project OPTIMAL (Ref: Grant Agreement No: 101007963) and CATALYSE (Ref: Grant Agreement No: 10183092).

Modelling\simulation, optimization and performance assessment of large-scale rotating packed bed (RPB)-based post-combustion carbon capture (PCC) process using concentrated MEA for large scale combined cycle gas turbine (CCGT) power plant

Abiodun Tolulope Okeleye, Olajide Otitoju, Toluleke Akinola, Meihong Wang\*

School of Chemical, Material and Biological Engineering, University of Sheffield, UK.

Emission of  $CO_2$ , a major greenhouse gas causing global warming is linked directly to  $CO_2$  emissions from combustion from power plants. Solvent-based post-combustion carbon capture (PCC) using packed bed (PB) technology is the most commercially deployed technology to capture  $CO_2$  from power plants. However, this technology requires high energy demands, high capital (CAPEX), and operating costs (OPEX). The replacement of conventional PBs with rotating packed bed (RPB) technology permits the use of MEA concentrations of well over 30 wt% which will significantly reduce the packing volume required, the size of the columns, and energy required for solvent regeneration. This change has the potential to lower both cost and energy consumption.

Existing studies on RPB-based PCC process have focused on CO<sub>2</sub> capture with a maximum capacity of 100TPD translating to almost 6MWe power plant (Jung et al., 2024a). Furthermore, existing studies (Jassim et al., 2007, Otitoju et al., 2023) on RPB absorbers also showed that using a higher MEA concentration (30 wt%-75 wt%) reduces column size, thus lowering the CAPEX of the RPB-based PCC process. In view of this, studies on large-scale RPB-based PCC (including RPB absorber and RPB stripper) capable of CO<sub>2</sub> capture from a 250MWe CCGT power plant will be needed. This study aims to develop steady-state models for whole RPB-based PCC process and implemented in Aspen Custom Modeller (ACM), model validation with experimental data, model scale-up, optimisation and a comprehensive technoeconomic assessment of a large-scale RPB-based PCC process using different MEA concentrations (30 wt%, 50 wt% and 75 wt%) for a 250MWe CCGT power plant.

**Model validation and scale-up:** The RPB absorber model will be validated using experimental data from (Jassim et al., 2007) while the RPB stripper will be validated with experimental data from (Cheng et al., 2013). The validated RPB absorber and RPB stripper models will be scaled up using the iterative scale-up procedure described by (Otitoju et al., 2023).

**Model simulation:** This will be done by exporting the RPB absorber and RPB stripper models as custom models from the ACM® platform to Aspen Plus® platform. These custom models will be used with other default Aspen Plus blocks® in Aspen Plus®, such as heat exchangers and pumps, to simulate a complete RPB-based PCC process.

**Optimisation**: This aims to minimize total annual cost comprising of the CAPEX and operating cost. This will be implemented by adjusting decision variables which includes design variables such as inner, outer radius and height of both RPB absorber and stripper and operational variables such as the rotor speed of both the RPB absorber and stripper and the solvent flow rate. It will be subject to constraints of  $CO_2$  capture rate of minimum of 90% and reboiler temperature that does not exceed 120 °C. This will be executed in Aspen Plus<sup>®</sup>.

**Technical and economic assessments (TEA):** For performance assessment, comprehensive TEA will be conducted using APEA<sup>™</sup> to estimate the direct costs associated with the absorber, stripper, and other components, CAPEX, and OPEX for the plant.

*Keywords:* Post-combustion carbon capture, Rotating packed bed, Scale-up, Technical and economic assessments, Optimisation, Combined cycle gas turbine power plant.

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Hybrid modelling\simulation and techno-economic performance assessment of direct air capture integrated with post-combustion capture using different solvents for ethylene plant

Yao Zhang <sup>a</sup>, Shengyuan Huang <sup>a</sup>, Jin Ma <sup>b</sup>, \*Meihong Wang <sup>a</sup>

<sup>a</sup> School of Chemical, Materials and Biological Engineering, The University of Sheffield, Sheffield S1 3JD, UK
 <sup>b</sup> Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, School of Information Science and Engineering, East China University of Science and Technology, Shanghai 200237, China

Carbon capture technology is increasingly becoming a hot research topic among researchers in order to address the issue of climate change due to elevated concentrations of carbon dioxide in the atmosphere. As post-combustion carbon capture (PCC) based on chemical absorption has been commercially deployed, a few studies began to exploring the potential for integrating direct air capture (DAC) with solvent-based post-combustion carbon capture. Through solvent recirculation, this new integrated process enables the reduction of energy consumption and the capture of more carbon dioxide. However, there may be significant differences in the performance of different solvents (e.g., MEA and PZ) when this integrated process is used. Therefore, a comparative technical economic assessment of the different solvents in this integrated process through modelling and simulation is necessary. However, due to the complexity of the process and the physical properties of the solvent, modelling and simulation of such an integrated process still face challenges of low accuracy and high computational demand. By embedding the physical information of the process into machine learning in the form of constraints, development of hybrid models can greatly reduce the complexity and computational demand of the model while ensuring the physical interpretability, providing a solid foundation for technical economic assessment based on modelling and simulation.

This study aims to develop a hybrid model of DAC integrated with PCC using different solvents for ethylene plant and carry out techno-economic performance assessment based on modelling and simulation. The model will be validated by pilot scale experiment data. The performance of MEA and PZ at different power plant load and carbon capture level will be compared. This study provides an advanced approach to the modelling of DAC integrated with PCC using different solvents, and the results of detailed comparative technical and economic assessment of its application to the ethylene plant are useful for process design by the industrial practitioners. It also provides guidance for modelling other complex processes, as well as newer solvent.

Keywords: Hybrid modelling, process simulation, direct air capture, post-combustion capture, process integration, different solvents

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# Opportunities and Challenges in Process Intensified CO<sub>2</sub> capture from Biomass (BECCS)

\*Muhammad Akram<sup>1</sup>, Kris Milkowski<sup>1</sup>, Abdulaziz Gheit<sup>1</sup>, Janos Szuhanszki<sup>1</sup>, Ihab Ahmed<sup>1</sup>, Jon Lee<sup>2</sup>, Mohamed Pourkashanian<sup>1</sup>

<sup>1</sup>Energy Innovation Centre (EIC), Department of Mechanical Engineering, University of Sheffield, Sheffield S10 2TN, UK

<sup>2</sup>School of Engineering, Newcastle University, Merz Court, Claremont Road, Newcastle upon Tyne NE1 7RU, UK

This paper presents data gathered during demonstration of post combustion  $CO_2$  capture technology with flue gases generated from biomass at the Energy Innovation Centre's waste to energy and  $CO_2$  capture facilities. Flue gas, with a  $CO_2$  content of  $\sim 10.5\%$ , generated by a 250 kWth biomass boiler was fed to a 1 tpd  $CO_2$  capture plant. For these tests Rotating Packed Bed (RPB) absorber was operated with a conventional packed bed desorber. The solvent used for Monoethanolamine,  $\sim 35$ wt%. Desorber pressure was maintained at 1.5 bara. Solvent flow rate was varied to achieve different liquid to gas ratios (1.8 to 3). Pressurised hot water (PHW) was used for desorbing  $CO_2$  and setpoint of the PHW was changed to achieve desired capture efficiency.  $CO_2$  loadings and solvent concentrations were measured using Mettler Toledo auto-titrator. Particulates content of the flue gas was measured, and particulates were collected for further analysis at the boiler exit and absorber inlet by Electrical Low-Pressure Impactor (ELPI®+) manufactured by Dekati®.

The particulate samples were analysed by ICP-OES to investigate the impact of metals in the flue gas coming from the biomass on the solvent degradation. The results indicate that around 93% of the particulates measured at the boiler exit were lost in the flue gas ductwork, likely due to the long length of the flue gas transfer pipework and condensation within them. Moreover, particulates seem to have been fragmented during the journey. The ICP analysis has shown that K, Zn, Na and Fe were present in the highest amounts in the particles with most of the metals present in the size range of  $0.1 \text{ to } 0.3 \text{ } \mu\text{m}$ .

Solvent samples were collected and analysed with ICP-MS and Ion Chromatography to quantify build-up of metals and anions in the solvent over time. Potassium, Calcium and Sodium were found to be present in significant amounts in the solvent over the 116 hrs test period. However, Fe, Mg and other metals were found in small quantities, <2mg/kg of solvent. Build-up of anions as measured by Ion Chromatography indicated that Formate was present in the highest amount followed by nitrate and Nitrite. Oxalate was found to be the lowest at ~2ppm.

During the tests capture efficiency was mostly around 85-88% while reboiler duty was 4-5 MJ/kg of CO<sub>2</sub> captured. The minimum reboiler duty was observed at L/G ratio of ~2. The project has highlighted some key practicality issues during post combustion capture from biomass flue gases such as flue gas variability, carry over of particulates and metals and solvent degradation. There is very limited information on this subject in open literature. The short-term tests presented here can serve as a starting point for further longer-term investigations into the impact of biomass flue gas contaminants on the solvent behaviour and the solvent management requirements during CO<sub>2</sub> capture from biomass flue gases.

Keywords: CO<sub>2</sub> capture, bioenergy, biomass, process intensification

Acknowledgement: The authors want to acknowledge the financial support provided by Industrial Decarbonisation Research and Innovation Centre (IDRIC). Experimental facilities of the Energy Innovation Centre (EIC) at the University of Sheffield, have been used for the experimental work.

# Session 2A. Biomass/Waste 1 Wednesday, 10<sup>th</sup> September

Multi-Objective Optimisation of Waste-to-Resource Management for Small-Island Developing States.

Sherard Sadeek<sup>1</sup>, Arun Mangra<sup>1</sup>, Keeran Ward<sup>2</sup>, Maria M. Papathanasiou<sup>3,4</sup>, Dhurjati Chakrabarti<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, The University of the West Indies, St. Augustine, Trinidad and Tobago, <sup>2</sup>School of Chemical and Process Engineering (SCAPE), University of Leeds, Leeds, LS2 9JT, UK, <sup>3</sup>Sargent Centre for Process Systems Engineering (SCPSE), Imperial College London, South Kensington Campus, London SW7 2AZ, UK, <sup>4</sup>Department of Chemical Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

Sustainable municipal solid waste (MSW) management is a pressing global issue, with prominent challenges such as landfill overuse, poor recycling, limited funding, and infrastructure hurdles particularly affecting small-island developing nations (SIDS). The balance between environmental and economic objectives is crucial for driving optimal decision-making, aiding SIDS in achieving a sustainable transition towards cleaner productivity. Our model offers a multi-objective framework for understanding how MSW fractions- plastic, organics, paper and textiles- can be sustainably managed across three (3) techno-economicenvironmental scenarios linked to landfilling, recycling and incineration. The model superstructure examines waste collection, transport, sorting and final disposal with Pareto optimal solutions outlining current and future scenario and location-specific economic and environmental trade-offs. Our results illustrate a 63% reduction in CO<sub>2</sub> emissions compared to current landfilling business-as-usual (BAU) operations, from complimenting greater recycling and incineration into waste processing and disposal within land-use constraints and growing population densities. However, these reductions accompany increased levelised waste management costs from US\$59 to USD\$134 per tonne. Furthermore, sensitivity analyses performed on organic and plastic waste fractions and sorting and landfilling costs illustrate optimal waste flows and transportation models, providing insights into the decentralisation and debottlenecking of core disposal technologies to inform better waste management practices and integrate new fiscal policies. Ultimately, our waste management model provides a holistic overview of a growing problem among SIDS, with strong incentives and solution support to drive the sustainable transition towards greater resource circularity and efficiency across the MSW life cycle.

Keywords: Mixed-Integer Linear Programming, Multi-Objective Optimisation, Waste Technology, Life-cycle Assessment, Sustainable Development.

### Resource Assessment of Water Hyacinth in India and it's Bioenergy Potential

\*Ryan Longley<sup>1</sup>, Andrew Ross<sup>1</sup>, Keeran Ward<sup>1</sup>, Gaurav Nahar<sup>2</sup>

<sup>1</sup> School of Chemical and Process Engineering, University of Leeds, UK
<sup>2</sup> Defiant Renewables, Pune, Maharashtra, India

Water hyacinth leads to huge environmental, ecological, and socioeconomic impacts in subtropical regions. It is now found on every continent except Antarctica causing considerable challenges for riparian communities and economic challenges for local and national governments. The methods of control and management of water hyacinth have thus far been largely unsuccessful. This study aims to combine remote sensing resource assessment tools and laboratory scale bioenergy conversion data to predict the potential for valorising water hyacinth to bioenergy. The overall aim is to promote the sustainable management of water hyacinth and develop a circular bioeconomy in India.

**Resource Assessment**: The resource assessment of water hyacinth at the chosen locations was achieved using the open-source remote sensing software Google Earth Engine (GEE). Remote sensing was the most desirable method to meet the specific objectives as it can be executed remotely, it provides rapid quantitative data, which can be applied to different regions. Furthermore, remote sensing also allows for the visualisation of data for entire water bodies and can be used for monitoring coverage over long time periods.

Remote sensing data was obtained for the aquatic vegetation coverage at five different water bodies in several regions of India where water hyacinth was known to be present. Data for water surface area and percentage vegetation coverage over a period of five years was used to determine the average annual distribution of water hyacinth biomass. From the 5 locations monitored the average maximum vegetation coverage observed was 55.4%.

**Bioenergy Conversion Calculator:** The bioenergy conversion approaches considered for this study were based on their suitability for use with aquatic/lignocellulosic biomass feedstocks Data was obtained from literature studies for anaerobic digestion, fermentation, hydrothermal carbonisation, and hydrothermal liquefaction. From this data robust correlations between biomass resource and bioenergy output could be determined.

The average product yields for biomethane; bioethanol; hydrochar; and biocrude were  $0.17m^3/kgWH_{(dry)}$ ;  $0.22kg/kgWH_{(dry)}$ ;  $50.42wt\%WH_{(dry)}$ ; and  $31.21wt\%WH_{(dry)}$ , respectively, with reported HHVs,  $39.80MJ/m^3$ ; 26.70MJ/kg; 18.69MJ/kg; and 27.10MJ/kg, respectively. The energy potential of water hyacinth was compared with the top three agricultural residues in India; wheat straw, rice straw, and sugarcane. The total harvest area for wheat; rice; sugarcane; and water hyacinth was  $31.45x10^6$  ha;  $43.78x10^6$  ha;  $4.57x10^6$  ha; and  $1.57x10^6$  ha respectively, whilst the energy potential per hectare was 80.88GJ/ha; 48.45GJ/ha; 452.43GJ/ha; and 146.39GJ/ha, respectively. This shows that water hyacinth has a higher energy potential per unit area than wheat and straw residue.

Keywords: bioenergy, resource assessment, water hyacinth, remote sensing

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Characterisation of chars produced from washed and thermochemically pretreated wood biomass – an intermediate biofuel for hydrogen production

Lusani Mulaudzi<sup>1</sup>, Samuel A. Iwarere<sup>1</sup>, \*Michael O.Daramola<sup>1</sup>

<sup>1</sup> Sustainable Energy and Environment Research Group (SEERG), Department of Chemical Engineering, University of Pretoria, Pretoria, South Africa

The global production of industrial scale quantities of hydrogen (H<sub>2</sub>) is currently heavily reliant on thermochemical conversion of fossil fuels, which has negative environmental connotations inherent in the conversion of fossil fuels. Biomass is currently being explored as an alternative feedstock to either supplement or replace fossil fuels in H<sub>2</sub> production, largely through adaptation of the thermochemical processes designed for fossil fuels.

There are however drawbacks to using biomass in thermochemical conversion processes, which are a result of the (generally) high ash content, nature of the ash, and poor fuel properties of raw biomass. These drawbacks limit the quantity of biomass that can be used in conversion process due to problems that arise related to equipment and operational issues, poor quality of products, mass and energy transfer limitation, low energy efficiencies, etc. Washing pre-treatment and thermochemical pre-treatment are techniques that are most commonly employed to tackle the problems of ash and poor fuel properties respectively. Mineral acids are commonly used for the washing pre-treatment step, and hydrothermal carbonisation (HTC) and torrefaction are mostly employed for the thermochemical pre-treatment step.

Both washing and thermochemical pre-treatment methods alter the structure (make-up) and composition of the pre-treated biomass, which could be due to changes effected on the surface or the organic matrix of the biomass. The result is a biomass product with (various) properties from those of the starting material. Consequently, the pre-treated (both washing and thermochemical) biomass requires a comprehensive characterisation to effectively determine the degree to which alteration has been effected, and to determine the potential suitability of the resulting pre-treated (intermediate) biomass as a feedstock for H<sub>2</sub> production through thermochemical conversion.

As such, the current study aims to perform characterisation of wood biomass derived hydrochars (from HTC) and biochars (from torrefaction) produced by a combination of washing and thermochemical pretreatment methods, with an intention of producing a fuel suitable for H<sub>2</sub> production by thermochemical conversion. Washing pretreatment will be conducted using the aqueous phase derived from the HTC process to ensure sustainability, and thermochemical pretreatment will include HTC and torrefaction. Characterisation of the chars will focus on evaluation of the energy properties/parameters, ash composition, functional groups, surface morphology and elemental make-up, surface area/porosity, and transformation of the carbon structure. Analysis of effluents from the washing pretreatment step will also be performed to enhance evaluation of the interaction between the different pretreatment steps.

*Keywords:* Biofuel, Characterisation, Char, Hydrogen, Pretreatment, Thermochemical conversion, Wood biomass

Acknowledgement: This work is supported by York Timbers.

Utilising electrochemical hydrogenation for the mild upgrading of Pinewood and Wheat straw bio-oils

Cesar Catizane<sup>1</sup>, Ying Jiang<sup>2</sup>, Scott Banks<sup>3</sup>, Joy Sumner<sup>4</sup> and Stefano Mori<sup>1</sup>

- 1. School of Water, Energy and Environment, Cranfield University, Cranfield, MK43 0AL, UK
  2. Renewable and Sustainable Energy Research Centre, Technology Innovation Institute, Abu Dhabi, UAE
  - 3. College of Engineering and Physical Sciences, Aston University, Birmingham, B4 7ET, UK
  - 4. Franco-Australian Centre for Energy, Swinburne University of Technology, Melbourne, Australia

Electrochemical hydrogenation (ECH) is a promising technique for upgrading bio-oils by selectively hydrogenating and deoxygenating oxygen-rich compounds under mild conditions. This study investigates the ECH of the oily phase of bio-oils derived from slow pyrolysis of wheat straw and pinewood, utilising a PtRu/ACC electrode and methanol as the catholyte. Sodium chloride (NaCl) and tetrabutylammonium hexafluorophosphate (TBAHFP) were evaluated as additives to enhance electrolyte conductivity which had detrimental impacts on electrode stability. GC-MS and FTIR analyses revealed that phenolic compounds were preferentially hydrogenated, resulting in reduced unsaturation and increased alcohol content. While NaCl improved conductivity, it caused significant cathode corrosion due to chloride-induced degradation. TBAHFP, though less corrosive, led to secondary reactions, such as the formation of trimethyl phosphate, which facilitated the methylation of phenolic compounds. SEM imaging confirmed additive-specific degradation patterns on the cathode, with TBAHFP showing unexpected surface damage despite its inert properties. The findings highlight the trade-offs between additive performance and material stability, providing insights into optimising ECH conditions for bio-oil upgrading. This work underscores the potential for tailored additive selection to enhance bio-oil quality, advancing its viability as a renewable fuel alternative.

#### Pyrolysis gas and biochar generation for five woods

Aysha Irstad<sup>1,2</sup>, G.E. Andrews<sup>1\*</sup> and H.N. Phylaktou<sup>1</sup>

<sup>1</sup>University of Leeds, UK, <sup>2</sup>University of Engineering & Technology, Lahore, Pakistan

Biomass Pyrolysis Gas (BPG) generation and biochar formation for 5 wood types were investigated using hard and soft woods: pine, acacia, eucalyptus, sycamore, dry ash. The cone calorimeter with an air box was used with nitrogen flow replacing the normal air flow. Heated (190°C) gas sample lines and a 190°C heated FTIR were used to measure the BPG released in hot vapour form. Provided the temperature of the BPG is maintained by transfer pipe insulation, the BPG gas could be supplied to a burner and a suitable burner has been developed by the authors.

Hydrocarbons and oxygenated hydrocarbons were produced with CO. Some gases were pyrolysed over the temperature range  $80-500^{\circ}$ C: CO, xylene, formaldehyde, acetaldehyde, acrolein, tri-methyl benzene, toluene, phenol. Other gases were pyrolysed at high temperatures in the range  $350-500^{\circ}$ C: methane, ethane, formic acid, acetic acid, methanol, ethanol, acetone, furfural, furfural alcohol, p.creosote.

The five woods had a range of char and volatile yields, as summarised in Table 1. The char contained a large fraction of the wood mass and the typical GCV of char is 30 MJ/kg. This energy could be recovered in a separate burner or be gasified to produce hydrogen, but a more effective use is to add to soil to enhance the CO<sub>2</sub> adsorption of the soil from the atmosphere.

The volatlile mass balance from FTIR emissions was in very good agreement with the mass loss from the load cell used in the cone calorimeter, as shown in Table 1. The cumulative energy content of the different pyrolysis products and of the remaining char gave comparable energy content to the GCV of the wood determined by bomb calorimetry.

The cumulative volatiles formed were, in order of amount, formic acid, xylene, CO, trimethylbenzene, acetic acid, acrolein, toluene and 21 other species. The total volatile mass by FTIR and the flammable species mass are shown in Table 1 together with the GCV of the flammable mass as MJ per kg of total volatiles. The GCV of the BPG is low, in the range 10-16 MJ/kg, which together with the CO<sub>2</sub> and water vapour in the BPG is difficult burn, but has been achieved.

Table 1: Proportion of wood converted to char, volatiles, flammable volatiles and their GCV.

Biomass	Final biochar	Total Volatile Mass loss	Volatile gas Mass from FTIR %	CO/HC/HCO Volatiles % mass of wood	GCV of volatiles at 450°C MJ/kg <sub>volatiles</sub>
Pine wood	27.7%	72.3%	76.3%	40%	14
Eucalyptus wood	35.5%	64.5%	67.0%	28%	16
Acacia wood	32.2%	67.8%	71.9%	30%	10-20
Dry ash wood	29.5%	70.5%	75.0%	34%	10
Sycamore wood	28.4%	71.6%	75.6%	33%	13

Keywords: bioenergy, biomass pyrolysis gas, bio-char

Acknowledgement: Aysha Irstad would like to thank the University of Lahore for a Scholarship.

# Improving combustion and gasification performance of refuse derived fuel using torrefaction

\*James Banks1, Richard Marsh1, Julian Steer1

<sup>1</sup>Cardiff University, Cardiff, UK

While being an abundant resource for thermal treatment and waste-to-energy applications, Refuse Derived Fuel (RDF) has properties that make it challenging for processes such as combustion and gasification. This study investigates the potential of torrefaction at modest temperatures (<350°C) to upgrade RDF into an improved fuel source by increasing thermochemical characteristics and reducing the contaminants commonly found in wastes.

A commercially available RDF was torrefied at temperatures between 200 and 350°C in a low oxygen environment for residence times of 30 and 60 minutes. Raw and torrefied samples were then tested to assess their potential behaviour in a combustion and gasifying environment. Proximate and Ultimate analysis, including chlorine analysis using XRF, Ion Chromatography and mineral composition of the subsequent ash were determined. In addition, particle size, mass yield and energy density were measured.

Torrefaction provided an increase in energy density, but with minimal mass loss and demonstrated an upgraded fuel with only small changes to calorific value. In addition, torrefaction decreased the chlorine content in the fuel, which will potentially increase the lifetime of boiler and gasifier hardware as reduced chlorine content reduces the amount corrosion caused by chlorine byproducts such as hydrochloric acid.

Keywords: torrefaction, RDF, chlorine, gasification

Acknowledgement: This work is supported by Resilient Decarbonised Fuel and Energy Systems Doctoral Training Program

### Session 2B Gasification/Pyrolysis Wednesday, 10th September

Pyrolysis/non-thermal Plasma/catalysis of Waste Plastics for the Production of Liquid Fuels and Chemicals

Jie Gu, Paul T. Williams \*

School of Chemical and Process Engineering, University of Leeds, Leeds, UK

This study investigates the pyrolysis coupled with non-thermal plasma assisted catalysis of waste plastics (polypropylene) using a ZSM-Y catalyst, focusing on the effects of catalytic temperature and plasticto-catalyst mass ratio on product composition in relation to the production of liquid fuels and chemicals. Initial experiments investigated the pyrolysis/catalysis of polypropylene to compare with the non-thermal plasma/catalysis process. The results for pyrolysis/catalysis showed that as the catalytic temperature increases, gas yield rises, particularly at higher catalyst ratios (2:2 or 1:1), while liquid yield reaches its maximum at 500°C under lower catalyst ratios (2:1 or 1:0.5). Gas composition analysis reveals that propylene (C<sub>3</sub>H<sub>6</sub>) is the dominant product, with higher selectivity observed under the 2:2 ratio, whereas lower catalyst ratios (2:1) favor the formation of smaller hydrocarbons such as methane (CH<sub>4</sub>) and ethylene (C<sub>2</sub>H<sub>4</sub>), especially at higher temperatures. Hydrogen (H2) yield increases with catalytic temperature, peaking at 650°C under the 1:1 ratio, suggesting enhanced catalyst activation at higher temperatures. Oil product analysis shows that aromatic hydrocarbons dominate, with BTEX (benzene, toluene, ethylbenzene, and xylene) accounting for 78.06% of the total liquid fraction and styrene (C<sub>8</sub>H<sub>8</sub>) reaching 57.08%. Additionally, minor amounts of polycyclic and conjugated olefins were detected, indicating complex reaction pathways. These findings demonstrate that optimizing catalytic temperature and catalyst ratio can effectively control product distribution, improve selectivity toward target compounds, and enhance the efficiency of plasticspyrolysis.

In addition, pyrolysis/non-thermal plasma/catalysis of polypropylene using the ZSM-Y catalyst was also investigated. The results showed that the introduction of the non-thermal plasma produced a marked increase in monocyclic aromatic hydrocarbons (e.g. ethylbenzene) while polycyclic aromatic compounds decreased in concentration.

Keywords: hydrothermal liquefaction, direct HTL, two-stage HTL, biocrude

Gasification of Whisky Distillery Waste for Distillery Heat

### Session 2B Gasification/Pyrolysis Wednesday, 10th September

Gordon Andrews\*<sup>1,2</sup>, Herodotus Phylaktou<sup>1</sup>, Ramon Quinonez Acre<sup>2</sup>, Francis Olanrewaju<sup>2</sup>, Richard Wakeman<sup>2</sup>, Steve Smith<sup>2</sup>, Ray Massey<sup>2</sup> and Ian Bownes<sup>3</sup>

<sup>1</sup>University of Leeds. Leeds, UK, LS2 9JT. <sup>2</sup>Clean Burner Systems Ltd. 11 Caputhall Road, Deans Industrial Estate, Livingston, UK. EH54 8AS. <sup>3</sup>Colorado Construction and Engineering. 11 Caputhall Road, Livingston, UK. EH54 8AS.

The present work uses whisky industrial waste biomass for the decarbonization of the distillery and can be applied to any industrial heat process with biomass waste generation. The principle distillery wastes are draff, pot ale and spent lees and these are all wet wastes. The authors have shown that there is sufficient waste biomass energy from the distillery industry to evaporate all the water and provide the energy to operate the distillery. There are also many other sources of wet wastes, particularly in farm wastes slurries, that could be used as an industrial fuel. A process that could simultaneously dry the biomass and produce energy, would be preferable as the waste could be used directly from the process, retaining the sensible heat.

TGA analysis of draff shows that 50% of the mass is devolatilised between 250° and 370°C. By heating up to 550°C there was a release of 80% of draff as volatiles. Heating also dries the biomass. The batch air gasifier design that was used was similar to smaller scale commercially available domestic log gasifiers, with a preburner for ignition and heating of the logs. A batch gasifier has a batch of biomass waste material and the gasification rate is set by the oxygen supply from a pre-burner, which must operate very lean to provide heat and oxygen for the gasification heat release. The aim was to pass the biomass gasification gas (BGG) from the gasifier directly to the BGG Jet Mix burner, retaining the sensible heat, and to burn it using co-firing with NG. The BGG Jet Mix burner had 8 axial air jets with 8 radial jets fired between the axial air jets and the radial jets were fed with BGG. The NG to support the flame stability was fired on the centreline of the radial BGG jets. The power turn-down flame stability for NG was very good, but with BGG in the radial jets the flame was not stable due to the high water and nitrogen content. Stable flames were achieved by co-firing with NG. The BGG burner could be operated on hydrogen for zero carbon emissions.

A  $30\text{m}^3$  cubic gasifier was used with refractory walls. This had a problem with high thermal inertia and when empty it took 10 hours at 230 kW on the preburner to reach  $200^{\circ}\text{C}$  air outlet temperature and  $500^{\circ}\text{C}$  after an additional 14 hours at 300 kW. With 750 kg of straw and wet draff biomass in the present work, the heating was faster due to heat release from the biomass. The pre-burner at 280 kW enabled  $350^{\circ}\text{C}$  BGG gas outlet temperature to be achieved, which would dry and devolatilize most of the outer biomass layers and achieved significant heat release from the BGG. The BGG burner was designed to achieve 2MW thermal output and initially 1 MW was provided by the NG fuel with 15% O<sub>2</sub> at the flame outlet. The BGG gases from the gasifier consumed some of the surplus BGG burner O<sub>2</sub> and at  $350^{\circ}\text{C}$  at the gasifier outlet the BGG burner outlet was 11.8% and the 3.2% oxygen consumed showed that BGG heat release had been achieved. The BGG flammable content was CO and hydrocarbons (speciated using a heated FTIR). There were problems of BGG flame stability and this was shown to be a lean flame blow out, which could be controlled by keeping the BGG burner flame on NG only to give a burner oxygen output of <10%. The BGG burner combustion efficiency was >99%. The blue flame on NG became yellow with the hydrocarbon rich BGG.

Keywords: bioenergy, biomass, industrial burners,

Acknowledgement: This work is supported by UK DESNZ Green Distilleries Programme

Direct Chemical Looping Gasification of Biochar/Biomass: A Pathway to Efficient Syngas Production

### **Gasification/Pyrolysis Wednesday, 10<sup>th</sup> September** \*Maryam Awode<sup>1</sup>, Begum Tokay<sup>2</sup>, Colin E. Snape<sup>1</sup>, Fatih Güleç<sup>1,2</sup> Session 2B

<sup>1</sup>Low Carbon Energy and Resources Technologies Research Group, Faculty of Engineering, University of Nottingham, Nottingham NG7 2TU, United Kingdom. <sup>2</sup>Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, United Kingdom.

Rising carbon emissions from fossil fuel consumption are accelerating global warming, contributing to extreme weather events, sea-level rise, and biodiversity loss. The urgent need for sustainable energy alternatives has driven interest in carbon capture technologies, with chemical looping emerging as a promising approach for mitigating emissions while enabling cleaner fuel production. As a crucial component of carbon capture and utilisation strategies, chemical looping enables efficient conversion of biomass to syngas, reducing reliance on fossil fuels and promoting carbon-neutral energy systems. However, optimising process conditions and oxygen carrier (OC) compositions remains a challenge for improving efficiency and scalability.

This study investigates the gasification of biochar derived from White Wood (WW) and Coffee Grounds Residue (CG) using Fe-based oxygen carriers in a chemical looping process. Specifically, the effects of temperature (700-900°C), oxygen carrier-to-fuel ratio (0.1-0.3), and OC composition - including Fe-based carriers with Co, Mn, and Ni additives- on gasification performance are systematically examined. Transition metal oxides are expected to enhance oxygen transport capacity, reaction kinetics, and syngas selectivity, influencing both carbon conversion efficiency (CCE) and product distribution. By optimising these parameters, this study aims to advance biomass/biochar utilisation, providing insights into the role of operating conditions and material properties in maximising syngas yields and carbon utilisation efficiency.

OCs were synthesised via coprecipitation and characterised using SEM-EDX, XRD, and XPS to determine their structural and morphological properties. SEM revealed variations in particle morphology influenced by the choice of precipitating agents, while XRD identified Fe<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>O<sub>3</sub>, NiO, Al<sub>2</sub>O<sub>3</sub>, FeMnO<sub>3</sub>, and spinel phases as the dominant crystalline components. Although XRD did not detect the presence of Alsupport in the composites, XPS and EDX confirmed its incorporation, validating the synthesis process. These findings provide critical insights into the physicochemical properties of Fe-based OCs, which play a crucial role in their reactivity, stability, and overall performance in biomass chemical looping applications. Preliminary experiments demonstrated that higher than 95 vol.% of the carbon conversion efficiency is possible with biochar gasification under Fe<sub>2</sub>O<sub>3</sub> with stochiometric ratio of OC:Fuel of 0.2. The results of this study will contribute to the ongoing development of advanced chemical looping technologies by refining process parameters and optimising OC compositions. By addressing key challenges in biomass-based chemical looping, this research supports the transition towards cleaner energy systems, offering a sustainable approach syngas production while reducing carbon emissions.

Keywords: Biochar, Biomass, Chemical Looping Gasification, Carbon Conversion Efficiency, Syngas Production, Carbon Capture.

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# European Power Sector emissions: Are we sure Gas is better than Coal? Stewart Bradley

Uniper Technologies Ltd

The decarbonisation of the power sector in Europe continues to see the closure of coal stations and the expansion of renewables supported by gas-fired generation. This transitioning correlates with declines in GHG emissions at a national level but it has been questioned if the same gains are being realised at the global level. The rapid increase of the international LNG market coupled with improved methane emissions quantification change the GHG lifecycle analysis of gas used for power generation.

One controversial analysis concludes that US LNG imported into Europe has a greater GHG footprint than coal-fired generation once upstream methane emissions are considered. Whilst there is a consensus that US methane emissions have been under-reported historically, the conclusion that gas-fired generation may have a greater impact on the climate than coal is misleading. As Europe imports the majority of its fossil energy the issue of accounting for upstream emissions remains important, particularly due to variation in regulation of GHG emissions between countries that produce natural gas.

The EU's Methane Regulation (EUMR) introduced in 2024 includes requirements intended to address emissions at producer-level for fossil energy imported into the EU. Whilst it introduces comprehensive monitoring requirements on up- and mid-stream operators in the EU it additionally obliges importers to ensure their non-EU production sources are equivalent. The requirements on EU operators and importers increase incrementally over time, culminating in a cap on the methane intensity of fossil energy imports in 2030.

Keywords: methane, emissions, regulation

### Influence of Model Butyl-based Biofuel Blending with HVO Biodiesel on Engine Performance and Emissions

\*K.S. Hernández-Domínguez $^1$ , S. Wiseman $^1$ , H. Li $^1$ , A.S. Tomlin $^1$ 

<sup>1</sup>School of Chemical and Process Engineering, University of Leeds, Leeds, United Kingdom, LS2 9JT

Heavy-duty vehicles and off-road machinery commonly depend on compression ignition (CI) engines, which utilise diesel as the primary fuel source. A replacement for these fossil fuels is needed, such as lower-carbon alternatives. At the same time, the EU Renewable Energy Directive (REDII) mandates an increased use of advanced biofuel components within liquid fuel blends to reduce greenhouse gas emissions. It is, therefore, important to investigate the impact of using alternative fuels on engine performance to ensure that they will improve compliance with emissions standards. Advanced biofuels present a viable option to satisfy the criteria of current and future emissions standards and regulations while improving air quality. These biofuels, also classified as second-generation biofuels, are mainly produced from lignocellulosic feedstocks. Acid-catalysed alcoholysis serves as a potential method for producing liquid biofuels. The reaction of lignocellulosic material with alcohol, used as a solvent, would produce a complex mixture of products, which includes the alcohol used as the solvent, an alkyl levulinate and the corresponding ether as three of the leading products in the mixture [1].

A series of model blends was previously defined to represent the final products of alcoholysis, varying the blending levels of n-butyl levulinate (BL), di-n-butyl ether (DNBE), and n- butanol (BuOH) with ultra-low sulfur diesel (ULSD), while also adjusting the composition of each biofuel component [2]. A new set of blends was also proposed, incorporating hydrotreated vegetable oil (HVO) biodiesel as a substitute for ULSD as the base fuel in the blends due to its promising combustion properties and the possibility of replacing diesel without modifying engines. This study focuses on the emissions and performance of a Yanmar L100V CI engine as part of a generator set fueled with this potential lignocellulosic-derived model biofuel blended with HVO biodiesel in different ratios. Ignition delays (ID) were calculated from the crank angle and engine RPM data. Gaseous emissions were measured using a Horiba MEXA7100D and a Gasmet DX4000 FTIR, total particle number (PN) using a Cambustion DMS500, and particulate matter (PM2.5) was captured on filter papers. All blends, including pure HVO biodiesel, had shorter IDs compared to diesel, affecting engine performance and emissions, favouring the reduction of nitrogen oxides (NOx=NO+NO2). Emissions of CO, total hydrocarbons (THC) and NOx were reduced relative to diesel. Exhaust concentrations of volatile organic compounds such as formaldehyde and hexane also decreased relative to diesel. PM2.5 and the total PN reduced for the set of model blends relative to pure HVO and ULSD upon the addition of biofuel. Emission indices of CO were lower than the Stage V limits defined in BS2869, whilst slight exceedances were shown for THC and NOx.

Keywords: Advanced biofuels, Compression Ignition Engine, Emissions, Particulate Matter.

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### Application of ammonia water in a Venturi tube

\*Serhii Horianoi <sup>1,2</sup>; Igor Volchyn<sup>1,3</sup>, Andrii Yasynetskyi <sup>1,2</sup>

<sup>1</sup>Thermal Energy Technology Institute, NAS of Ukraine <sup>2</sup>National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnical Institute", Kyiv, Ukraine <sup>3</sup>National University of Food Technologies, Kyiv, Ukraine

Increasing the environmental requirements for energy production stimulates the modernisation of gas cleaning equipment for combustion plants. A significant part of them is equipped with wet Venturi scrubbers as dust removal facilities. The possibility of using wet Venturi scrubbers as devices for complex flue gas cleaning from particulate matter and sulphur dioxide is considered. For this purpose, mathematical modelling and experimental studies were carried out. In the study, an aqueous solution of ammonia in droplet form was proposed as a reagent and medium for capturing the dust particles. In a Venturi tube, droplets are dispersed by increasing the gas flow velocity in the throat to 70-100 m/s, which helps to reduce the size of droplets and increase their total contact area with the gas phase. The analytical calculation established the dependence of the distance between drops on the spaying density according to the power law -(1/3).

**Dust removal:** In mathematical modelling, measures to increase the efficiency of particulate deposition on droplets in the Venturi tube diffuser were evaluated. The efficiency of particulate matter removal can be increased by increasing the spray density and narrowing the throat of the Venturi tube. The calculated efficiency of particulate matter capture by droplets of 150  $\mu$ m size at a specific liquid flow rate of more than 0.5 kg/nm3 was above 99.9%.

**Desulphurization:** The use of an aqueous ammonia solution as a reagent ensures that sulphur dioxide is bound by the reaction:

$$SO_2 + 2NH_3xH_2O + O_2 = (NH_4)_2SO_4 + H_2O$$

The sulphur dioxide enters the reagent droplets by diffusion and has to travel a distance of 5-6 droplet diameters during its stay in the Venturi tube. The use of the Fourier transforms in the mathematical modelling of the process allowed us to obtain an analytical formula for estimating the time required to capture sulphur dioxide molecules in the Venturi tube. According to the results of mathematical modelling, a practical complete absorption of sulphur dioxide on 150  $\mu$ m ammonia water droplets with an ammonia content of less than 0.3% was obtained.

**Experimental studies:** During the experimental study, the process of sulphur dioxide absorption by an aqueous ammonia solution was studied. Air was used as the gas phase, into which sulphur dioxide was supplied at a flow rate of 6 l/min, which ensures a sulphur dioxide concentration of 1500 ppm. The specific consumption of aqueous ammonia solution was 0.6 kg/m<sup>3</sup> of model gas. The concentration of ammonia in the aqueous solution corresponded to the stoichiometric mole ratio  $NH_3/SO_2 = 1.9-2.0$ . As a result, a sulphur dioxide capture efficiency of 98.15 % was achieved.

Keywords: flue gas, ammonia, particulate matter, sulphur dioxide, complex cleaning

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### Optimizing Ship Engine Performance and Emissions Under Transient Operating Conditions

Mojibul Sajjad<sup>1</sup>, Thuy Chu Van<sup>1</sup>, Zoran Ristovski<sup>1</sup>, Richard J. Brown<sup>1</sup>, Meisam Babaie<sup>2</sup> and \*Ali Zare<sup>3</sup>

<sup>1</sup> International Laboratory for Air Quality and Health, QUT, Brisbane, QLD 4000, Australia <sup>2</sup> School of Mechanical Engineering, University of Leeds, Leeds, UK <sup>3</sup> School of Engineering, Deakin University, 75 Pigdons Rd, Geelong, Victoria 3216, Australia.

The maritime industry is increasingly focused on improving energy efficiency and reducing emissions in line with global decarbonisation goals. This study investigates ship engine performance and emissions under transient operational conditions, particularly during acceleration, deceleration, and low-load manoeuvring. The research integrates findings from experimental test bed studies and on-board ship measurements to assess the applicability of the propeller law (engine power proportional to rpm³) in predicting fuel consumption and emissions in real-world conditions.

During steady-state operation, ship engine loading typically follows the propeller law, and most fuel consumption models use engine load as a primary predictor. However, this study highlights the limitations of propeller laws in accurately representing engine behaviour in port and coastal areas, where transient operational conditions dominate. Comparative analysis across three complementary research approaches—test bed engine studies, on-board ship measurements, and numerical modelling—demonstrates that transient operational conditions significantly influence ship propulsion efficiency, fuel economy and emission outputs. For example, during acceleration, the demanded load significantly lags the actual engine response. These transient effects are more pronounced at higher rpm change rates, influencing brake-specific fuel consumption (BSFC) and emission profiles. At low operational loads, BSFC increases significantly, reflecting inefficient fuel utilisation. Higher specific fuel consumption at lower loads contrasts with more stable BSFC at higher loads, suggesting that partial loading conditions pose challenges for fuel efficiency and emission control.

Emission rates of NOx, CO, PM, and PN show a strong correlation with engine parameters and transient conditions. Experimental testbed results and on-board ship measurements indicate that low-load emission correction factors are consistently below fleet emission inventory values, whereas higher load correction factors align more closely with established estimates. Furthermore, NOx emissions tend to be higher at lower rpm change rates, while PM and particle number (PN) emissions increase at higher rpm change rates. These discrepancies highlight the necessity of refining emission estimation models to incorporate transient operational effects.

This study contributes to the broader field of decarbonising maritime transport by providing actionable insights into optimising ship propulsion systems. The findings emphasise the necessity of incorporating transient operational factors into regulatory frameworks and emission inventories to enhance environmental sustainability in the shipping sector. Future research should focus on refining computational models and exploring alternative fuel pathways, such as ammonia and hydrogen, to further mitigate maritime emissions in alignment with global sustainability goals.

Keywords: manoeuvring, transient operation, diesel engine exhaust, emission factor

#### Economic Assessment for Chemical Recycling from Mixed Plastic

Samaila Hassan<sup>a</sup>, Gerardo Martínez-Narro<sup>a</sup>, Anh N. Phan<sup>a\*</sup>.

<sup>a</sup> School of Engineering, Newcastle University, Newcastle upon Tyne, NE1 7RU, United Kingdom.

Among the plastic waste recycling technologies, pyrolysis has been found to be suitable for addressing the problem of mixed plastics in plastic feed streams and to fully understand the economics of this technique for efficient implementation, a techno-economic analysis has been conducted for the pyrolysis of mixed plastic waste to produce gas for electricity generation and naphtha range hydrocarbons to be reintegrated back into the refinery for circularity. It was predicted that at a capacity of 100 tonnes per day the pyrolysis plant of mixed plastic waste (20 % HDPE, 28.5 % LDPE, 27.5 % PP, 9 % PS, and 15 % PET) was economically feasible with an estimated capital expenditure of around £5.6 million and an annual operating cost of around £3 million. The payback time would be around 3 years where the pyrolysis oil minimum selling price was estimated to be £384.9/tonne with a corresponding cumulative NPV of over £200 million. A sensitivity analysis for the 100 tonnes per day plant found that a feedstock cost of £39/tonne with corresponding heavy and light pyrolysis oils selling prices respectively of £450 and £551.2 per tonne resulted in a payback time of 3 years while a £157/tonne cost with same respective products prices resulted in a payback time of over 8 years. Similar analysis against the pyrolysis oil selling price results in payback time of about 2 years at selling price of £697 per tonne while a selling price of £110 results in a non- economically viable project over the entire project timeframe. A scale up from 100 tonnes per day to 200 and 500 tonnes per day shows an increase in cumulative NPV from about £200 million to over £580 million and over £1730 million respectively. These economic results show responsiveness to feedstock costs, the operating capacity, and the products selling prices. Furthermore, economic performance of four different scenarios were analysed and compared:

(1) Base case scenario targeting a crude oil grade product for potential blending with crude oil upstream refinery, (2) With wax recirculation targeting naphtha-range oil for potential blending at the steam cracker unit of the refinery, (3) Power plant incorporated to produce electricity as additional revenue source and (4) Simultaneous wax recirculation and electric power generation from optimized gas production.

Keywords: Plastic waste, sustainability, Aspen plus, process simulation, sensitivity analysis.

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# Integrated CO<sub>2</sub> capture and utilisation (ICCU) using CaO based dual functional materials for syngas production

\*Chunfei Wu¹, Yuanyuan Wang¹, Xiaotong Zhao¹

<sup>1</sup> Queen's University Belfast, Belfast, UK

CO<sub>2</sub> capture and utilization (CCU) technologies pave the way to a net-zero future on the premise of applying fossil fuels, however, are restricted by the high cost. Integrated CO<sub>2</sub> capture and utilization (ICCU) eliminates the intermediate steps, such as CO<sub>2</sub> compression and transportation, by in-situ upgrading the captured CO<sub>2</sub>, hence representing a promising technology. Plenty of researches paid efforts on designing dual functional materials to achieve CO<sub>2</sub> capture and catalytic conversion by incorporating CO<sub>2</sub> adsorbents (e.g. MgO and CaO) and catalysts (e.g. Ni and Ru). Few attentions were concentrated on the catalytic performance of adsorbents in the absence of catalytic active sites. Herein, we reported an ICCU process achieved by integrating CO<sub>2</sub> capture with reverse water gas shift reaction using simple and low-cost CaO as both sorbent and catalyst. By switching the feeding gas from CO2 source to H<sub>2</sub> isothermally, up to 75% of captured CO<sub>2</sub> was 100% converted into CO at 600-700 °C and the cycle performance of CaO was significantly improved under ICCU condition. In addition, the simulation confirms the significant economic advantage compared to similar traditional processes. The concept could also be achieved over natural materials (e.g. marble stone), and handling the realistic flue gas conditions. Further introducing potassium into the CaO system could enhance the catalytic performance by improving the selectivity of carbonates direct hydrogenation. Overall, as a low-cost net-zero tech, ICCU using CaO exhibits both impressive cost-effectiveness and potential for industrial deployments.

Keywords: Carbon capture, integrated CO<sub>2</sub> capture and utilisation, CO<sub>2</sub> utilisation

Acknowledgement: This project has received funding from the European Union HORIZON TMA MSCA Staff Exchanges (HORIZON-MSCA-2021-SE-01), grant agreement no 101086071, project name "CUPOLA — Carbon-neutral pathways of recycling marine plastic waste".

# Comprehensive Energy Utilization of Fluoride-salt-cooled High-temperature Small Modular Nuclear Reactor

\*Associate Professor Quanbin Zhao1, Prof Daotong Chong1, Prof Junjie Yan1

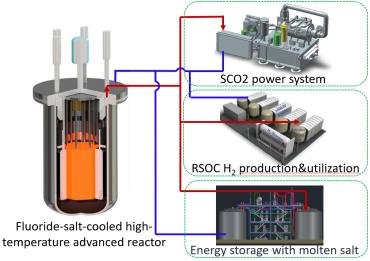
<sup>1</sup> Xi'an Jiaotong University, Shannxi Province, China,

Fluoride-salt-cooled High-temperature reactor(FHR), as a Generation IV small modular nuclear reactor, is characterized by compactness, high temperature, and inherent safety. The high operation temperature can provide various application scenarios, such as energy and power plant, provide high-temperature process heat for hydrogen production with reversible solid oxide fuel cell (RSOC), energy storage with molten salt, etc. However, few studies on the operational characteristics of the coupled system with FHR and other systems, especially for the electricity and hydrogen combined production. This talk will cover the following three aspects:

**Power generation**: The supercritical carbon dioxide (SCO<sub>2</sub>) Brayton cycle is chosen as the energy conversion system for power plant, owing to its excellent characteristics high efficiency, compactness, and modular manufacturing capability. The coordinated matching configurations for SCO<sub>2</sub> Brayton cycle are investigated firstly. Optimized configuration and design parameters are obtained with intelligent optimization algorithm method. The coordinate coupling operation characters for SCO<sub>2</sub> cycle and FHR are further investigated with dynamic code, and optimized control strategies are developed to guarantee the safety and flexibility of the coupled system.

**Hydrogen production and utilization:** The high-temperature FHR can provide high temperature process heat for hydrogen production with reversible solid oxide fuel cell (RSOC) stack. Therefore, the system configurations for RSOC system are studied. Based on the energy and temperature demand of the RSOC stack, an optimized system configuration is proposed with high temperature fluoride-salt preheater. Further, the key factors affecting the transient response rate of the RSOC stack were studied and an optimized control strategy with air reflux are proposed.

**Energy storage with molten salt:** The energy storage system can reduce the control numbers and amplitudes of FHR during the system load rapid and frequent changes. Also, the molten salt energy storage is of great significance for improving the efficiency and response rate of the power generation system and hydrogen production system. The paper investigates the configuration and storage capacity of the molten salt energy storage system for the FHR, power generation system and hydrogen production system with different operation requirements. Finally, the dynamic response characteristics of energy storage system is analysed to obtain the advanced control strategy for energy storage system.



*Keywords:* Fluoride-Salt-cooled Reactor, SCO<sub>2</sub> power system, Hydrogen production with RSOC, Energy storage with molten salt

# Comparison of Micro- and Meso-Pore Analysis Techniques to Understand Carbon Capturing Capability of Plant Derived Biochar

\*Baldeep Kaur<sup>1</sup>, Atul Sharma<sup>1</sup> and Michael Bradley<sup>1</sup>

<sup>1</sup> The Wolfson Centre for Bulk Solids Handling Technology, University of Greenwich, Central Avenue, Chatham Maritime, Kent, UK.

Carbon capture and storage (CCS) in bioenergy sector aims to neutralise the carbon footprints to generate green energy. Biochar is one of the major waste-products in bioenergy sector which holds the capability to capture carbon from the environment. Biochar has many other useful applications, such as, it is used as a soil nutrient enhancer, containment sorbent, carbon sequester, catalyst and energy storage material. The performance of biochar is dependent mainly on two factors: the porosity and surface area. Biochar produced from different raw materials exhibit different measurements of surface area and porosity. This research will focus on the biochar derived from plant-based biomass.

**Biochar:** The biochar samples under investigation are derived from the plant-based biomass, hence contains cellulose, lignin and hemicellulose as main components. Hemicellulose decomposes within 220-315°C, cellulose being highly stable decomposes within 315-400°C, and lignin due to its complex structure decomposes within 150-900°C. Lignin is one of the main contributors to the surface area and porosity in the biochar (Leng *et al.* 2021).

**Surface area and porosity measurements:** Measurements of surface area and porosity of biochar is a major challenge. Biochar usually contains high moisture content, usually around 40%. It has been observed that drying of biochar samples before BET analysis alter the delicate structure of micro- and meso-pores, hence affects the accurate measurements of these quantities (Maziarka *et al.* 2021). Alternative methods, such as, cyclohexane vapour sorption analysis measures the surface area and porosity reliably without disturbing the delicate micro- and meso-pore structure of biochar samples. This research compares the measurements of the surface area and porosity of biochar samples analysed through BET technique using Nitrogen gas as an adsorbent and cyclohexane vapour sorption method to determine pore size and surface area for better understanding of suitability of measurement techniques.

Keywords :biomass, carbon absorption, sorption, carbon capture storage and utilisation, bioenergy.

Acknowledgement :The authors acknowledge the support in undertaking experimental measurements by Surface Measurement Systems Ltd., UK.

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Leng, L., Xiong, Q., Yang, L., Li, H., Zhou, Y., Zhang, W., Jiang, S., Li, H., Huang, H., (2021), An overview on engineering the surface area and porosity of biochar, Science of The Total Environment, *763*, 144204. (<a href="https://doi.org/10.1016/j.scitotenv.2020.144204">https://doi.org/10.1016/j.scitotenv.2020.144204</a>)

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### Comparing the Performance of MOFs and Amines as Carbon Capture Technologies through Life-Cycle Assessment

\*Nicholas Landon<sup>1</sup>, Henry Owen<sup>1</sup>, Orla Williams<sup>1</sup>, Jon Mckechnie<sup>1</sup>, Rebecca Ryder- Brown<sup>2</sup>, Selina Ambrose<sup>2</sup>, Akos Cseke<sup>1</sup>, Edward Lester<sup>1</sup>

<sup>1</sup> University of Nottingham – Faculty of Engineering, University Park, Nottingham, UK, NG7 2RD, <sup>2</sup> Promethean Particles – 1-3 Genesis Park, Midland Way, Nottingham, UK, NG7 3EF.

The need for carbon capture technologies that can remove CO2 from industrial emission sources, in an energy efficient manner has never been greater. This has led to a greater research focus on innovative solutions to the carbon capture challenge. Currently, amine-based technologies are more widely deployed than any other technology, though the environmental concerns and high regeneration energy usage show the overall inefficiency of these materials.

Metal organic frameworks (MOFs) are solid sorbent materials that have been shown to be efficient at CO2 capture, and research is being conducted to evaluate their effectiveness in reducing environmental impact and energy usage. Life-Cycle Assessment (LCA) is a tool allowing for a complete cradle-to-cradle overview of a product's life-cycle. Currently, there are virtually no studies which compare the environmental impact of amines and MOFs for CCS.

This study uses CCS plant performance data modelled in the Integrated Environmental Control Model (IECM), an open source tool for calculating the performance, emissions, and cost of a fossil-fuelled power plant, to generate a comparative LCA of Amine and MOF CCS from a biomass power station in the SimaPro LCA software, using the ecoinvent v3.11 database and ReCiPe 2016 Midpoint (H) impact assessment method. The models involve finding the relevant input quantities (materials, energy etc) in the available databases, constructing each process step, then extrapolating the data to determine the environmental impact. This study provides timely and useful information on how MOF and amines CCS systems operate, their comparative environmental impact and identifies improvements for future models.

Keywords: carbon capture, life cycle assessment, metal organic framework, amine, SimaPro, ecoinvent

Acknowledgement: This work was supported by the Engineering and Physical Sciences Research Council (EPSRC) Centre for Doctoral Training in Resilient Decarbonised Fuel Energy Systems [grant number EP/S022996/1] and Promethean Particles. The authors would like to thank all those involved in the project for their support and assistance.

The Difficulties of Modelling the Manufacture of Carbon Capture Technologies for Life Cycle Assessment

\*Nicholas Landon<sup>1</sup>, Orla Williams<sup>1</sup>, Jon Mckechnie<sup>1</sup>, Rebecca Ryder-Brown<sup>2</sup>, Selina Ambrose<sup>2</sup>, Scott Priest<sup>2</sup>, Akos Cseke<sup>1</sup>, Edward Lester<sup>1</sup>

University of Nottingham – Faculty of Engineering, University Park, Nottingham, UK, NG7 2RD, Promethean Particles – 1-3 Genesis Park, Midland Way, Nottingham, UK, NG7 3EF.

The need for carbon capture technologies that can remove CO2 from industrial emission sources, in an energy efficient manner has never been greater. This has led to a greater research focus on innovative solutions to the carbon capture challenge. Currently, amine-based technologies are more widely deployed than any other technology, though the environmental concerns and high regeneration energy usage show the overall inefficiency of these materials. The deficiencies provide a target for research into alternative technologies to improve upon.

Metal organic frameworks (MOFs) are solid sorbent materials that have been shown to be efficient at CO2 capture, and research is being conducted to evaluate their effectiveness in reducing environmental impact and energy usage. However, there are still many gaps that need filling.

Life-Cycle Assessment (LCA) is a tool allowing for a complete cradle-to-cradle overview of a product's life-cycle, using real-world data to inform computer models of the processes involved in manufacturing, using, disposing and recycling materials. Very few have been conducted for MOFs, but understanding how each stage is affected and can be refined and improved is crucial to implement the materials on an industrial scale.

LCA studies on MOF manufacture have been conducted in SimaPro, using the ecoinvent v3.11 database and ReCiPe 2016 Midpoint (H) impact assessment method. They involve finding the relevant input quantities (materials, energy etc) in the available databases, constructing each process step, then extrapolating the data to determine the environmental impact. However, a number of issues have presented themselves while creating these manufacturing models: **Materials from scratch**: Input materials that are not readily available in the databases must be created from scratch, using chemical formulae to work out stoichiometrically how to construct these materials. Since the materials made this way aren't verified by any external regulator, validation by recreating those available in this method and comparing them is required.

**Region of origin:** A number of input materials are available as an averaged 'global' value, but also broken up into different streams from a variety of sources. A common MOF precursor is sourced from China, which has a far greater environmental impact than the averaged 'global' or Europe equivalents. Changing region of origin would greatly reduce the overall process impact.

**Waste treatment streams:** The definition of waste treatment options in ecoinvent is limited by the industries that have provided data, and thus are either very specific or don't cover numerous elements. While the waste out of each process for MOF manufacture can be broken up between each material, there is less differentiation between components in the database. As such, we must try to find the most applicable endpoint for each, taking into account type of material (e.g. inert or hazardous waste) and final destination (e.g. landfill or incineration).

*Keywords :* carbon capture, life cycle assessment, metal organic framework, manufacture, SimaPro, ecoinvent

Acknowledgement: This work was supported by the Engineering and Physical Sciences Research Council (EPSRC) Centre for Doctoral Training in Resilient Decarbonised Fuel Energy Systems [grant number EP/S022996/1] and Promethean Particles. The authors would like to thank all those involved in the project for their support and assistance.

Hybrid State of Charge Estimation for Lithium-Ion Batteries Using Kalman Filters and AI: Enhancing Accuracy and Sustainability

\*Mansur Mustapha<sup>1</sup>, Dr. Arunachalam Sundaram<sup>2</sup>

[1][2] University of Salford, Salford, UK

Sustainability underpins modern efforts to balance resource consumption with conservation, ensuring availability for future generations This global shift has brought about the adoption of greener ways of thinking, often leading to a transition towards electrical solutions. Batteries have seen significant growth in usage over the past few years due to the shift from fossil fuels to electricity generation. The use of batteries in devices comes with its challenges, particularly in detecting the amount of electrical energy remaining, or the state of charge (SoC). This work addresses how to effectively measure the state of charge of lithium-ion batteries by merging older techniques with newer technologies, such as the Kalman filter, and leveraging artificial intelligence (AI).

This research aims to help Battery Management Systems (BMS) better calculate the remaining electrical energy in a battery while enjoying the inherent advantages of SoC estimation. The main question this research seeks to answer is: "How can the accuracy, robustness, and real- time capability of state of charge (SoC) estimation in lithium-ion batteries be improved for applications like electric vehicles and energy storage systems?"

The study leverages key battery parameters—nominal capacity, terminal voltage, current, and temperature—as inputs for the Kalman filter, which mitigates noise and provides an initial SoC estimation. This output, along with historical SoC data, serves as input to an AI model utilizing neural networks. The hybrid system captures complex nonlinear battery behaviours and dynamically refines SoC estimates.

The main outcome of this hybrid approach is an estimated 5–10% improvement in accuracy over the standard Kalman filter, enhancing robustness to noise and capturing complex nonlinear battery behaviours. Compared to AI-only models, the hybrid approach offers an additional 2–5% improvement through real-time dynamic updates from the Kalman filter.

A 5% improvement in SoC estimation can reduce overcharge and over-discharge occurrences, preserving battery health. This could extend the life of a lithium-ion battery in an electric vehicle, which typically lasts eight years, by an additional 10 to 14 months. Improved range estimation could alleviate range anxiety among drivers, as a 5% accuracy improvement can reduce errors in range predictions. These advancements underscore the potential of the hybrid method to optimize battery performance, extend operational life, and reduce costs. Such improvements are crucial for achieving sustainable, reliable energy solutions in high-impact industries.

*Keywords:* State of Charge (SoC), Lithium-Ion Batteries, Kalman Filter, Artificial Intelligence (AI), and Battery Management Systems (BMS).

Acknowledgement: This is work was carried out at Automotive and Autonomous Vehicle Technology Labs (AAVT) at the University of Salford.

# Fabric Waste Derived Carbon Based Electrode Materials for Energy Storage Applications

Yavuz Gökçe<sup>1</sup>, Gabriela Duran-Jimenez<sup>2</sup>, \*Emine Yagmur<sup>3,1</sup>, Savaş Yaglikci<sup>4</sup>, Fatih Güleç<sup>3,2</sup>

<sup>1</sup>Department of Chemical Engineering, Faculty of Engineering, Ankara University, Tandogan, 06100 Ankara, Turkiye.

<sup>2</sup>Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, UK.

<sup>3</sup>Low Carbon Energy and Resources Technologies Research Group, Faculty of Engineering, University of Nottingham, Nottingham NG7 2TU, UK.

<sup>4</sup>Department of Energy Systems Engineering, Faculty of Engineering, Ankara University, Golbasi 06830 Ankara, Turkiye.

The textile industry is one of the industrial sectors with the lowest recycling rate. Although textile wastes can theoretically be completely recycled, the recycling rate in practice is relatively low; 15-20%. The proliferation of new and functional textile products due to the change in the desired properties of textile products and the fast fashion trend complicates the composition of textile products. The complex composition of waste makes classification and fibre separation more difficult, increasing recycling costs. The growing global population leads to higher textile production and fast fashion, which results in more textile waste. The challenges associated with textile recycling have prompted researchers to conduct studies exploring the utilisation of waste in a circular perspective. The objective of this study is to transform cotton dust, which is produced during the textile manufacturing process and cannot be utilised subsequently, into carbon-based electrode materials for energy storage through upcycling. The primary motivation for this study is to upcycle cotton dust into high-value carbon-based materials, thereby reducing greenhouse gas emissions from disposal, which tends to be the combustion of waste. The investigation focused on the impact of crucial parameters, such as the pre-carbonisation temperature and the activation impregnation ratio, on the surface characteristics and energy storage capabilities of the resulting carbon-based electrodes. The effect of these parameters on the material's structural properties was characterised through BET surface area and pore size distribution analyses. The energy storage performance of the cell was evaluated using a range of analytical methods, including cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). Results showed that activated carbon samples with a surface area exceeding 2000 m<sup>2</sup>/g could be produced. Notably, the surface area of the samples produced at a pre-carbonisation temperature of 500 °C and subsequently carbonised/activated at 800 °C demonstrated a substantial surface area of 2261 m<sup>2</sup>/g. The supercapacitor cell of these samples exhibited a specific capacitance of 131 F/g at a current density of 1 A/g in the presence of a 6 M potassium hydroxide electrolyte, demonstrating the effectiveness of wastederived electrode materials in energy storage applications. Furthermore, the samples demonstrated 98% long-term electrochemical stability after 20,000 charge-discharge cycles, indicating their reliability and durability in real-world scenarios.

Keywords: Cotton, Activated Carbon, Upcycling, Energy Storage.

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#### IMPULSE® Cleaning and its Applications in the Power Industry

\*Thomas Ball<sup>1</sup>, Guy Sharp<sup>1</sup>, Gerry Riley<sup>1</sup>

<sup>1</sup> RJM International, Winchester, UK

With the move away from coal to biomass and waste the problems with ash deposition have increased. The higher levels of alkali species in the ash of biomass and waste feedstocks lead to higher fouling rates which can be particularly corrosive given the higher levels of chlorine in these fuels. These problems manifest themselves as unreliable operation of the plant, with frequent unplanned outages and poor thermal performance. As many of these plants are debt funded it has resulted in numerous plant closures.

Traditional cleaning technologies such as soot blowers struggle to provide effective cleaning in these applications, with plants having to use supplementary techniques such as Online Cleaning to maintain operation. Sites have looked for more permanent solutions such as explosion cleaning technologies. This presentation will describe the theory behind this new application of explosive cleaning being deployed in the UK. Although new to the European markets it is a proven technology with over 300 units installed in the USA. IMPULSE® Cleaning is a unique explosion cleaning technology which utilises the key benefits of all explosion cleaning technologies, non-line of sight cleaning and no parasitic load consumption but without moving parts. The unique nature of this system allows it to maintain boiler efficiency through its proactive cleaning cycle.

We will present a case study of the implementation of this system on a waste wood advanced gasification plant. These plants have been notoriously unreliable. For this installation, cleaning units have been installed in the gasifier, evaporator and economiser sections of the plant. The paper will discuss the background to the technology and the engineering challenges associated with the project.

The installation within the gasifier, where temperatures are operating in excess of 1000°C, is normally considered not possible due to the high temperatures resulting in fused slag rather than fouling. However, in combination with a Flue Gas Recirculation system, the material formation is friable allowing for IMPULSE® Cleaning to help control the build-up of deposits which in the past have shed and defluidised the bed necessitating a lengthy and costly unplanned outage.

The units installed in the boiler and economiser have two objectives to maintain the thermal performance of the unit and control pressure drop across the plant which limits the generation as the ID fan is constrained.

The results show a meaningful improvement to the performance of the plant. The efficiency of the system has been maintained from as clean, and the lower back-end temperatures are allowing for increased generation (increased ID fan capacity). The gasifier has been kept significantly cleaner and the bed is healthier meaning that the bed has not required replacement on the shutdown.

Keywords: Explosion Cleaning, Boiler Efficiency, Fouling, Slag

Acknowledgement: PowerPlus Cleaning Solutions

### **Session 3C Combustion Processes 1 Thursday, 11<sup>th</sup> September**

#### Investigation into Hydrogen Pre-ignition Induced by a Single Oil Droplet

Olayinka Ramonu, Junfeng Yang\*

School of Mechanical Engineering, University of Leeds, Leeds, LS2 9JT, United Kingdom

Pre-ignition, an abnormal phenomenon is a critical issue in hydrogen combustion, altering its auto-ignition properties, flame development and propagation, and overall combustion dynamics. The origin of this abnormal and destructive phenomenon is believed to emanate from several factors, such as hot surfaces or spots, accumulation of dirt or dust, and lubricating oil droplets or deposits, which may result in a deflagration to detonation transition of hydrogen mixture. Despite several attempts to understand and mitigate these crucial challenges to hydrogen combustion, this problem persists. Moreover, hydrogen-air mixture pre-ignition induced by a single oil droplet has not been well studied yet.

This study employs the Leeds optical Rapid Compression Machine (RCM) to investigate the pre-ignition of a hydrogen-air mixture induced by a single oil droplet from two commercial oils (oil A and oil B) with distinctive formulations. The optical RCM adapted with a pressure acquisition tool is utilised to visualise the event of the single oil droplet inducing pre-ignition in a stoichiometric hydrogen-air mixture in the RCM at the end of compression temperature and pressure  $T_{eoc} = 950$ K and  $P_{eoc} = 22$  bar, respectively. The oil droplet of 0.8µL, equivalent to 1.16mm diameter, is placed on a metal wire and suspended in the middle of the combustion chamber.

The result reveals that oil A vaporises quickly and pre-ignites the surrounding hydrogen-air mixture, thereby significantly reducing the ignition delay time (IDT), and, in the end, a detonation-like bright spot was observed. On the contrary, oil B exhibited a late ignition after the autoignition of the hydrogen-air mixture, with an indication that the mixture's propagating flame vaporised and ignited the oil droplet. These results indicate that the oil formulation plays a major role in promoting pre-ignition, with Oil A exhibiting more susceptibility.

Conclusively, this study presents detailed insights into the pre-ignition of a hydrogen-air mixture induced by a single oil droplet and contributes to the advancement of mitigation approaches towards efficient hydrogen combustion.

Keywords: Hydrogen, pre-ignition, oil droplet

#### Compastion i rocesses I

#### Torrefaction of spelt husks to increase its fuel properties

\*Abubakar Halidu<sup>1</sup>, Anh Phan<sup>2</sup>, Paul Bilsborrow<sup>2</sup>

<sup>1</sup> Federal Polytechnic Nasarawa, Nigeria, <sup>2</sup> Newcastle University, Newcastle upon Tyne, UK

As a pre-treatment for various thermochemical processes, torrefaction is the moderate pyrolysis of biomass at temperatures between 200 and 300°C in an oxygen-free atmosphere to improve its heating value, improved grindability, and storability. Temperature clearly affected torrefaction product yields, according to torrefaction results. Spelt husks were torrefied in this investigation at 200, 250, and 300°C in an inert nitrogen atmosphere at a heating rate of 20°C.min<sup>-1</sup> and residence times ranging from 15 to 60 minutes, respectively. Analysis was done on the impact of residence time and torrefaction temperatures. The findings demonstrated that the higher heating values (HHV) and grindability were improved by the investigated torrefaction temperatures. Char yield dropped as torrefaction temperatures increased, while gas and liquid yields improved.

Higher torrefaction temperatures increase HHV and carbon content while decreasing volatiles, oxygen content, and energy output. With a residence period of 15 minutes and a torrefaction temperature of 250°C, the maximum energy yield of almost 97% was achieved. When compared to the non-torrefied spelt husks, which had an HHV of 17.56 MJ kg $^{-1}$ , the torrefied husks at 300°C with a residence time of 15 minutes showed the largest increase in HHV, 30.88 MJ kg $^{-1}$ . The grindability was enhanced and oxygen was eliminated as CO<sub>2</sub>, CO, and H<sub>2</sub>O by raising the temperature from 200 to 300°C. The liquid product had little potential for additional use in the petrochemical sector and was primarily water with a considerable acidity.

**Objective of the Study:** To evaluate spelt husks potential for use as solid biofuel in order to improve its energy density, grindability, and combustion efficiency as well as make it more compatible with coal cofiring in power plants.

**Materials and Methods:** The spelt husks torrefaction experiment was conducted in a stainless steel reactor with an internal diameter of 14 cm and a height of 28 cm. Forty (40) g ( $\pm$ 0.5) of biomass was fed into the reactor, which was then heated to the desired temperature of 200, 250, and 300°C, respectively. The oxidation and ignition were eliminated by using a heating rate of 20°C min<sup>-1</sup> and a nitrogen flow rate of 60cm<sup>3</sup> min<sup>-1</sup>. As the residence period for each targeted torrefaction temperature, the sample was left in place for 15 to 60 minutes. The torrefaction experiment using spelt husks was carried out in a stainless steel reactor which has an internal diameter of 14 cm and a height of 28 cm in which 40 g ( $\pm$ 0.5) of the biomass was fed and then heated to a preferred temperature of 200, 250 and 300°C respectively. A heating rate of 20°C min<sup>-1</sup> was used under a nitrogen flow rate of 60cm<sup>3</sup> min<sup>-1</sup> in order to eliminate ignition and oxidation. The sample was allowed to be held for a duration of 15-60 mins as the residence time for each desired torrefaction temperature. Following the procedure, the solid products were taken from the reactor that had been cooled to a temperature of less than 50°C, while the liquid products were taken from the condenser that had been kept at 0°C while submerged in an ice bath. The non-condensable gas samples were collected using gas bags in triplicate for gas chromatography (GC) analysis. Prior to being examined for grindability, the samples were obtained in order to determine the solid yield, liquid yield, gas yield, proximate analysis, and HHV.

Keywords: Torrefaction, temperature, spelt husks, residence time, higher heating values

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A comparison of pre-treatment approaches for enhancing the biogas yield from water hyacinth

Betul Esen<sup>1</sup>, Jessica M.M. Adams<sup>2</sup>, Andrew B. Ross<sup>1</sup>

<sup>1</sup>School of Chemical and Process Engineering, University of Leeds, Woodhouse Lane, Leeds, LS2 9JT, <sup>2</sup>Institute of Biological, Environmental & Rural Sciences, Aberystwyth University, Aberystwyth, SY23 3EE

Water hyacinth (WH) is a highly invasive macrophyte which dominates freshwater bodies in the developing world, causing considerable environmental and economic impacts. It is often removed and dumped, resulting in the release of GHG emissions. It is becoming generally recognised that the utilisation of the biomass can reduce GHG emissions associated with its disposal, and it represents a novel biomass supply chain for generating bioenergy and bioproducts because of its fast growth rate and accessibility. WH is a fibrous biomass that exhibits limited biodegradability by anaerobic digestion (AD) when processed in its raw state. It generally requires pre-treatment to increase its biodegradability. This study investigates different pre-treatment approaches, including steam explosion (SE), hydrothermal pre-treatment (HTT) and hydrodynamic cavitation (HC).

WH has a high cellulose and hemicellulose content and a low lignin content. It typically contains 90-95 wt% moisture content, its volatile matter (db) is approximately 75 wt%, and ash content of 20-30 wt% ash. The dry matter typically contains 16 18 wt% crude fibre, 20 wt% crude protein, 18-50 wt% hemicellulose, 17-35 wt% for cellulose and 1-12 % lignin content (Gaurav et al., 2020). WH samples have been collected from Lake Victoria, Uganda, after which the biomass is air-dried and oven-dried to a moisture content under 10%. Characterisation of the WH includes proximate, ultimate analysis and biochemical and elemental analysis. Pre-treatment by steam explosion (SE) was performed in 2 bar (120°C), 5 bar (150°C), and 15 bar (200°C) thermal conditions. Hydrothermal treatment (HTT) was performed by heating hot compressed water at 120°C and 150°C for 1 hour. Hydrodynamic cavitation (HC) using an orifice/venture design has been conducted at 50°C and 7 bar at different retention times (5 and 15 min). Following pre-treatment, the resulting slurries were analysed for their Biochemical Methane Potential (BMP) using an AMPTS II under mesophilic conditions for 30 days.

Pre-treatment significantly improves the biodegradability of WH, resulting in increased bio-methane production compared to untreated WH. For pre-treatment by SE, the biomethane yield increases with increasing temperature since the higher severity results in more breakdown of the macromolecular structure due to hydrolysis. Biodegradability increases by almost 75% following the different pre-treatments.. SE significantly increases the biomethane yield by 140- 180 % for 120°C and 200°C, respectively. At 200°C, the fibrous nature of the biomass is reduced dramatically, producing a pumpable fluid. After HTT, a similar improvement is observed with an increased BMP of 178% yield at 150°C. However, the highest efficiency seems to be at a higher retention time of HC, with 213% BMP yield.

Keywords: anaerobic digestion, pretreatments, water hyacinth

Integration of biohydrogen production from food waste into existing anaerobic digestion systems: samples pretreatment and process stability

\*Cynthia Okoro-Shekwaga1

<sup>1</sup> University of Leeds, Leeds UK

Biological hydrogen production from organic wastes (like food waste) presents a great opportunity for a sustainable hydrogen economy. Food waste has quite a complex composition, therefore, dark fermentation (DF) which provides a complex microbial ecosystem, becomes the most suitable biological biohydrogen production process for food waste. DF occurs through the activities of anaerobic fermentative bacteria characterised by the same biochemical reactions of the fermentation stages (acidogenesis and acetogenesis) of the well-established anaerobic digestion (AD) technology. This presents a unique opportunity to integrate DF into AD systems, given the widespread technical know-how of the AD technology globally.

Moreover, AD systems offer a good source of  $H_2$ -producing bacteria (HPB), like Clostridium, and so, the liquid effluent from AD (digestate) is often used as inoculum (seed) for DF processes. However, digestate also contains communities of other  $H_2$ -consuming bacteria (HCB) that could inhibit the DF process, therefore, it must be pretreated to inactivate the HCB, consequently, enabling an enrichment of the HPB. The most common method of achieving this is by subjecting only the inoculum to extreme heat (known as heat shock) and combining this with FW (with or without pretreatment).

The present study seeks to reduce multi-level pretreatment of the inoculum and FW by a combined inoculum/FW heat-shock pretreatment process and identify the optimal process conditions, such as starting pH, for the DF process. In this study, the author demonstrates that this approach allows better process stability, evidenced by improved system pH recovery and higher fermentation rates. This is particularly important for a continuous DF/AD process, whereby, maintaining optimal pH is important for process stability and improved fermentation rates during DF increases the downstream AD rate.

The conventional DF approach of pretreating the inoculum independently from the substrates creates multiple levels of operation along with associated energy and cost implications. Some AD systems, operate a pasteurisation unit at 70°C–80° C temperature for the substrate before feeding into the AD. The pasteurisation unit in existing systems can be optimised for inoculum/FW pretreatment at onsite operating temperature, which could help reduce the potential energy and operating cost associated with DF, and presents an opportunity for easy retrofitting of DF into existing AD systems.

Keywords: food waste, dark fermentation, anaerobic digestion, biohydrogen

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# Generation of Biogas from Continuous Anaerobic Co-digestion of Agro-waste and Chicken Droppings

\*Esther O. Babatunde¹ and Lukhanyo Mekuto¹

<sup>1\*</sup>Department of Chemical Engineering, Faculty of Engineering and Built Environment, University of Johannesburg, Johannesburg, South Africa.

The current state of the energy sector demonstrates the unreliability of non-renewable energy sources; thus, researchers have shifted their focus to renewable energy sources for energy production. One distinct renewable energy source is biomass because it offers a renewable energy source and improves the environment's wellness by lowering environmental impacts and pollution. Biogas production from biomass through anaerobic digestion (AD) is one way to generate energy. This occurs through the decomposition of organic matter by microorganisms. This presentation concerns the generation of biogas, which focuses on the pre-treatment and conversion of biomass using anaerobic digestion.

The feedstock will be pretreated to remove dirt and contaminants, mixing various feedstocks to ensure the right proportion and carbon to nitrogen (C:N) ratio and may involve the addition of water. It will provide data on process conditions, material, and feedstock issues. Biogas production through the anaerobic digestion technology provides more advantages over other forms of bioenergy production. It is one of the most efficient and environmentally friendly technologies for bioenergy production. It is useful since it reduces carbon dioxide emissions. This technology aids in regulating waste disposal. The residues from this process can be utilized as fertilizers for arable land. Biomass treatment under anaerobic conditions is highly dependent on the composition of biomass. Anaerobic Digestion is a degradation process consisting of four main stages namely hydrolysis, acidogenesis, acetogenesis, and methanogenesis.

**Hydrolysis:** The experimental procedure here will be based on breaking down of complex organic matter, (biomass) into simpler molecules like sugars and amino acids by microbes secreted from inoculum. The inoculum in this work will be obtained from the residue (waste) generated from fruit processing industries.

**Acidogenesis:** During this stage the acidogenic bacteria convert the simple sugars and amino acids into volatile fatty acids (VFAs), ammonia, carbon dioxide, and hydrogen sulphide.

**Acetogenesis:** In this stage, acetogens convert the products from acidogenesis (ethanol and fatty acid), mainly organic acids, into acetic acid, carbon dioxide, and hydrogen.

**Methanogenesis:** In the final stage, methanogens utilize the products from the previous stages (acetic acid, hydrogen, and carbon dioxide) to produce methane and carbon dioxide. The proposed research is to investigate the use of biomethane potential (BMP) for the continuous anaerobic co-digestion of treated biomass, e.g., in the form of solid material. Therefore, the pretreatment of biomass such as fruit peels, chicken droppings, and the addition of inoculum will be fed into a digester under anaerobic digestion will be conducted. This will, in general, lead to the formation of biogas, which can then be stored before being either refined further into biomethane for vehicle fuel or for injection into the gas grid or burned in a combined heat and power engine to produce electricity and heat, or burned in a gas boiler to produce heat for local use.

Keywords: Biogas; Agro-waste; Anaerobic digestion; Degradation; Renewable energy; Biomass.

Acknowledgment: The authors would like to thank the University of Johannesburg, South Africa, for providing research facilities and the technical staff members in the Department of Chemical Engineering Technology, and PEET, UJ, for their support.

#### Making Waste Carbon Negative: Integrating Carbon Capture with EfW's

\*Sinéad Goodall 1

<sup>1</sup> Suez Recycling and Recovery UK

**EfW's and their Potential for Carbon Capture:** As we have moved away from landfill, we have significantly increased our use of Energy from Waste (EfW) plants. EfW's plants are a hygienic way to treat unrecyclable waste, they also help us reduce environmental impact when compared to landfill by avoiding methane emissions and leachate generation.

EfW's extract energy in the form of steam and electricity while treating waste. Through this energy production this again reduces the wastes carbon intensity, with the reuse of ash as building aggregate, and recovery of metals also adding a second life to a portion of the waste. However, (although still less polluting than landfill) due to the nature of the feedstock it is a very carbon intense process. In general, an EfW will generate 1 tonne of  $CO_2$  per tonne of waste incinerated.

EfW's have a unique position when implementing carbon capture and storage (CCS). Around half of all waste processed comes from biogenic origins (food and garden waste, unrecyclable paper/cardboard, wood, textiles etc.). This means that if CCS was implemented on an EfW it would have an overall carbon negative effect, as 50% of its emissions are from non-fossil sources.

EfW's are also primarily left with CCS as a solution as there is currently no large-scale alternative to decarbonise this waste. Unlike other sectors there's no electrification or fuel replacement options that the sector can implement for significant decarbonisation. Other than CCS decarbonisation options include removing some of the fossil sources (predominantly plastics) from the waste stream before incineration.

**SUEZ's Teesside Plants:** SUEZ has four EfW plants in the Teesside area. These sites in 2024 alone processed over 1m tonnes of waste, generated 411,847 MWh of electricity and exported 459,161 MW $_{th}$  of steam, producing 951,610 tCO $_2$ . For these sites the average biogenic fraction was 53.6 % meaning that with carbon capture our negative emissions for 2024 would have been 510,134 tCO $_2$ .

**Integrating Carbon Capture:** SUEZ is studying two possible carbon capture scenarios and has completed pre-FEED studies covering all four of its EfW's in the East Coast Cluster. For the STV site the proposal is to build one large facility to cover all five incineration lines, compared to the Wilton 11 site which will build two carbon capture lines one for each of the EfW lines.

One of the main issues associated with carbon capture facilities is their high energy demand. The integration of the steam from the existing EfW with the proposed carbon capture facility comes with challenges. Similar to the EfW CCS projects in the HyNet cluster, SUEZ is exploring preliminary options to supply steam to the carbon capture facility through a back pressure turbine, which would supply both the steam at the required conditions and the electricity required to power the plant.

Other integration studies SUEZ are currently exploring to progress their carbon capture project include, cooling options, water effluent treatment, and reducing energy demand.

Keywords: Carbon Capture, Energy from Waste

Acknowledgement: This work is supported by Suez Recycling and Recovery UK.

Mechanisms of using NaCl-CaCl<sub>2</sub> molten solar salts in enhancing the integrated CO<sub>2</sub> capture and utilization via reverse water gas shift (ICCU-RWGS) process with CaO alone

Xiaotong Zhao<sup>1</sup>, Bo Zong<sup>1</sup>, Jia Hu<sup>1</sup>, Yulan Han<sup>1</sup>, Yingrui Zhang<sup>1</sup>, Chunfei Wu<sup>1,\*</sup>

<sup>1</sup> School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast BT7 1NN, UK

This research investigates the integration of NaCl-CaCl<sub>2</sub> molten solar salts with CaO in the Integrated CO<sub>2</sub> Capture and Utilization via Reverse Water Gas Shift (ICCU-RWGS) process, aiming to enhance CO<sub>2</sub> conversion efficiency. The study demonstrates that combining NaCl-CaCl<sub>2</sub> molten salts with CaO significantly improves the CO<sub>2</sub> capture and CO generation rates compared to using CaO alone. Experimental data show a CO<sub>2</sub> conversion of 56.99 % at 650 °C, with an average CO<sub>2</sub> capture rate of 0.64 mmol g<sup>-1</sup> min<sup>-1</sup> and a CO generation rate of 0.23 mmol g<sup>-1</sup> min<sup>-1</sup>. X-ray photoelectron spectroscopy (XPS) and in-situ analyses reveal that the eutectic behavior of NaCl-CaCl<sub>2</sub> facilitates the dissolution of CaO, enhancing its capacity for CO<sub>2</sub> uptake. Mechanistic studies suggest that the molten salt environment accelerates the desorption and conversion of CO<sub>2</sub>, primarily through interactions involving adsorbed oxygen species. These findings offer critical insights for optimizing the ICCU-RWGS process, paving the way for more efficient solar-driven CO<sub>2</sub> capture and conversion systems.

Keywords: CO<sub>2</sub> capture, CaO, molten salts, reverse water gas shift, integrated carbon capture and utilization.

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# Can Carbon-Based Materials from Waste Fabrics Provide a Sustainable Solution for CO<sub>2</sub> Capture?

\*Emine Yagmur<sup>1,2</sup>, Gabriela Duran-Jimenez<sup>3</sup>, Yavuz Gokce<sup>2</sup>, Savaş Yaglikci<sup>4</sup>, Orla Williams<sup>3</sup>, Edward H. Lester<sup>3</sup>, Fatih Güleç<sup>1,3</sup>

<sup>1</sup>Low Carbon Energy and Resources Technologies Research Group, Faculty of Engineering, University of Nottingham, Nottingham NG7 2TU, UK.

<sup>2</sup>Department of Chemical Engineering, Faculty of Engineering, Ankara University, Tandogan, 06100 Ankara, Turkiye.

<sup>3</sup>Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, UK.

<sup>4</sup>Department of Energy Systems Engineering, Faculty of Engineering, Ankara University, Golbasi 06830 Ankara, Turkiye.

The rapid pace of the fashion industry has led to an alarming increase in fabric and clothing waste, posing significant environmental challenges in the UK, Turkiye, and globally. In the UK alone, over 200,000 tonnes of fabric waste are annually discarded into landfills, contributing to environmental pollution and resource depletion. Current efforts to reuse and recycle clothing have not sufficiently addressed the escalating volume of fabric waste, necessitating innovative solutions. This project aims to address the critical issue of fabric waste by developing a sustainable and circular approach to upcycling them into valuable resources such as advanced carbon materials (ACM). The development of solid adsorbents for CO<sub>2</sub> capture is gaining significant attention as a sustainable alternative to conventional amine-based absorption processes. Solid sorbents offer advantages such as lower energy requirements, enhanced stability, and reusability, making them suitable for scalable CO<sub>2</sub> capture applications. The objectives of this project are to i) develop and optimise a thermal process for upcycling waste fabrics to ACMs, and ii) investigate their application in CO<sub>2</sub> capture to validate their utility and market value.

This study covers the upcycling of various fabric wastes including cotton, polyester, elastane, and wool through different thermal conversion methods such as i) conventional and ii) microwave heating processes to produce ACMs for CO<sub>2</sub> capture. Parameter optimisation was investigated to understand the relationship of operating parameters such as microwave power (100-1000W), conventional heating temperatures (400-800 °C), activating agent, and residence time on the development of pore structure in the ACMs. The physicochemical properties of ACMs were comprehensively characterised using surface area (BET) and pore structures (BJH), surface morphology (SEM), with thermogravimetric analysis (TGA) for CO<sub>2</sub> capture tests. The findings showed that the surface area of ACMs produced with KOH at 800 °C in conventional heating systems was 2000 m<sup>2</sup>/q with a CO<sub>2</sub> capture capacity of 13%.

By producing high-value products such as ACMs, the project demonstrated a viable circular economy model within the textile industry, contributing to sustainable energy technologies and environmental conservation.

Keywords: Waste fabric, Activated Carbon, CO2 capture, Carbonisation, Chemical Activation.

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# Integrated CO<sub>2</sub> capture and utilisation (ICCU) using CaO based dual functional materials for syngas production

\*Chunfei Wu¹, Yuanyuan Wang¹, Xiaotong Zhao¹

<sup>1</sup> Queen's University Belfast, Belfast, UK

CO<sub>2</sub> capture and utilization (CCU) technologies pave the way to a net-zero future on the premise of applying fossil fuels, however, are restricted by the high cost. Integrated CO<sub>2</sub> capture and utilization (ICCU) eliminates the intermediate steps, such as CO<sub>2</sub> compression and transportation, by in-situ upgrading the captured CO<sub>2</sub>, hence representing a promising technology. Plenty of researches paid efforts on designing dual functional materials to achieve CO<sub>2</sub> capture and catalytic conversion by incorporating CO<sub>2</sub> adsorbents (e.g. MgO and CaO) and catalysts (e.g. Ni and Ru). Few attentions were concentrated on the catalytic performance of adsorbents in the absence of catalytic active sites. Herein, we reported an ICCU process achieved by integrating CO2 capture with reverse water gas shift reaction using simple and low-cost CaO as both sorbent and catalyst. By switching the feeding gas from CO2 source to H<sub>2</sub> isothermally, up to 75% of captured CO<sub>2</sub> was 100% converted into CO at 600-700 °C and the cycle performance of CaO was significantly improved under ICCU condition. In addition, the simulation confirms the significant economic advantage compared to similar traditional processes. The concept could also be achieved over natural materials (e.g. marble stone), and handling the realistic flue gas conditions. Further introducing potassium into the CaO system could enhance the catalytic performance by improving the selectivity of carbonates direct hydrogenation. Overall, as a low-cost net-zero tech, ICCU using CaO exhibits both impressive cost-effectiveness and potential for industrial deployments.

Keywords: Carbon capture, integrated CO2 capture and utilisation, CO2 utilisation

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# Evaluating the Effectiveness of Spraying PVA Glue with Water to Supress and Bind Biomass Wood Pellet Dust.

Savchenko, V.a, Lester, E.a, Güleç F.a, Williams, O.a

<sup>a</sup>Faculty of Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, UK

Dust generated during the transportation and handling of biomass wood pellets poses significant environmental and industrial challenges. In-situ systems to bind and contain dust could help reduce the risk of fire and dust propagation in transportation systems, whilst minimising material losses and increase the overall efficiency of the power generation system. This experiment investigates the development of a biomass dust binding system and assess the effectiveness of binding biomass dust particles using a spray solution of diluted PVA. A sealed 20 litre clear container was used to simulate controlled conditions.

Biomass wood pellet dust of varying particle size combinations was placed into the container (< 60 g/m³) to avoid fire and explosions according to HSE with a compressed air connection to create an airborne dust environment within the sealed container. A compressed air spray system applied a mixture of water and PVA glue into the container. Changes in particle size, weight, and dispersibility were measured before and after treatment to evaluate the binding effect. The experiments were recorded using a high-speed camera to evaluate the binding effect. Preliminary findings suggest that adding PVA glue to water improves the binding of dust particles, reducing their tendency to become airborne again. This approach shows potential as a low-cost dust mitigation strategy in industrial settings, offering both environmental and occupational safety benefits.

Keywords: biomass wood pellets, dust, PVA glue, water, spray system, dispersibility.

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# Comparative Analysis of Low- and High-Impact Forces on the Disintegration of Wood Pellets

Savchenko, V.a, Lester, E.a, Güleç F.a, Williams, O.a

<sup>a</sup>Faculty of Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, UK

Dust formation from biomass pellets continues to be an operation issue for bioenergy plants. There is little research in the area of how low and high impact forces influence the breakdown of biomass pellets in transportation systems. This study aims to address this gap in knowledge by investigating the effect of high and low mechanical impact forces on the breakdown of biomass wood pellets and the consequent dust generation for biomass transportation and handling applications.

This study uses 3 batches of a commonly used biomass pellet in large scale bioenergy systems, one commercially available pellet (Balcas energy wood pellets), and one torrefied "black" pellet. The influence of low mechanical forces seen in transportation was simulated using a tapped density tests for low-impact repetitive situations such as conveyor belts. Pellets were tapped for varying taps up to 50,000 taps, and the mass of the broken down pellet was recorded. Minimal breakdown was observed, with less than 0.1% degradation, indicating low impact tapping type action is not responsible for pellet breakdown in transportation systems.

A ball mill without balls at varying speeds and durations was used to simulate high-impact conditions. After testing, the samples were sieved in a sieve shaker for 8 size classes to obtain their particle size distribution (PSD). Subsequently, PSD analysis was performed to quantify the extent of pellet breakdown under the various low and high impact test conditions. the ball milling tests showed that high-impact forces significantly contribute to pellet disintegration, leading to increased dust generation. The findings highlight the critical role of high-impact forces in dust formation during biomass handling and transportation.

*Keywords:* dust, biomass, wood pellets, sieving, particle size, cumulative mass.

Acknowledgement: This work was supported by the Engineering and Physical Sciences Research Council (EPSRC) Centre for Doctoral Training in Resilient Decarbonised Fuel Energy Systems [grant number EP/S022996/1] and Net Zero Research (NZR). The authors would like to thank all those involved in the project for their support and assistance.

Pre-Treatment of Municipal Solid Waste using dry, saturated steam in rotating autoclaves to present a homogenous, high percent biomass product for sustainable, solid, liquid, and gaseous biofuels.

Pete Metcalf, Tom Wilson, Sheila Hughes, Rebecca Addy

Wilson Bio-Chemical Ltd.

The management of municipal solid waste (MSW) presents a critical challenge in the transition toward a circular economy. The effective management and valorisation of municipal solid waste (MSW) are essential for advancing circular economy strategies. This study investigates the Wilson System®, an advanced autoclave-based pre-treatment technology that utilizes dry, saturated steam in rotating autoclaves to transform MSW into Wilson Fiber®—an energy-dense, cellulose-rich material with significant potential for sustainable biofuel application. Through controlled thermal and mechanical processing, the Wilson System® homogenizes the incoming raw MSW waste stream, producing a sustainable 90-95% biogenic product available to be converted to solid fuel for CHP and liquid and gaseous biofuel for transportation, particularly SAFs.

Wilson Fiber® serves as a versatile resource for second-generation biofuel, driving innovation in renewable energy from a sustainable global asset. Its consistent composition makes it particularly well-suited for bioethanol, biobutanol, hydrogen and sustainable aviation fuel (SAF)—key components of a low-carbon future. Furthermore, when integrated with carbon capture strategies, this process offers a potentially carbonnegative solution, reducing landfill dependency and mitigating methane emissions.

This presentation will report the latest findings on the functional applications of Wilson Fiber® with respect to its practical use as a torrefied product in CHP and existing incineration plants. This is particularly significant for the proposed expansion of the UK Emissions Trading Scheme to cover all large-scale incineration and CHP installations. The results underscore the viability of the Wilson System® as a scalable and industrially adaptable method for improving Municipal and Commercial waste valorisation, supporting the transition toward sustainable energy, carbon-zero pathways, and circular economy principles.

**Keywords**: municipal solid waste, organic waste, cellulose fibre, steam autoclaving, Wilson System, Wilson Fibre, process technology, carbon zero sustainable bioproducts, torrefaction, sustainable aviation fuel, biobutanol, bioethanol.

Energy, Exergy, Economic and Environmental Analysis of an Integrated Coal-Biomass Gasification Fuel Cell System for Low-Carbon Energy generation and Methanol production

Sa Li<sup>1</sup>, \*Xiao Wu<sup>1</sup>, Meihong Wang<sup>2</sup>

National Engineering Research Center of Power Generation Control and Safety,
 School of Energy and Environment, Southeast University. Nanjing, China.
 Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, S1 3JD, UK

Integrated Coal Gasification Fuel Cell (IGFC) systems have garnered significant attention for their high efficiency and minimal impact on overall efficiency when coupled with carbon capture systems.

This study proposes a novel Integrated Coal-Biomass Gasification Fuel Cell (ICBGFC) system to enhance energy efficiency, reduce carbon emissions, improve operational flexibility, while enabling polygeneration of power, heat and methanol. The system primarily utilizes coal as a feedstock, supplemented by biomass co-gasification, and integrates a solid oxide fuel cell (SOFC) for cascaded energy utilization. Additionally, methanol synthesis is incorporated to diversify energy outputs, addressing various end-user demands while improving system flexibility.

Model of the ICBGFC is developed based on the commercial software of Aspen Plus for operating performance evaluation. The entire model consists of nine subsystems: the Air Separation Unit (ASU), Coal and Biomass Sizing, Coal Gasification, Gas Purification, Water-Gas Shift (WGS), SOFC, Methanol, Combined Heat and Power (CHP), and Carbon Capture and storage (CCS).

A 4E (Energy, Environment, Economy, and Exergy) assessment framework is then adopted to comprehensively evaluate the technical, environmental and economic performance of the ICBGFC system. Furthermore, the impacts of key parameters, such as biomass mixing ratio and gasification temperature, on overall system performance are analyzed.

Key findings indicate that biomass co-gasification significantly reduces the carbon footprint of the ICBGFC. When combined with CCS, the ICBFC can achieve near-zero or even negative carbon emissions. The ICBGFC system demonstrates higher thermal efficiency than conventional coal-fired power plants while offering flexible polygeneration capabilities. Additionally, the incorporation of methanol production enhances overall system flexibility by allowing adjustments in methanol output while maintaining stable gasification system operation.

This study presents a novel technical pathway for the low-carbon utilization of coal.

Keywords: Integrated Coal-Biomass Gasification Fuel Cell, Polygeneration, Carbon Capture, 4E(Energy, Environment, Economy, and Exergy) Analysis, Modeling

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### **Session 5A** China Clean Energy Research Friday, 12<sup>th</sup> September

# Integration of direct air capture and green hydrogen for sustainable fuel production

Eni Oko

Newcastle Upon Tyne University, NE1 7RU, UK.

Climate change, attributed to rising atmospheric CO<sub>2</sub> levels, prompted global action through the 2015 Paris Agreement by 196 countries to keep global warming below 2°C while pursuing a 1.5°C target by 2100. However, due to the current atmospheric CO<sub>2</sub> level, the slow pace of large-scale decarbonization rollout and the short time frame required to reach net zero, the aspiration of the Paris Agreement cannot be achieved without large-scale atmospheric CO2 removal. The EU, for instance, will require a cumulative atmospheric greenhouse gas removal of about 20-70 GtCO2 by 2100 to meet its Paris Agreement obligations (Daggash et al. 2019. International Journal of Greenhouse Gas Control 81, 181-198). In recent years, direct air capture (DAC) has become recognised as a promising atmospheric CO<sub>2</sub> removal technology with positive results outcomes from commercial demonstration projects by Carbon Engineering in Canada and Climeworks in Europe (Gutknecht et al. 2018. Energy Procedia 146, 129-134). The aerospace industry and other hard-to-abate industries are increasingly embracing DAC as a complementary solution for fuel-switching to sustainable fuel. Consequently, there are eighteen pilot DAC projects in operation worldwide, with government and private sector funding commitments towards its development on the increase. DAC cost as a promising technology is still high at  $\leq 115 - 310/\text{tCO}_2$ , due to its energy-intensive nature, typically > 0.6 GJ/tCO<sub>2</sub>-electricity and > 4.2GJ/tCO<sub>2</sub>-thermal (Fasihi et al. 2019. Journal of Cleaner Production 224, 957-980.). Management of CO<sub>2</sub> also presents further challenge for direct air capture implementation. A typical solution to CO2 management will comprise the integration of hydrogen production within the process to provide opportunity to hydrogenate CO<sub>2</sub> to obtain sustainable fuel configuration. This project explored large-scale integration and techno-economic analysis of green hydrogen integration and catalytic CO2 hydrogenation to obtain dimethyl ether, a potential fuel substitute for diesel.

**Keywords:** Green hydrogen, sustainable fuel, process modelling, techno-economic analysis

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### **Session 5A** China Clean Energy Research Friday, 12<sup>th</sup> September

Experimental study on hydrogen production by methanol reforming under multiple conditions: temperature gradient regulation and product selectivity optimisation

Runze Feng, Quanbin Zhao, Ming Liu, Daotong Chong, \*Junjie Yan

Xi'an Jiaotong University, Xi'an, China.

With the growing demand for hydrogen as a clean energy source, methanol-water vapor reforming has emerged as a critical technology for hydrogen production due to its high energy density and operational simplicity. However, the synergistic effects of the water-to-methanol ratio (S/C) and temperature on product selectivity remain unclear, and existing studies predominantly focus on optimizing individual parameters. In this study, the effects of S/C ratio (1:1-1.6:1) and reaction temperature (503.15-533.15 K) on reaction performance were systematically investigated. Theoretical analysis reveals that at an S/C ratio of 1:1, the primary reaction products are H<sub>2</sub> and CO<sub>2</sub>, with only trace amounts of CO. Increasing the S/C ratio from 1:1 to 1.6:1 enhances methanol conversion by 23.2% (from 76.2% to 99.4%). Experimental results under fixed conditions (S/C = 1.2:1, feed rate = 45 mL/min) demonstrate a non-monotonic temperature dependence: methanol conversion peaks at 513.15 K (67.3%) and then declines to 59.1% at 533.15 K, while CO<sub>2</sub> selectivity decreases from 96% to 92.1% across the temperature range of 503.15-533.15 K. This study highlights that the synergistic regulation of S/C ratio and reaction temperature significantly governs methanol conversion and product selectivity. Additionally, the gravity-assisted effect of the vertical reactor further optimizes reactant distribution and mass transfer efficiency. These findings reveal the nonlinear interplay between S/C ratio and temperature, providing both theoretical and experimental insights for optimizing hydrogen production reactor operation.

Keywords: methanol reforming, hydrogen production, water-alcohol ratio, temperature gradient

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Unravelling Atomic-Scale Mechanisms and Parameter Synergies in Coal Supercritical Water Gasification: A ReaxFF Molecular Dynamics Study

Ruiqi Mu<sup>1</sup>, Ming Liu<sup>1</sup>, Jingqi Gao<sup>2</sup>, Kai H. Luo<sup>2</sup>, \*Junjie Yan<sup>1</sup>

<sup>1</sup> State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, China. <sup>2</sup> Department of Mechanical Engineering, University College London, Torrington Place, London WC1E 7JE, UK.

Coal remains a cornerstone of global energy systems, supplying over 35% of worldwide electricity generation and serving as a critical resource for industrial applications. However, the conventional coal utilization through direct combustion has caused severe environmental pollution and high carbon emissions. Among the existing thermochemical approaches, supercritical water gasification (SCWG) is a transformative technology for clean hydrogen production and carbon capture, offering a sustainable pathway to decarbonize coal-based energy systems.

To obtain atomic-scale resolution and dynamic reaction insights beyond the capabilities of experiments and system-level simulations, reactive force field molecular dynamics (ReaxFF MD) simulations are employed to investigate the coal SCWG process. This work focuses on revealing fundamental reaction pathways, optimizing key operational parameters, and evaluating the feasibility of alternative transport medium, such as CO<sub>2</sub>, to enhance gasification efficiency and system sustainability. By providing in-depth molecular-level insights, this study aims to offer valuable theoretical guidance for the optimization and large-scale application of coal SCWG technology.

**Mechanisms**: This study provides a detailed reaction mechanisms of coal decomposition during SCWG, tracking the breakage and transformation of molecular structures at the atomic level. To clarify the conversion of coal into gaseous products, radical interactions and the evolution of key intermediates are thoroughly examined. Additionally, the formation pathways of primary gaseous products, H<sub>2</sub> and CO<sub>2</sub>, are explored to identify critical reaction routes and key influencing factors.

**Parameters**: The performance and efficiency of coal SCWG are highly sensitive to operational parameters. To gain molecular-level insights into parameter optimization, the effects of key operational parameters, including reaction time, gasification temperature and coal water slurry concentration, on hydrogen production, carbon conversion efficiency, and by-product formation in coal SCWG process are investigated. Furthermore, the role of oxygen addition in modulating gasification performance is explored to differentiate the mechanisms of SCWG, supercritical water partial oxidation, and supercritical water oxidation.

**Transport medium**: Conventional coal SCWG systems primarily utilize  $H_2O$  as the transport medium considering its high diffusivity and solubility. However,  $H_2O$ -based systems are highly energy-intensive during the heating process due to the large specific heat capacity and low heating rate. To address these limitations and enhance carbon recycling, supercritical  $CO_2$  has emerged as a promising alternative transport medium, offering distinct advantages such as a lower critical point and in-situ carbon utilization potential. In this study, the transport medium of  $H_2O$  and  $CO_2$  in coal SCWG are systematically compared using ReaxFF MD simulation, and their distinct gasification mechanisms and the synergistic effects within hybrid medium systems are also explored.

Keywords: Coal gasification, Supercritical water, Hydrogen production, ReaxFF molecular dynamics

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### Performance Analysis of a Coal-Biomass Co-fired Boiler Based on Numerical Simulation

Lingxiao Chen<sup>1</sup>, Xiao Wu<sup>\*1</sup>, Meihong Wang<sup>2</sup>

<sup>1</sup>National Engineering Research Center of Power Generation Control and Safety, School of Energy and Environment, Southeast University, Nanjing 210096, China,

<sup>2</sup>Department of Chemical and Biological Engineering, University of Sheffield, Sheffield, S1 3JD, UK.

Biomass, with its characteristics of carbon neutrality and renewability, has become the fourth-largest energy source after coal, oil and natural gas. Currently, coal-fired power generation accounts for over 70% of power generation in China. The direct co-firing of biomass in the coal-fired power plant (CFPP) requires less equipment retrofit, making it a promising low-carbon transformation pathway for the CFPPS. In addition, biomass has low nitrogen(N) and sulfur(S) contents and less ash compared with coal, which can effectively reduce the emissions of nitrogen oxides ( $NO_x$ ), sulfur oxides ( $SO_x$ ), and soot, bringing good environmental benefits.

However, there are several technical challenges in directly co-firing. The co-firing conditions, such as biomass types, co-firing ratios, co-firing positions and excess air coefficients, affect the combustion characteristics and the pollutant emission characteristics of the boiler.

For this reason, this study focuses on a 1000MW ultra-supercritical opposed-firing concentric firing boiler system. Computational fluent dynamics (CFD) model of the boiler furnace is developed and validated. Based on the model, numerically simulations on the velocity field, temperature field and pollutant emissions are then carried out. The combustion characteristics of the furnace, as well as the benefits of carbon and pollutant emission reduction, are explored under different co-firing ratios, co-firing positions and excess air coefficients. The safe and stable operating conditions with the best economic and environmental benefits are then proposed.

This research outcome can provide a reference for the design and operation of biomass-coal co-fired boilers.

*Keywords:* biomass and coal co-firing, Numerical Simulation, carbon emission reduction, pollutant emission reduction

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Mass flowrate measurement of gas-liquid two-phase CO<sub>2</sub> flow under CCS conditions

Caiying Sun<sup>1,3</sup>, Yong Yan<sup>2\*</sup>, Wenbiao Zhang<sup>3</sup>, Ding Shao<sup>3</sup>

<sup>1</sup> Inner Mongolia University of Science & Technology, Baotou, China, <sup>2</sup> Beihang University, Hangzhou, China, <sup>3</sup> North China Electric Power University, Beijing, China.

During the long-distance transportation process in Carbon Capture and Storage (CCS), slight temperature and pressure changes in the pipeline will lead to significant changes in the phase of CO<sub>2</sub>, resulting in gas-liquid two-phase CO<sub>2</sub> fluid. Under the condition of gas-liquid two-phase flow, Coriolis flowmeters can be used to measure and output the apparent mass flowrate of the fluid. However, due to the complex and variable nature of multiphase flows, the measurements made by Coriolis flowmeters are affected by gas-liquid decoupling and fluid compressibility. The combined effects of these two factors significantly reduce the accuracy of flowrate measurement. Based on Coriolis flowmeters and capacitive sensors, a new hybrid theory-data-driven method for measuring the mass flowrate of CO<sub>2</sub> in gas-liquid two-phase flow is proposed.

**Methodology:** As shown in Fig. 1, the theoretical model is based on the measuring sensors and parameters, and the output results of the Coriolis mass flowmeter are corrected by calculating the decoupling error and compressibility error. However, there is still a significant gap between the corrected mass flowrate of the theoretical model and the real mass flowrate due to the complexity of the fluid, which can be corrected by data-driven model. The data-driven model is built based on the fluid state parameters provided by the Coriolis flowmeter and differential pressure transmitter, combined with soft sensing algorithm.

**Experimental Evaluation:** On the horizontal and vertical test sections in the  $CO_2$  gas-liquid two-phase flow platform, parameters required for theoretical models, such as gas volume fraction (GVF), pressure, temperature, vibration frequency, and apparent mass flowrate, can be obtained using sensors such as Coriolis flowmeters and capacitance sensors. A theory-data -hybrid driving model for mass flowrate measurement in pure  $CO_2$  two-phase flow is established by using the algorithms of deep neural network (DNN) and least squares support vector machine (LSSVM). The experimental results show that both algorithms can correct the mass flowrate error for most pure  $CO_2$  gas-liquid two-phase flow conditions to within  $\pm$  2.5%, which is the process requirement for CCS.

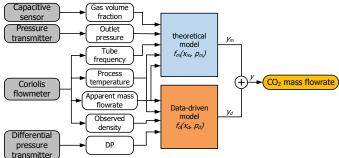


Fig.1 Overall strategy for the mass flowrate measurement of gas-liquid two-phase CO<sub>2</sub> flow

*Keywords :* CCS transportation, Gas-liquid two-phase flow, Coriolis flowmeter, Hybrid method, mass flowrate

Acknowledgement: This work is supported by Natural Science Foundation of China.

An improved NSD optical flow method for dynamic feature extraction and combustion state identification of burner flames

Sixu Pu, Jian Li, \*Chuanlong Xu,

National Engineering Research Center of Power Generation Control and Safety, School of Energy and Environment, Southeast University, Nanjing, China

The flame combustion state of the boiler burner in coal-fired power plants is critical to the overall combustion efficiency and safety of the furnace. With the development of digital imaging technology, a non-invasive method for flame detection has been provided and widely applied to various fuels and combustion conditions. Currently, flame combustion state diagnosis primarily relies on the analysis of static features extracted from flame images. These methods typically depend on single-frame images for flame feature extraction and are unable to effectively capture the correlations between multiple frames. The lack of dynamic description of the flame leads to limitations in combustion state diagnosis, making it difficult to comprehensively and accurately assess the flame state of the burner.

To address the aforementioned issues, this paper proposes an improved Non-Smooth Data (NSD) optical flow method to analyze the dynamic characteristics of flames. Considering the high-speed movement of the burner outlet flame and the inaccuracies in optical flow estimation, a multi-scale analysis approach based on the image pyramid algorithm is introduced. By computing optical flow at different resolutions, this method effectively captures motion information across multiple scales, thereby reducing estimation errors caused by insufficient resolution. Furthermore, the complex environment inside the boiler, characterized by rapid changes in background light intensity and blurred flame boundaries and textures, poses challenges to the stability of optical flow computation. To enhance robustness, a Lorentzian function and noise parameters are incorporated as robust enhancement functions to mitigate the influence of outliers and improve the adaptability and stability of the algorithm in complicated conditions. Additionally, to accommodate variations in flame morphology under changing load conditions, adaptive adjustment parameters are introduced, allowing for dynamic regularization parameter adjustment based on the gradient magnitude of the image.

To further validate the accuracy and applicability of the algorithm, a flame image acquisition system was established on a 660MW opposed combustion boiler, and the flame states under different load conditions were analyzed. Five key dynamic features, including optical flow pulsation energy, were extracted from the optical flow data to quantify the flame's motion characteristics. The results indicate that as the load decreases, the optical flow pulsation energy decreases. Under fixed load conditions, when the flame combustion is stable, the optical flow pulsation energy fluctuates within a range of approximately 0.1. When the air and coal flow rates are improperly regulated, the optical flow fluctuates significantly, indicating that the flame combustion state is unstable. This provides a quantitative indicator for flame stability, making it more suitable for real-time monitoring and diagnosis of boiler burner flames.

Keywords: Coal-fired power plant, Burner, Flame stability, Optical flow, Dynamic characteristics,

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Simulation, analysis and performance study of Direct Air Capture and Piperazinebased Post-combustion Carbon Capture for Large-scale Biomass-fired Power Plant

Shengyuan Huang<sup>1</sup>, Yao Zhang<sup>1</sup>, Jin Ma<sup>2</sup>, \*Meihong Wang<sup>1</sup>

<sup>1</sup> School of Chemical, Materials and Biological Engineering, The University of Sheffield, Sheffield S1 3JD, UK

<sup>2</sup> Key Laboratory of Smart Manufacturing in Energy Chemical Process, Ministry of Education, School of
Information Science and Engineering, East China University of Science and Technology, Shanghai 200237, China

A series of environmental problems caused by the increasing concentration of CO2 in the atmosphere have attracted more and more attention by researchers worldwide. CO2 can be captured from large single source such as power plants. CO2 can also be captured directly from the air. This study aims to integrate post-combustion carbon capture (PCC) from biomass-fired power plant and direct air capture (DAC). Such a PCC chemical absorption plant integrated with DAC process is still a very new research topic in the world. The integrated carbon capture process will achieve negative carbon emissions.

At the present stage, DAC and solvent-based PCC still face two challenges: high cost and high energy consumption. In DAC process, low CO2 concentration in the air means low driving force for mass transfer. Integrating DAC unit with PCC system will reduce total solvent energy consumption by circulating PZ solvent between DAC and PCC. Meanwhile, the feedstock of power plant is biomass, which could achieve negative carbon emissions with additional carbon capture from air. In addition, the electricity from biomass power plant could support the integrated carbon capture system when electricity grid is off peak.

In this study, the process simulation in Aspen Plus® will include integrated DAC and PCC process. Both use packed column and PZ solvent. Information on biomass-fired power plant will come from literature. Each process model will be validated using pilot scale experimental data. Technical and economic performance assessment of this integrated process will be performed through process simulation. Different power plant loads and carbon capture levels will be studied to achieve better system performance and energy consumption performance. The research can be useful for government decision making and also the industrial practitioners.

*Keywords:* Post-combustion carbon capture, chemical absorption, direct air capture, negative emissions, process simulation, process integration

Acknowledgement: The authors would like to thank the financial support of the EU RISE project OPTIMAL (Grant Agreement No: 101007963).

## Solar-driven direct air capture and CO<sub>2</sub> utilisation for syngas production using CH<sub>4</sub>-fluidised solar calcination

Yide Han, \*Meihong Wang

Department of Chemical and Biological Engineering, The University of Sheffield, Sheffield S1 3JD, UK

Direct air capture and CO<sub>2</sub> utilisation (DACCU) can serve as a carbon-neutral feedstock for producing value-added chemicals and fuels. This enables the deep decarbonisation and paves the way for a circular economy. However, current liquid solvent-based direct air capture (L-DAC) is mainly driven by nature gas combustion. To achieve sustainable decarbonisation though L-DAC with potential CO<sub>2</sub> utilisation, a transition to renewable energy-powered process is essential. This study proposes a novel solar energy-powered DACCU process and evaluate its performance at the commercial scale.

This study aims to develop a novel design of the solar-driven L-DAC system with CO<sub>2</sub> utilisation by integrating solar calcination and carbonates dry reforming of methane (CaDRM) reaction on a CH<sub>4</sub>-based fluidised bed. Thus, CO<sub>2</sub> is directly captured from the air and then utilised for syngas production driven by solar energy. The whole process will be modelled and simulated in Aspen Plus<sup>®</sup> with Fortran routines.

Techno-economic assessment will be conducted for a 1 Mt CO<sub>2</sub>/yr solar-driven DACCU plant, which is based on the individual unit operation data from the pilot plant, numerical scale-up and process simulations. The simulation results will indicate material balance, energy consumption and cost evaluation. The preliminary results indicate that the total cost of DACCU process is much cheaper than the stepwise processes. Therefore, the insights gained from this study will inspire more research towards commercial deployment of DACCU at large scale.

Keywords: Direct air capture, CO<sub>2</sub> utilisation, solar calcination, syngas production, process modelling and simulation, techno-economic assessment

Acknowledgement: The authors would like to thank the financial support of the EU RISE projects OPTIMAL (Ref: Grant Agreement No: 101007963) and CATALYSE (Ref: Grant Agreement No: 101183092).

### Adsorption Breakthrough Study of CO<sub>2</sub>/CH<sub>4</sub> Separation in a Vacuum Pressure Swing Adsorption using Water-based Aluminium Fumarate Metal Organic Framework (MOF)

Mukondeleli K. Muluvhu<sup>1</sup>, Nicholas M. Musyoka<sup>2</sup>, Michael O. Daramola<sup>1,\*</sup>

<sup>1</sup>Sustainable Energy and Environment Research Group (SEERG), Department of Chemical Engineering, Faculty of Engineering, Built Environment and Information Technology, University of Pretoria, Hatfield Campus, Pretoria, South Africa

<sup>2</sup>Centre for Nanostructures and Advanced Materials (CeNAM), Chemicals Cluster, Council for Scientific and Industrial Research (CSIR), Pretoria, South Africa.

Refining biogas to produce biomethane is critical and more research is still needed to identify, investigate, and evaluate the adsorbents that can potentially refine biogas. There are many factors to consider in the selection of the best candidate adsorbents and most of them might be good at separation but may have environmental or cost constraint associated with their synthesis, preparation, or availability. Another important aspect in refining biogas is the separation of carbon dioxide from methane. Depending on the scale of the refining, it is important to choose a cost-friendly but effective technology. Adsorption is a spontaneous exothermic process which depends on the properties of the adsorbent material. The process is based on molecular characteristics and the affinity of a gas to the adsorbent material. Pressure swing adsorption is a well-known gas separation technology where the adsorbent is subjected to pressure changes for adsorption and desorption of the adsorbate. One promising adsorbent for CO<sub>2</sub> is Aluminum Fumarate (Al-Fum) metalorganic frameworks (MOFs).

**Experimental:** The synthesis of Al-Fum MOF was investigated by utilizing tap water as a replacement for deionized water. The resulting product was pelletized using granulation technology, exploring two organic binders, namely PVA and PVDF. The physical properties of Al-Fum and its CO<sub>2</sub> adsorption performance were examined. Effect of binder (e.g. 5 wt% of PVA and PVDF) on the mechanical performance and the adsorption performance of the adsorbent was also studied. Additionally, VPSA (Vacuum Pressure Swing Adsorption) experiments were conducted at 293 K to ascertain the breakthrough curves of CO<sub>2</sub>, CH<sub>4</sub>, and the CO<sub>2</sub>/CH<sub>4</sub> mixture

**Results:** The results show that the use of PVA yielded pellets with superior mechanical strength, withstanding up to 21 N, though it displayed a slightly lower BET surface area of 886 m²/g. On the other hand, Al-Fum pellets obtained with PVDF were weaker, withstanding only 11 N, but demonstrated a slightly higher BET surface area of 952 m²/g. Adsorption equilibrium isotherms for CO<sub>2</sub> were measured at 298 K and 273 K, and their behaviour was similar to that of the Type II adsorption isotherm. The CO<sub>2</sub> coverage area at 293 K and 1.0 bar was 699 m²/g. The breakthrough curves showed that Aluminum fumarate MOF had a higher affinity towards carbon dioxide than methane. Methane took approximately less than 15 seconds to break through, while carbon dioxide took between 150 and 180 seconds to breakthrough.

Keywords: Breakthrough, CO2 adsorption, MOFs, Methane, Biogas

Application of Response Surface Methodology (RSM) to the Synthesis of Chitosan Applicable in Post-Combustion CO<sub>2</sub> Capture

Keren Osler<sup>2</sup>, Olawumi O. Sadare<sup>1</sup>, Olugbenga O. Oluwasina<sup>3</sup>, Michael O. Daramola<sup>1,\*</sup>

 <sup>1</sup>Department of Chemical Engineering, Faculty of Engineering, Built Environment and Information Technology, University of Pretoria, Hatfield 0028, Pretoria, South Africa.
 <sup>2</sup>School of Chemical and Metallurgical Engineering, Faculty of Engineering and the Built Environment, University of the Witwatersrand, Private Bag X3, Wits 2050, Johannesburg, South Africa.
 <sup>3</sup>Department of Chemistry, Federal University of Technology, P.M.B.704, Akure, Ondo State, Nigeria

Carbon dioxide capture is essential for reducing  $CO_2$  emissions in an attempt to mitigate climate change. This study focused on chitosan as an alternative non-toxic biodegradable polymer that can be utilized as an adsorbent for  $CO_2$  capture.

**Experimental:** The chitosan was extracted from brown crab shell chitin. The effect of experimental variables (NaOH concentration, temperature, and synthesis time) on the degree of deacetylation (DDA) of the synthesized chitosan was studied using Response Surface Methodology (RSM). Fourier Transform Infrared (FTIR) was used to examine the functional groups and determine the DDA of the synthesized chitosan. The data generated from the experiments were used for the development of an empirical model to explain both the main effect and the interactive effect of the variables on the synthesis. A thermogravimetric analyzer (TGA) was used to evaluate the performance of chitosan for CO<sub>2</sub> capture.

**Results:** Approximately 50 mg of chitosan was exposed to pure CO<sub>2</sub> (100 % CO<sub>2</sub>) at varying temperatures (25, 35, and 45 °C) and varying flow rates (flowrate 45, 60 and 75 mL/min), under a pressure of 1.1 bar for 120 minutes. Results showed that the empirical model developed from this study significantly predicts the DDA of chitosan, based on the NaOH concentration, temperature, and time used for synthesis. In addition, about 0.27 mmol CO<sub>2</sub>/g adsorption capacity was obtained for chitosan at 25 °C and 60 mL min<sup>-1</sup> feed flow rate, making chitosan a promising material for advanced CO<sub>2</sub> capture and utilization technology.

**Keywords:** Carbon Capture and Storage; Chitosan; Degree of deacetylation; Response Surface Methodology

Pilot Plant Study of MCFC with Co-production of Hydrogen: CO2 Management and Achieving Negative Emissions

\*Luma Sh. Al-Saadi <sup>1</sup>, Maria Fernanda Rojas Michaga<sup>2</sup>, Jenny Jones<sup>3</sup>, Timothy Cockerill<sup>4</sup>, M Pourkashanian<sup>2</sup>

<sup>1,2,3</sup> School of Chemical and Process Engineering (SCAPE), Leeds University, <sup>2</sup> School of Mechanical, Aerospace and Civil Engineering, Sheffield University.

Molten carbon fuel cells (MCFC) offer a way to capture carbon dioxide from biomass combustion while having the flexibility to simultaneously produce electricity, heat, and hydrogen, depending on operational preference and economics. There are several techniques for separating the produced hydrogen, and it is unclear which is the most effective. Aspen Plus was used to examine the relative merits of membrane separation, pressure swing adsorption (PSA), and cryogenic separation as potential approaches to separate **hydrogen** from the anode gases in an MCFC plant using biogenic flue gas from feedstocks such as wood chips. PSA has a high recovery ( $\leq 20 \%$  loss) and purity ( $\geq 99.99\%$ ) making it the most desirable option for small-scale applications compared to membrane separation, with a recovery rate typically > 97% only when three membranes are used. Due to its complexity and energy needs, cryogenic separation is best suited for large-scale operations. It can achieve recovery rates exceeding 90% but requires extensive cooling and careful control of low temperatures. Furthermore, in larger-scale facilities with higher gas volume and more recovery possibilities, recycling the tail gas stream may provide benefits that are not possible at smaller scales. The environmental evaluation of the analysed configuration results in a global warming potential (GWP) of 0.157 kgCO<sub>2</sub>eg/t of CO<sub>2</sub> captured for a cradle-to-gate approach. However, when the transport and storage of CO<sub>2</sub> are included, the GWP result is -0.94 kgCO<sub>2</sub>eg/t of CO<sub>2</sub>. This highlights the negative emissions nature of this configuration, which can produce electricity and hydrogen while capturing CO2. The novelty of this study is that it identifies ways of improving the efficiency of carbon dioxide capture processes by using MCFC technology with hydrogen co-production in a biogenic setting. The results highlight the promise of MCFC systems in achieving global climate goals and enabling a sustainable energy transition.

*Keywords:* Molten Carbonate Fuel Cell (MCFC), Hydrogen co-production, CO<sub>2</sub> capture, Negative emissions, Aspen Plus

Low  $NO_x$  Burners for Hydrogen: Why the  $NO_x$  can be lower than for Natural Gas.

\*Gordon Andrews<sup>1, 2</sup>, Herodotus Phylaktou<sup>1</sup>, Ramon Quinonez Acre<sup>2</sup>, Ray Massey<sup>2</sup>, Richard Wakeman<sup>2</sup>, Jim Maxfield<sup>2</sup> and Steve Smith<sup>2</sup>

Leeds University, Leeds, UK,
 Clean Burner Systems Ltd., Livingston, Preston and Rugby, UK.

The Hy4Heat UK Government programme of hydrogen burner development required the same environmental standards as for natural gas (NG), which means the same or lower NO<sub>x</sub>. The peak flame temperature for NG-air is 2238K and for hydrogen (H<sub>2</sub>) it is 2393K, both at and equivalence ratio, Ø, of 1.05. NO<sub>x</sub> formation is primarily controlled by the peak flame temperature and so if both flames were operated premixed at Ø=1.05 then the NO<sub>x</sub> would be much higher for H<sub>2</sub> than NG. Many NG burners operate premixed in domestic heat applications, cookers, fires and boilers. These burners will flash back if H<sub>2</sub> replaces NG and so the NG design cannot be used on H<sub>2</sub> and burners must operate with diffusion flames with separate air and fuel admission holes. The NO<sub>x</sub> is then controlled by the rate at which gas and air mix. This paper addresses the performance of dual fuel NG/H<sub>2</sub> burners and shows why the NO<sub>x</sub> emissions can be lower than for NG.

The Wobbe index for hydrogen is about 6% lower than for NG, so that for the same delivery gas pressure and same fuel hole size, 6% less energy will be delivered (GCV basis) with hydrogen. A dual fuel burner for NG/H<sub>2</sub> should operate at the same flame temperature and thermal power for the same heat application. A NG burner that meets CO emission regulations, will for the highest thermal efficiency operate at a flame temperature of 2195K at  $\emptyset = 0.95$  and dry oxygen of 1.3%. For hydrogen to achieve this temperature the  $\emptyset$  would be 0.80. However, the UK guidance for hydrogen burners (PAS4444) requires that a hydrogen burner operates with unburnt hydrogen at <1000ppm and this requires operation at  $\emptyset$  < 0.75, where the flame temperature is 2091K. The air flow required to deliver these conditions may is the same, so the burners can operate on the same air fan supply or natural draught air supply. If the delivery pressure is the same then for the same hole size the Wobbe Index difference will reduce the hydrogen delivered energy by 6%, which reduces the  $\emptyset$  to 0.7, where the dry oxygen is 4.6% and the flame temperature is 2011K. This is 184K lower than the NG flame condition and this is the main reason why the NO<sub>x</sub> emissions for hydrogen can be lower than for NG, if the gas and air are well mixed.

The  $NO_x$  emissions from a hydrogen diffusion flame burner are controlled by the rate at which the gas and air mix and this is controlled by the burner design. The ratio of the hydrogen to methane jet velocity for the same gas supply pressure is 2.83. Thus, a hydrogen diffusion flame fire with diffusion jet gas impingement on a metal or ceramic surface, will have much greater impingement jet mixing due to the higher jet velocities with hydrogen, compared with methane and this leads to lower  $NO_x$  with hydrogen. Also, as hydrogen contains no hydrocarbons there is no route to prompt  $NO_x$  formation and the proportion of  $NO_x$  that is  $NO_2$  is also reduced. The paper will demonstrate hydrogen/NG  $NO_x$  ratios for the same thermal power input, using round jet gas holes, of 0.8 for open gas fires, 0.64 for glass fronted gas fires and 0.25 for a 70 kW industrial burner. All these heat applications meet the current  $NO_x$  standards on both fuels. The assumption, in the literature on hydrogen for heat, that  $NO_x$  will increase is not true and  $H_2$  burners can reduce the environmental impact of heat. Only poorly designed  $H_2$  burners will increase  $NO_x$ .

Keywords: hydrogen, NOx, burners

Acknowledgement: UK DESNZ Hy4Heat and Green Distilleries programmes.

#### Neural ODE Method for NH3/H2 Combustion Chemistry Acceleration

Sipei Wu<sup>1</sup>, Wenkai Liang<sup>1</sup>, \*Kai Hong Luo<sup>1,2</sup>

<sup>1</sup> Tsinghua University, Beijing, China, <sup>2</sup> University College London, London, UK.

Due to the ongoing climate crisis and increasing levels of atmospheric carbon emissions, it is imperative to explore zero-carbon fuels and carbon-neutral combustion technologies to reduce greenhouse gas emissions and meet the stringent pollutant regulations. To accurately address the chemical kinetics, burning characteristics, and NOx emissions across various combustion devices, it is essential to employ detailed mechanisms in simulations. However, computing reacting flows with detailed chemistry is often prohibitively expensive due to the complexity of reaction mechanisms and the numerical stiffness arising from disparate chemical time scales. While recent advancements in deep neural networks (DNNs) offer potential for efficiently capturing the dynamics of stiff chemistry, its application to dual-fuels with drastic differences in reactivity such as ammonia (NH3) and hydrogen (H2) remains challenging. Constructing a universal model with limited parameters is especially difficult.

To enhance the efficiency of combustion chemistry simulations, we propose the DNN framework that could predict the kinetics of fuel blends of low-reactivity fuel NH3 and high- reactivity fuel H2, highlighting its applications to binary fuels with significant reactivity differences. We develop a systematic "sampling-training" workflow to overcome the challenge of generalizing DNN models to widely applicable fuel properties. This workflow involves three improvements:

- 1. Base manifold: The unity Lewis number laminar flames are leveraged as an economical thermochemical base manifold, given their similarities with turbulent flame profiles.
- 2. Randomization: Randomization is a necessary step to enhance model generalization and robustness. A continuously controllable randomization method is introduced to balance model capacity and computational efficiency by adjusting key parameters.
- 3. Training details: A physics-based loss function based on mass conservation and heat release rate accuracy ensures stable long-term predictions.

Two key hyperparameters that control data and model complexity are optimized to balance prediction accuracy and computational efficiency. The well-trained DNN model was coupled with CFD codes to simulate challenging turbulent combustion cases across a wide range of turbulent intensities and fuel compositions. Our approach is validated against simulations of planar premixed turbulent flames and temporally-evolving jet flames across a diverse range of unburnt temperatures, pressures, time steps, equivalence ratios, and mixing ratios. The results show nearly identical scalar fields and highly accurate statistical outcomes, even under intense turbulence and after  $O(10^4)$  DNN model calls, achieving chemical acceleration factors of up to  $7\times$  (CPU) or  $30\times$  (GPU), and an overall acceleration of up to  $5\times$  (CPU) or  $10\times$  (GPU).

*Keywords :* turbulent combustion, detailed chemical mechanism, combustion chemistry acceleration, deep neural network, manifold sampling, physics-based training.

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Selective catalytic reduction systems for ammonia combustion in heavy- duty engines-a modelling study

\*Madhumitha Rajendran<sup>1</sup>, Kevin Hughes<sup>2</sup>, William Nimmo<sup>3</sup>

<sup>123</sup> The University of Sheffield, Sheffield, UK

Ammonia (NH<sub>3</sub>) dual-fuel (DF) combustion in engines has gained significant research attention; however, studies on exhaust treatment systems for NH<sub>3</sub> and its fuel blends in compression ignition engines remain limited. Our gas-phase kinetic modeling study on combustion has revealed that N<sub>2</sub>O emissions, a potent greenhouse gas that is negligible in diesel combustion, are released in higher concentrations during cold starts and at very fuel- lean equivalence ratios, particularly at lower ammonia energy shares. Additionally, NH<sub>3</sub> combustion leads to increased water vapor and H<sub>2</sub> emissions, the impact of which on the selective catalytic reduction (SCR) system's NO<sub>x</sub> reduction efficiency remains unexplored.

This study employs catalytic surface kinetic modeling to assess the  $NO_x$  reduction efficiency of a commercial three-way catalyst under varying fuel-air equivalence ratios and diverse driving conditions, such as cold starts. A transient inlet flow into a perfectly stirred reactor model is simulated using ANSYS Chemkin-Pro. The transient exhaust flow data are derived from gas-phase kinetic modeling that investigates  $NO_x$  formation mechanisms from  $NH_3$  combustion with n-heptane, employing validated Tian and reduced n-heptane reaction mechanisms. The direct injection (DI) model, newly integrated into ANSYS Chemkin-Pro, effectively simulates DF combustion kinetics and predicts engine-out exhaust gas composition across varying fuel blend ratios, air-fuel equivalence ratios ( $\Phi$ ), compression ratios (CR), fuel injection timings, and durations. The NO molar conversion results have been experimentally validated using a fixed catalytic bed reactor.

This presentation will discuss key findings from both the modelling and experimental studies, including the effects of unburned NH<sub>3</sub>, H<sub>2</sub>, and hydrocarbons (HC) in the exhaust on SCR system performance under both fuel-lean and fuel-rich conditions—a combination not previously examined in a single study. Additionally, N<sub>2</sub>O emissions have been specifically measured using gas chromatography. NO and NO<sub>2</sub> emissions have been measured using chemiluminescence. The surface composition of both fresh and spent SCR catalysts has been analyzed using Energy Dispersive X-ray Spectroscopy (EDS).

This research is led by the University of Sheffield in collaboration with industrial partners Eminox Limited and Interkat Catalyst GmbH, both specialists in exhaust after-treatment system design and catalyst manufacturing. The boundary conditions for the study were finalized in consultation with industry partners to ensure applicability to existing vehicle fleets with minimal modifications.

*Keywords:* low-carbon dual fuel combustion and emission characteristics in heavy-duty engines, ammonia, catalyst surface kinetic modelling

Acknowledgement: This work is supported by UKRI EPSRC and Eminox Limited, UK.

#### Experimental investigation of NOx, NO emissions in combustion vessel

\*Rawan Alkandari<sup>1</sup>, Junfeng Yang<sup>1</sup>, Meisam Babaie<sup>1</sup>, Amir Nourian<sup>2</sup>

<sup>1</sup> University of Leeds, Leeds, UK, <sup>2</sup> University of Salford, Manchester, UK

The demand for achieving zero carbon emissions is increasing. Carbon-free hydrogen fuel is favored as it produces no direct carbon dioxide emissions, making it a key fuel for decarbonizing various sectors. However, the utilization of hydrogen combustion raises concerns regarding elevated NOx emissions. This leads to potential health and safety risks for personnel in the workplace. The study describes an experimental investigation to measure the NOx and NO levels in a unique fan-stirred combustion vessel. A Horiba analyzer with CLD detector was installed in the vessel exhaust to collect the measurements. The fuel utilized for this research includes hydrogen mixture and hydrogen blend mixtures to reduce NOx and NO emissions. An extensive set of parameters has been selected for the hydrogen mixture at atmospheric temperature with an equivalence ratio range of  $0.5 \le \phi \le 1.2$ , at a pressure of 1 bar. The study was conducted to examine the effect of laminar flame cases and turbulent flames on NO and NOx concentrations after combustion. In laminar hydrogen premixed combustion flames, the highest NOx level is observed at an equivalence ratio of 0.8. The combustion of lean conditions exhibited higher levels of NOx and NO compared to the rich condition. Regarding turbulent hydrogen flames, results indicate that under lean conditions, increasing the fan speed tends to reduce NOx and NO levels, while the opposite effect is observed when increasing the fan speed under rich conditions. The experimental results were compared to numerical NO level predictions based on the GRI mechanism using CHEMKIN software.

Keywords: hydrogen, lean combustion, laminar flame, NOx, turbulent flames, combustion vessel

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## Navigating the Path to Net Zero Emission: Biofuels Development in Indonesia

\*Ferry Fathoni<sup>1,2</sup>, Effie Kesidou<sup>1</sup>, Muhammad Mufti Rifansha<sup>3</sup>, Dinda Syira Tiftazani<sup>4</sup>

<sup>1</sup> University of Leeds, Leeds, UK, <sup>2</sup> PT Pertamina (Persero), Jakarta, Indonesia <sup>3</sup> Institute Technology of Bandung, Bandung, Indonesia, <sup>4</sup> University of Padjajaran, Bandung, Indonesia.

Biofuels have become an eco-innovation pathway for some countries to pursue net-zero emission targets. Our study utilises a multi-level interview approach to examine the factors influencing biofuels development in Indonesia. The development of palm oil-based biodiesel has received significant support from mandatory use policies in transport, power generation, and industry. Likewise, incentive mechanisms have created economies of scale to compete with fossil fuels. Abundant feedstock availability, adequate infrastructure networks, and collaborative innovation among stakeholders have accelerated biodiesel development. However, compatibility with existing diesel engines has been a challenge as the government's roadmap is to increase the proportion of biodiesel gradually. This research also explores the hurdles that developing countries face in developing biofuels. Environmental issues related to Indonesia's biofuel supply chains have provided an opportunity to develop hydrotreated vegetable oil by utilising used cooking oil. However, processing investment remains a significant obstacle to developing this cleaner biofuel. Furthermore, hydrogenated vegetable oil and bioethanol are still struggling due to inadequate incentive mechanisms. Fiscal and non-fiscal policy support plays a critical role in the sustainable development of biofuels.

Keywords: biofuels, eco-innovation, drivers, barriers, net zero emission

Acknowledgement: This work is supported by PT Pertamina (Persero).

#### Modelling tools to assess low-carbon hydrogen routes to reach net zero

\*Carolina Font-Palma<sup>1</sup>, Will Bowling<sup>2</sup>, Matthew Joss<sup>2</sup>

<sup>1</sup> School of Engineering, University of Hull, Hull, Hul 7RX, UK, <sup>2</sup> Energy Systems Catapult, 7<sup>th</sup> Floor, Cannon House, Birmingham, B4 6BS, UK

The latest UK Hydrogen strategy delivery update has set up a roadmap that allocates up to 4 GW for hydrogen derived from methane reforming or biomass gasification with CCS (or CCUS- enabled hydrogen) and up to 6 GW for hydrogen via the electrolytic route by 2030. CCUS-enabled hydrogen projects are expected to become live as part of the Cluster sequencing process and the expansion of track-1 and track-2 projects. Net Zero Teesside Power (NZT Power) has entered the execution phase to become the world's first gas-fired power station with CCS and it is expected final decisions for the HyNet Hydrogen Production Plant 1 (HPP1) and the Teesside Hydrogen CO2 Capture project. The Environment Agency expects more than 95% of CO2 produced to be removed from the reformer flue gases from post-combustion carbon capture, in order to keep the carbon intensity as set in the Low Carbon Hydrogen Standard (LCHS) below the limit of 20 gCO 2e/MJ LHV of produced hydrogen. The LCHS includes the emissions from the hydrogen processes as well as the energy supply. For hydrogen production via the electrolytic route, renewable energy supply is essential, such as wind and solar, however, their intermittency is a challenge to keep up the electrolytic hydrogen production combined with storage.

The Energy Systems Catapult has developed technology-agnostic modelling tools. One is the Energy System Modelling Environment (ESME) Flex, a techno-economic whole system model, to aid balancing energy supply and storage technologies for energy networks for specific geographic regions and timeframes. ESME Networks looks at energy system designs at local level to identify the infrastructure needed. Thus, this project builds on previous developed models and complementary skills in the team to tackle the complexity and challenges of integrating a flexible low-carbon hydrogen system into a dynamic energy system. The novelty of this project derives from the need to assess pathways which contain novel technology elements that are not proven at the scale needed for the current targets.

This work provides insights into key technology performance parameters, e.g. efficiencies, emissions. Thus, technology specific modelling results are imported into ESME tools to perform whole systems analyses. Aspen Plus® process simulation software is used to model the CCUS- enabled hydrogen unit processes, e.g. compressors, heat exchangers, reactors of the selected hydrogen routes. Aspen Process Economic Analyzer (APEA) is used to appraise the impact of process designs and to size and estimate the costs of the standard equipment modelled.

Keywords: hydrogen, modelling, process simulation, whole system analysis

*Acknowledgement:* This work is supported by Researchers in Residence Innovation Scheme from Innovation Launchpad Network+.

### Scale-up of a Fluidised Bed Reactor for Sorption-Enhanced Steam Methane Reforming using CPFD Simulation

\*Chinonyelum Udemu¹, Carolina Font Palma¹

<sup>1</sup> School of Engineering, University of Hull, H

Scaling fluidised bed reactors from laboratory to commercial scales poses hydrodynamic challenges due to complex multiphase flows. Various scaling rules for fluidised beds aimed at maintaining hydrodynamic similarity across different system sizes have been proposed. However, verifying these rules experimentally is highly complex due to difficulties in adjusting structural dimensions and process variables while keeping key dimensionless parameters constant. This work combined computational particle fluid dynamic (CPFD) simulation and the principle of similarity to scale up a sorption-enhanced steam reforming (SE-SR) of methane process for hydrogen production operating in the bubbling regime. SE-SR process combines steam reforming and CO<sub>2</sub> capture in a single reactor vessel, enhancing hydrogen yield. As the steam reforming and water-gas shift reactions proceed, the sorbent immediately captures the produced CO<sub>2</sub> through carbonation. This continuous CO<sub>2</sub> removal shifts the reaction equilibrium toward increased hydrogen and CO<sub>2</sub> production, following Le Chatelier's principle.

The scaling criteria proposed by Glicksman (G) and Horio et al. (H) were applied to scale SE-SR of methane from a bench-scale reactor to, first, a 1 MW bubbling fluidised bed reactor. Computational simulations using CPFD software are conducted to evaluate the reliability of these scaling rules. The methodology involved deriving similarity relationships by nondimensionalising the governing equations in the CPFD model for fluidised beds. The similarities in methane conversion and bed voidage trends were examined between the scaled-up model and a validated bench-scale reactor model, across varied gas velocities and particle sizes. Whilst similarity was generally demonstrated qualitatively, minor deviations beyond  $\pm 10\%$  tolerance emerged under more vigorous bubbling and with finer particles. Nonetheless, over 90% of scaled model data agreed closely with bench-scale trends, validating the scaling criteria and approach. Model G and H simulations achieved near-identical results, though Model G required slightly larger reactor dimensions and mass.

Then, the system with 1 MW hydrogen production capacity was scaled up to larger 50 MW and 150 MW scales to examine the scale effects. The analysis highlighted the observed differences in bubble distribution and particle entrainment within the reformer at the different scales. The CPFD analysis of SE-SR conducted in this work for 1-150 MWth hydrogen production capacity has aided in understanding the micro-level details of the process, which are critical during the initial stages of technology development and scale-up.

Keywords: sorption-enhanced, CPFD, blue hydrogen, scale-up

Acknowledgement: Authors acknowledge the funding and support of Net Zero Research, UK.

## Green Methanol Production from FCC Unit Flue Gas in Basrah Refinery: A Circular Economy Approach

\*Nadeen Al-Janabi, Reem F. Badr

Ministry of Oil/ Baghdad/ Iraq

The global average atmospheric CO2 concentration was 417 ppm in 2022, which is around 40% higher compared to its level in the 1850s of only 280 ppm. Industry sector like steel, cement, oil refining and petrochemicals are directly responsible for more than 24% of global CO2 emissions with 9.0 Gt of CO2 emitted globally according to 2022 EPA report. Among the heavy industries, oil refining accounts for quarter of these emissions with around 6%, of which typically 25–35% of the refining sector emissions arises from the regenerators in Fluid Catalytic Cracking (FCC) units.

As a part of CO2 emissions' reduction, the Circular Carbon Economy approach has gained significant attention recently which implies the conversion of CO2 emissions into a highly value added raw materials.

In this study, the feasibility of methanol production from industrial flue gas emissions of an FCC unit under construction in the Basrah refinery has been investigated. CO2 capture capacities from FCC unit using post combustion capture reached around 90% from total emissions (flue gas) in which CO2 in flue gas percentage of (15-20%) scenarios has been studied.

The captured CO2 together with green hydrogen produced by water electrolysis and solar photovoltaic (PV) power was used to produce green methanol in a production plan designed using AspenHysys software with total capacity of 0.2 MM ton per year. The small-size FCC unit, with 34,000 bpd feed, emits approximately 0.28 MM tons of CO2 annually to the atmosphere.

Compared to previous works, this paper evaluated the feasibility of producing methanol under realistic conditions, CO2 capture process, and economic green hydrogen production, based on several key indicators such as CAPEX composed of variable and fixed costs, proposed required OPEX based on several scenarios.

Keywords: Green Methanol, FCC Emissions, Circular Economy Approach

Manufacturing of green carbon for the iron and steel industry: Industrial Scale trials.

Shalini Graham<sup>1</sup>, Martijn Jeroen Dekker<sup>1</sup>, Jenny Marie Jones<sup>21</sup>, Scott O'Shaughnessy, Zoe Westoby

<sup>1</sup>Perpetual Next, Kraanspoor 36, 1033 SE, Amsterdam, Netherlands. <sup>2</sup>School of Chemical and Process Engineering, University of Leeds, Leeds, UK, LS2 9JT.

The iron and steel (I&S) sector is one of the biggest industrial emitters of CO<sub>2</sub>, contributing approximately 6% (3 Gt) of global CO<sub>2</sub> emission in 2021. There are two dominant routes for steel production globally:

- The blast furnace—blast oxygen furnace (BF-BOF) is a continuous process and is the dominant route: iron ore is reduced to pig-iron in the blast furnace using coal-derived coke. The hot iron then moves to the basic oxygen furnace to make steel.
- The electric arc furnace (EAF) is a batch process and uses electricity, and chemical energy to heat the iron-based charge (scrap iron, pig-iron, sponge iron (from the direct reduced iron, DRI, process). It is the main process for steel recycling and lower in carbon emissions than BF-BOF.

Opportunities for biomass-based/green carbon in the manufacture of I&S include fuel for providing heat requirements (torrefied biomass may be suitable for this) in the Tuyere injection and use as a chemical reductant of iron e.g. by partial substitution of coal/coke in the lump coke or the coke breeze by bio-charcoal. The substitution of biomass-based carbon into the BF-BOF has been investigated for more than 10 years. Some studies have considered torrefied biomass substitution in the Tuyere injection which provides heat in the BF and is limited based on maximum oxygen enrichment in the blast furnace of 25.4%. The higher the carbon content, the more suitable the bio-charcoal as a chemical reductant and replacement of coke. Fixed carbon (FC) contents >85% are a threshold for the industry for the replacement of anthracite in the BF, while >80% may be acceptable for use in the EAF. Such high FC contents are a challenge in industrial manufacture, both in terms of process control, and in terms of the technical specification and economics. This work presents industrial trials held at the Perpetual Next 1100 kg/h pilot torrefaction plant for producing a range of biocarbon materials which could be suitable to replace coal in these applications. Results of the trials are presented, complemented by literature and laboratory-scale studies to explore the interplay between FC and char yield and how these may be maximised.

Keywords: thermal pretreatment, biomass, industrial scale, iron and steel industry

## Opportunities to facilitate the decarbonisation of steelmaking through the recovery of process dust arisings from the steel industry

\*Julian Steer1, Richard Marsh1, Neil Williams2,

<sup>1</sup> Cardiff University, Cardiff, UK; <sup>2</sup> Celsa Steel Ltd, Castle works, Cardiff, UK

The steel industry is at a transition point as it seeks to decarbonise from the carbon intensive process of the blast furnace to other production methods compatible with UK industry. The UK exports large amounts of scrap steel every year and has an increasing proportion of renewable electricity generation making the lower emissions electric arc furnace (EAF) route a strong candidate to replace the current blast furnaces. Both TATA Steel and British Steel have announced a commitment to the EAF manufacturing route in the UK. However, all of the large industrial scale steelmaking processes, including the EAF, generate large quantities of process dusts, mill scales, and oil contaminated particulates. These dusts contain valuable iron and other metals such as zinc, aluminium, calcium etc which represent valuable products in their own right where they can be recovered. Companies aim to reduce the production of these dusts; recover the value from the inprocess arisings; and to deal with legacy stockpiles. Processes that facilitate this represent an opportunity to align more closely with the circular economy and achieve deeper decarbonisation and sustainability. The research presented in this paper describes these dusts; their characterisation; and an outline of the technologies for recovering these co-products by linking practical processes with more detailed surface and bulk sample analyses. Initial work includes a study of the potential of flash reduction techniques as an adaption of pyrometallurgical extraction with a lower energy requirement and lower capital expenditure.

Keywords: Electric arc furnace; scrap; dust; recycling; drop tube furnace.

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## Ammonia decomposition on Ru-CeO<sub>2</sub> layers for hydrogen production – A DFT Study

\*Nomcebo P. Motsa<sup>1</sup>, Daniel Oduma<sup>1</sup>, Cecil Ouma<sup>2</sup>, Eni Oko<sup>3</sup>, Michael O. Daramola<sup>1</sup>

<sup>1</sup> Sustainable Energy and Environment Research Group (SEERG), Department of Chemical Engineering, University of Pretoria, Pretoria, South Africa,

<sup>2</sup> HySA Infrastructure Center of Competence North-West University, Potchefstroom, South Africa, <sup>3</sup> Newcastle University, Newcastle upon Tyne NE1 7RU, UK.

Global warming and climate change challenges have pinpointed the hydrogen economy as an alternative to fossil fuel economy. The envisaged hydrogen economy cannot be realized without a proactive approach to novel materials design. Hydrogen is emerging as a game changer in the grand realm of clean energy value chain mainly because, as an energy vector, hydrogen is both an energy carrier and an energy source. However, despite this potential, several challenges limit large scale adoption of hydrogen including the fact that hydrogen is explosive and flammable, making it difficult to store and transport. One way of mitigating this bottleneck is chemical storage in molecular carriers. On this, liquid organic hydrogen carriers have gained dominance. However, they have not reached the level of technological maturity for large scale development and adoption. Molecules such as ammonia are likely to be good alternatives since their value chain is technologically mature and they can be used as feedstock in hydrogen production. Hydrogen is produced from ammonia mainly through catalytic decomposition. The catalyst that performs well in industry for NH<sub>3</sub> is ruthenium (Ru). However, Ru is expensive and scarce. Hence this study aims to reduce the amount of Ru through Ru-CeO<sub>2</sub> layered catalysis design (periodic slab models) and optimization, and subsequent adsorption and decomposition mechanism.

The study identified the stable adsorption sites for NH<sub>3</sub> decomposition products and calculated the activation energies for the rate-determining steps. The results indicate that NH<sub>3</sub> and N<sub>2</sub> adsorb strongly on the catalyst surface. The results also indicate that the NH<sub>3</sub> dehydrogenation step on the Ru-CeO<sub>2</sub> catalyst has a comparative activation energy to that of pristine Ru, making it a viable alternative to pure Ru. The findings suggest that a monolayer of ruthenium on CeO<sub>2</sub> offers a promising approach for efficient hydrogen production but needs to be further optimised to identify the suitable number of Ru layers necessary to further reduce the activation energies of the Ru-CeO<sub>2</sub> catalyst.

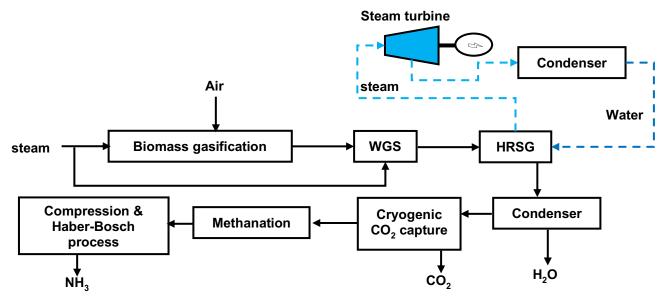
Keywords: Hydrogen, Ammonia, Ru-CeO<sub>2</sub>, Catalyst.

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Efficient Low Carbon Ammonia Production through Combined Biomass Gasification, Nitrogen Self-Sufficiency, and Waste Heat Recovery

Kazeem Mohammed a, Isaac Okereke a, Kerry McLaughlin b, Amirpiran Amiri a, \*

<sup>a</sup> Energy and Bioproducts Research Institute (EBRI), Aston University, Birmingham, UK
<sup>b</sup> Nium, Milton Park, Oxfordshire, UK



This study presents an integrated process for ammonia synthesis, combining air-steam biomass gasification and a steam turbine generator, with enhanced energy efficiency. By systematically adjusting the steam-air-biomass ratio during gasification, the process controls N<sub>2</sub> levels, ensuring sufficient N<sub>2</sub> from air for NH<sub>3</sub> synthesis as well as optimising H<sub>2</sub> generation via steam reforming. This approach eliminates the need for an air Separation Unit (ASU) for N<sub>2</sub> supply. The produced syngas undergoes water-gas shift reaction (WGSR), to maximise the H<sub>2</sub> production, followed by heat recovery using a heat recovery steam generator (HRSG) to drive the steam turbine for electricity generation as shown in the flowchart above. Subsequent steps include water vapour removal, cryogenic CO<sub>2</sub> capture, and methanation to eliminate residual CO and CO<sub>2</sub>, which are catalyst poisons in NH<sub>3</sub> synthesis. The target syngas composition achieves an H<sub>2</sub>: N<sub>2</sub> ratio close to 3:1, meeting ammonia synthesis requirements. Detailed chemical and thermal simulations of this concept were developed and simulated using Aspen Plus software and will be presented in this contribution. The results were validated, and a comparative analysis was performed to show the energy efficiency of our model compared to electrolysis pathway for ammonia production.

**Keywords:** Ammonia, hydrogen, biomass gasification, energy efficiency, H<sub>2</sub>: N<sub>2</sub> ratio optimization, nitrogen Self-Sufficiency

\*Corresponding author: Amirpiran Amiri

E-mail: <u>a.p.amiri@aston.ac.uk</u>, Tel: + 441212043169

## A Portable Dilution System for the Generation of Synthetic Biomethane Reference Materials

\*Oliver Williams<sup>1</sup>, Nur Ain Nazirah<sup>1</sup>, Dr Christopher Bamforth<sup>1</sup>, Lucy Culleton<sup>1</sup>

<sup>1</sup>National Physical Laboratory, Teddington, TW11 0LW, UK

Biomethane is expected to play a major role in Europe's green energy future. Blending biomethane into existing natural gas pipelines can quickly reduce fossil fuel consumption, facilitating the decarbonisation of energy gas networks.

The distinct and varied impurities which can occur in biomethane introduce novel challenges for those maintaining energy gas infrastructure. Ammonia may form corrosive and toxic compounds and combustion of siloxanes can produce abrasive deposits, all of which may damage existing gas infrastructure. Terpenes can mask stenching agents which are currently added to gas for leak detection, compromising safety. As such, there is a growing need for cost-effective purity analysis, to ensure that the biomethane injected into gas networks complies with EN 16723-1 (for injection into the gas grid) and EN 16723-2 (for vehicle use). The EURAMET 'Protocol for SI-traceable validation of methods for biomethane conformity assessment' project (BiometCAP) seeks to improve access to cost-effective, SI- traceable materials for the calibration and performance evaluation of commercially available biomethane purity analysers.

Conformity assessment of gas analysers is typically carried out using "static" reference standards; gas mixtures with known concentrations which can be used for calibration. The poor stability of components such as siloxanes, terpenes, and ammonia make it challenging to prepare traditional reference standards at low amount fractions of these analytes with low uncertainties. This means they need to be replaced regularly which is costly for end users.

NPL have developed a dynamic dilution system, based on thermal mass flow controllers, which allows users to produce multiple low-amount-fraction gas standards by diluting a single concentrated mixture. This could provide a long-lasting alternative to regularly purchasing sets of low-amount-fraction calibration materials which are currently required for the conformity assessment of biomethane analysers.

This presentation discusses the production of dynamic biomethane standards and their uncertainties. The following are considered: 0.1-20  $\mu$ mol mol<sup>-1</sup> ammonia in methane, 0.3-1 mg m<sup>-3</sup> total silicon in methane and 0.01-10  $\mu$ mol mol<sup>-1</sup> terpenes in methane. There is an explanation of how the system's design and passivation allow users to bypass challenges presented by static standards. Results from the evaluation of dynamic standards using existing chromatographic methods are discussed. The presentation concludes by assessing the system's suitability for the conformity assessment of commercially available biomethane analysers.

*Keywords:* biomethane, metrology, calibration, analysis, reference materials

Acknowledgement: BiometCAP 21NRM04 has received funding from the European Partnership on Metrology, co-financed from the European Union's Horizon Europe Research and Innovation Programme and by the Participating States.

## Green Solvent-Assisted Catalytic Hydrodeoxygenation of Bio-oil to Engine-Ready Drop-in Fuel

Jude A. Onwudili, Himanshu Patel

Aston University, Birmingham, UK

The conversion of bio-oil into sustainable, engine-compatible drop-in fuels offers a promising route to reduce reliance on fossil fuels and lower greenhouse gas emissions. However, the high oxygen content and chemical instability of raw bio-oil hinder its direct application as a fuel. This study explores a green solvent-assisted catalytic hydrodeoxygenation (HDO) process to upgrade bio-oil into high-quality hydrocarbons suitable for use in existing internal combustion engines. Initially, waste cooking oil (WCO) was treated with a titanium-based catalyst under an inert nitrogen atmosphere, yielding a hydrogen-rich liquid through a 'hydrogen autarky' approach. This process produced up to 90 wt.% of liquid product containing over 85% alkanes (in the gasoline-to-diesel range) and less than 3% oxygenated compounds. While the treated WCO shows strong potential as an alternative fuel, the limited availability of raw WCO constrains its scalability. To address this, we propose a two-step co-processing approach using bio-oil derived from pine sawdust combined with treated WCO in a 1:2 ratio. A series of bifunctional catalysts were systematically evaluated for their effectiveness in oxygen removal, hydrocarbon yield, and operational stability under moderate reaction conditions. The optimized system, employing a noble-metal-based catalyst, achieved an 85 wt.% yield of hydrocarbon-rich liquid, composed of approximately 90% alkanes and less than 5% residual oxygenates. The resulting fuel exhibited significantly improved physicochemical properties-including higher energy density, favourable viscosity, and enhanced volatility-meeting specifications for drop-in fuels compatible with existing internal combustion engines. Furthermore, the hydrocarbon product itself can function as a solvent medium for subsequent HDO reactions, thus minimizing reliance on fresh WCO and enhancing process sustainability. This green solvent-assisted HDO route not only offers a scalable and circular approach to bio-oil valorisation but is also tailored for decentralized deployment in regions like Nigeria, with the goal of powering agricultural machinery and supporting rural energy resilience.

## Solvent-Assisted Esterification: A Cost-Effective Strategy for Bio-oil Upgrading to Engine-Ready Drop-in Fuel

Himanshu Patel, Jude A. Onwudili

Aston University, Birmingham, UK

The advancement of sustainable and economically viable strategies for upgrading bio-oil into engineready fuels is critical for the future of bio-refinery technologies and the global shift away from fossil fuel dependence. Bio-oil, typically obtained via pyrolysis of lignocellulosic biomass, suffers from high oxygen content, acidity, and chemical instability-factors that limit its direct use in conventional combustion engines. This study presents a novel solvent-assisted esterification approach for bio-oil upgrading, integrating waste valorisation and green chemistry principles. Treated waste cooking oil (WCO), pre-processed via a titaniumbased catalytic system under an inert nitrogen atmosphere, served both as a reactive solvent and as a renewable hydrogen source. This treatment yielded ~90 wt.% of liquid product with over 85% alkanes (spanning the gasoline to diesel range) and less than 3% residual oxygenates. The high yields of alkanes indicated the possibility of in situ hydrogen generation for hydrogenation of C=C bonds during the WCO thermos-catalytic treatment. In the esterification process, treated WCO and bio-ethanol were employed alongside bio-oil derived from Indonesia-origin rice straw (in a ratio of WCO:bio-ethanol:bio-oil = 2:3:3). The reaction, catalysed by an inexpensive and reusable alkaline earth metal oxide under mild conditions, effectively esterified carboxylic acids and phenolics, significantly reducing the total acid number (TAN), while enhancing fuel miscibility, phase stability, and volatility. The resulting esterified bio-oil exhibited key improvements in physicochemical properties-lower acidity, reduced viscosity, and increased energy contentbringing it in line with diesel-range fuel specifications. Importantly, the upgraded bio-oil can be reused as a solvent medium for subsequent esterification cycles, reducing dependence on fresh WCO and contributing to process circularity. Additionally, its high miscibility with biodiesel enables seamless blending without the need for hydrogen-intensive hydrotreatment, making the process especially suitable for decentralized fuel production in regions with limited access to refining infrastructure or high-purity hydrogen. This solventassisted esterification strategy demonstrates a scalable, low-cost, and environmentally friendly pathway for transforming biomass-derived oils into engine-compatible drop-in fuels, reinforcing the broader vision of circular economy and carbon-neutral energy systems.

#### Upgrading of Biogas using Ex-situ Biochar Immobilised Bioreactor Approaches

\*Munira Alateeqi<sup>1</sup>, Andrew Ross<sup>1</sup>, Valerie Dupont<sup>1</sup>

There is an increasing interest in the upgrading biogas from anaerobic digestion, to produce high-quality biomethane. Numerous upgrading technologies have been developed to enhance the calorific value of biogas and reduce the levels of carbon dioxide. The focus of this study is to develop advanced technology for enhancing biogas quality using ex-situ biomethanation (ESB) incorporating biochar to immobilise hydrogenotrophic methanogens and convert hydrogen (H2) and carbon dioxide (CO2) to additional methane (CH4).

A range of biochar have been produced from different feedstocks and comprehensively analysed using a range of analytical techniques. The different propensity to immobilise microbial cultures have been investigated for the different biochars. Experiments have assessed the potential of biochar to act as a microbial support for biogas upgrading approaches. Biochemical methane potential tests (BMP) have been used to assess the efficiency of cell immobilisation and its role in enhancing biogas production. A laboratory-scale ex-situ biomethanation reactor for biogas upgrading has been designed and built. Biological upgrading uses hydrogenotrophic methanogens to convert CO2 and H2 into additional methane. Optimum biochar types have been tested with and without inoculate to understand the adsorption potential of the biochar and the biological upgrading potential of the methanogens. The potential for CO2 removal and biogas upgrading to additional biomethane is investigated.

**Microbial Immobilisation**: Methods have been developed to assess the influence of biochar properties on cell immobilisation through different tests and analysis. BMP tests and Scanning electron microscopy (SEM) have been performed to determine the viability of cell immobilisation and ensure the colonisation of methanogens on the surface and/or inside the pores of the biochar.

**Ex-situ Biomethanation:** A Laboratory-scale ex-situ biomethanation-packed bed bioreactor has been developed using biochar as the immobilisation support media capable of investigating gas adsorption characteristics and upgrading potential. It also enhances the mass transfer of hydrogen and carbon dioxide with methanogens enabling producing additional methane.

A mixture of model gases (H2/CO2) are employed to assess biogas upgrading. The biomethane produced is analysed by Gas Chromatograph with a Thermal Conductivity Detector.

Keywords: biogas, biochar, ex-situ biomethanation, immobilisation, methanogens

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School of Chemical and Process Engineering, University of Leeds, Leeds, UK

A Comparison of the Baseline Thermal Characteristics and Composition of Hydrochar and Pyrochar from Faecal Sludge and Water Hyacinth

\*Flora K. Chitalu<sup>1</sup>, Jenny Jones<sup>1</sup>, Andrew Ross<sup>1</sup>

<sup>1</sup> University of Leeds, Leeds, UK,

Biowaste-to-energy conversion presents a sustainable solution for energy utilisation and waste management in the Global South. Biowaste such as Faecal sludge (FS) and vegetative species such as water hyacinth (*Eichhornia crassipes*) are abundant yet underutilised biomass feedstocks with potential for solid fuel production. FS, a biowaste derived from human excreta and solid waste, is commonly collected from on-site sanitation systems such as pit latrines, while water hyacinth (WH) is an invasive aquatic plant causing ecological damage in many freshwater ecosystems including Zambia and Uganda, the focus of this study. While WH is lignocellulosic, FS is a non-lignocellulosic biomass material composed mainly of carbohydrates proteins, lipids and inorganics. However, both FS and WH are relatively high ash feedstocks, resulting in comparatively lower fuel quality. Converting these high-ash feedstocks into biochar through thermochemical processes such as pyrolysis and hydrothermal carbonisation (HTC) can enhance their energy value.

This study therefore investigates the combustion behaviour of dried FS and WH, as well as their derived biochar products from pyrolysis (200–800°C) and HTC (150–250°C), providing useful baseline data to determine the efficacy of the two processes. FS sourced from Lubigi WW- FSTP in Kampala, Uganda, while WH collected from Port Bell, Lake Victoria, will be utilised. A comparative assessment of the raw feedstocks and their resulting biochar will be conducted to determine how biomass composition and thermochemical processing influence fuel quality and combustion characteristics, considering the cellulosic and non-cellulosic nature of the feedstocks under study. This research will therefore provide insights into optimum technology for enhancing high-ash feedstocks for sustainable domestic and small-scale energy applications.

**HTC and Pyrolysis**: Pyrolysis is the established technology for biochar production in most parts of the world. Pyrolysis experiments will therefore be conducted to establish the "as is" quality of FS and WH derived pyrochar in current use for domestic and small-scale applications in the study area. Further pyrolysis runs will determine optimal process conditions for a minimised ash component. As an emerging technology under consideration, HTC experimental runs will also be undertaken to determine process influence on fuel properties, composition and combustion behaviour. From these analyses, the optimal conversion method for improving energy density, reducing ash related issues and enhancing the overall fuel quality will be ascertained.

**Feedstock and Biochar Characterisation:** The effect of pyrolysis and HTC on the various properties of FS and WH will be explored. Proximate and Ultimate analyses will determine the thermal and elemental changes that will occur after thermochemical processing. Furthermore, biochemical analysis will determine the prevalent structural components of WH and FS in relation to their lignocellulosic and non-lignocellulosic nature and provide critical insights into how these structures influence feedstock and biochar fuel behaviour.

**Combustion and Ash Analysis:** Combustion behaviour is investigated using thermogravimetric analysis (TGA) in air. Furthermore, analysis of the metal content and ash fusion behaviour will predict the propensity to slagging and fouling.

Keywords: Pyrolysis, Hydrothermal Carbonisation, Faecal Sludge, Water Hyacinth, Combustion

Acknowledgement: This work was carried out by the support of the Schlumberger Foundation and the University of Leeds under the International Network for Invasive Aquatic Plants (INIAP) Project.

### Increasing Fuel Flexibility of converted biomass boilers

B A Gudka, D P Maxwell and J M Jones\*

School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT.

Converting from coal to biomass-firing is one technology for decarbonising electricity generation. The operational availability of power plant is limited by factors such as meeting the particulate and gaseous emissions limits and the number of hours it is available to generate power. The fuel plays a large part in achieving good operation. Wood pellets are favoured for more reliable operation but carry a high price, and economics are difficult without subsidies. Substituting with cheaper fuels (lower quality) pose operational difficulties. This work seeks to extend the range of biomass that can be used in power stations, through optimised pre-treatment technologies. Potassium in biomass, especially in its volatile form, KCl and KOH, plays a key role in the ash deposition on boiler walls and heat-exchanger tubes causing slagging, fouling and corrosion. This leads to frequent plant shutdowns for maintenance purposes. Previous work has shown that removing the potassium via pre-treatment technologies can help to reduce this problem.

The main focus of this study is to develop a model which can enable plant operators to predict ash deposition rates using the potassium content of their fuels and the gas temperatures. The potential upgrading of the fuels by water washing to remove potassium salts is assessed for three fuels of interest: white wood pellets (as a baseline case); bagasse, and wheat straw. Both washed and unwashed fuels were studied in single-particle burning experiments in order to establish the release of potassium into the gas phase. The washing experiments show a 7, 52 and 25% removal efficiency of potassium for white wood pellets, bagasse and wheat straw respectively. In addition, a 33% removal efficiency was found for chlorine in wheat straw. Washed fuels burn slower than the corresponding unwashed fuels due a decrease in the catalytic effect of potassium on combustion. The washed fuels release lower absolute amounts of potassium into the gas phase upon combustion, although the fractions released during devolatilation and char burning change. The release of KOH is favoured over KCl for washed samples due to the higher K/Cl ratios for washed samples.

An empirical model is presented based on deposition data from the literature, such that deposition rates can be predicted based on K-content in the fuel and flue gas temperature. The model was validated for wheat straw only as there was a lack of data for other types of fuels. The developed model is then used to predict deposition behaviour for white wood pellets and bagasse. The predicted deposition rates are dependent on the K-content of the fuel, such that deposition rates are highest in wheat straw (0.8 wt% K), followed by bagasse (0.3 wt% K) followed by white wood pellets (0.1 wt% K). The model is also applied to the washed fuels and predict decreased deposition rates. This is most significant for bagasse, and it is clear that the deposition rate of washed bagasse can begin to approach the low values expected for white wood pellets. In this case 50% of the potassium content of the bagasse is removed by water washing, and the deposition rate decreases from 25 g/cm² h to 17 g/cm² h at 1172 K, compared to 15 g/cm² h predicted for white wood pellets.

Key words: Biomass, potassium, washing pre-treatment, ash deposition

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## Hydrothermal Liquefaction of Water Hyacinth and its comparison to different Invasive Aquatic Plants

\*Karim Ismail<sup>1</sup>, Patrick Biller<sup>2</sup>, Valerie Dupont<sup>1</sup>, Andrew Ross<sup>1</sup>

School of Chemical and Process Engineering, University of Leeds, UK Department of Biological and Chemical Engineering, Aarhus University, Denmark

Water hyacinth is a free-floating aquatic plant widespread across Asia and Africa, known for its significant environmental challenges. It obstructs waterways, disrupting aquatic ecosystems, reducing fish populations, and impeding recreational activities, navigation, and natural sediment flow. Often seen as an invasive waste, water hyacinth is typically removed and either discarded in landfills or left to decay along riverbanks and lakesides. Despite these environmental issues, it presents an untapped biomass resource for conversion into valuable bio-products.

Extensive research has explored its biochemical conversion into bioethanol and biogas through fermentation and anaerobic digestion, while a smaller body of work has focused on its thermochemical transformation via thermochemical conversion such as hydrothermal carbonisation, liquefaction and pyrolysis. Hydrothermal liquefaction (HTL) involves the processing of biomass in subcritical water at temperatures ranging from 300- 350°C producing a bio-crude, a gaseous and aqueous fraction, and a solid hydrochar. The aim of this study was to investigate the conversion of water hyacinth by Hydrothermal Liquefaction and compare its behaviour to other invasive aquatic plants. An initial screening was performed over a temperature range of 300-350°C with different KOH catalyst loadings in a batch hydrothermal reactor.

**Methodology:** The proximate, ultimate and biochemical content of the aquatic plants have been determined. Hydrothermal liquefaction experiments were determined in a 50ml high pressure reactor, rapidly heated in a sand bath. Experiments were performed with and without the addition of KOH as a catalyst. The liquefaction behaviour of water hyacinth has been compared to 3 other invasive aquatic plants (water lettuce, *lemna minor* and *azolla*).

**Results:** The highest yield of biocrude from water hyacinth are observed at 300C with a 2.8% KOH loading with the addition of KOH catalyst improving the yield of biocrude. Generally, the yields of biocrude are low and correlate well with water hyacinth having a high carbohydrate and low lipid content. Yields of biocrude are higher for *lemna minor* which has a higher lipid content although the levels of N in the biocrude are also higher. All bio- crude exhibit high levels of N-heterocycles in the biocrude with levels ranging between 2.8-

4.4 wt%. The ash content of the residual hydrochar is also high ranging between 56-71 wt%. The results indicate that the conversion of water hyacinth by hydrothermal liquefaction is feasible however yields are low in comparison to other feedstocks. The potential for co-liquefaction of aquatic plants with other feedstocks is discussed.

**Keywords:** Bioenergy, water hyacinth, Hydrothermal Liquefaction, invasive aquatic plants

Acknowledgement: this work is supported by the international strategy fund at the university of Leeds.

### Supercritical water liquefaction of waste plastics to produce oil high value fuels and chemicals

Maria Mathew<sup>1</sup>, Mohamad A. Nahil<sup>1</sup>, Paul T. Williams<sup>1</sup> \*, Andrew Ross<sup>1</sup>

<sup>1</sup>Chemical and Process Engineering, University of Leeds, Leeds, UK

Global plastic production approaches 400 million tonnes annually, with forecasts indicating a tripling by 2060. Inadequate recycling exacerbates waste accumulation, primarily disposed in landfills or ecosystems. Hydrothermal liquefaction (HTL) in supercritical water (T> 373.95 °C and P>22.12 MPa) presents a promising avenue for converting plastic waste by effectively breaking down complex polymers into valuable products such as liquid fuels and high value chemicals.

This study aims to evaluate the feasibility and efficiency of supercritical hydrothermal liquefaction (ScHTL) for the conversion of plastic waste—including low-density polyethylene (LDPE), polypropylene (PP), polystyrene (PS), polyethylene terephthalate (PET), and their mixtures—into liquid fuels and chemical feedstocks. Product yield and composition were assessed under varying reaction conditions to optimize process efficiency and mitigate the environmental impact of plastic pollution.

**Supercritical water hydrothermal liquefaction (ScHTL)** experimental setup employed a 75ml autoclave reactor with a thermowell and thermocouple for temperature measurement. Plastic pellets and water were added in varied ratios, not exceeding 24 ml per experiment. The reactor was sealed, purged with nitrogen, heated to 450°C and maximum pressure of 33 MPa, and maintained for 60-210 minutes. Experiments involving mixed plastics are conducted in a way that it optimises liquid product formation by minimising the solid production that hinders the experimental quality. After cooling, gas, solid and liquid samples were collected for analysis. Post-reaction, the liquid products were extracted using dichloromethane (DCM) and characterized via gas chromatography-mass spectrometry (GC-MS). Gaseous and aqueous products were analyzed using gas chromatography with thermal conductivity and flame ionization detectors (GC-TCD/FID) and high-performance liquid chromatography (HPLC), respectively. Solid residues, primarily derived from PET, were examined using Fourier-transform infrared (FT-IR) spectroscopy.

**Results:** High yields of oil (>97 wt.%) were obtained and contained a mixture of alkanes, alkenes, cyclic hydrocarbons, and aromatic hydrocarbons. The ScHTL of PS and PP predominantly yielded aromatic and alicyclic hydrocarbons, whereas LDPE conversion favored alkane formation. PET primarily produced solid terephthalic acid, which negatively impacted liquid yield in mixed plastic experiments. To counteract this, reaction conditions were systematically adjusted to enhance liquid production while minimizing solid residue formation.

This study highlights the potential of supercritical hydrothermal liquefaction as an effective and catalyst-free approach for converting plastic waste into valuable oil products. With consistently high oil yields and diverse product compositions, ScHTL emerges as a promising technology for mitigating plastic pollution and advancing resource recovery efforts.

Keywords: Plastics; Waste; Hydrothermal liquefaction; Supercritical; Fuel oils

Acknowledgement: This work is funded by UK Engineering and Physical Sciences Research Council (EPSRC) - University of Leeds Doctoral Training Partnership Scholarship

### Characterisation of Invasive Aquatic plants in India and their potential conversion by Anaerobic digestion

\* Andrew Ross<sup>1</sup>, Karim Ismail<sup>1</sup>, Srinivasan Balachandran<sup>2</sup>, Gaurav Nahar<sup>3</sup>

<sup>1</sup>School of Chemical & Process Engineering, University of Leeds, UK <sup>2</sup>Department of Botany, University of Visva-Bharati, Santiniketan 731235, West Bengal, India <sup>3</sup>Defiant Renewables, Chinchiwad, Pune, India

The aim of this study was to understand the anaerobic digestion behavior of different aquatic plants prevalent in India. Invasive Aquatic plants represent an underutilized resource for the production of bioenergy. They have a significant environmental impact and are often removed and dumped resulting in large GHG emissions. The management and utilization of this under-utilized resource has huge opportunities if converted to biogas using anaerobic digestion. Different species of invasive aquatic plants have been collected from water bodies across India including Water Hyacinth (*Eichhornia Crassipes*), Water lettuce (*Pistia Stratiotes*), Water Fern (*Azolla*) and Duckweed (*lemna minor*). Samples have been characterised for their biochemical and elemental composition (cellulose, hemicellulose, lignin, protein, CHNSO, VM and metals) and compared. The Biochemical Methane Potential (BMP) of each biomass has been determined using an AMPTS under mesophilic conditions using inoculum from a wastewater treatment plant.

*Pistia Stratiotes* has the highest BMP potential producing almost 200ml CH<sub>4</sub> g VS <sup>-1</sup> without any pre-treatment. It also has the faster biogas production rate of all the aquatic biomass studied. The second best performing aquatic biomass is *lemna minor* which produces 150ml CH<sub>4</sub> gVS<sup>-1</sup>. *Eichhornia Crassipes* generates between 100-220 ml CH<sub>4</sub> gVS<sup>-1</sup> and *Azolla* produces the lowest BMP at around 30 ml CH<sub>4</sub> gVS<sup>-1</sup>. Water hyacinth (WH) is regarded as the most prolific of the invasive aquatic plant species and while anaerobic digestion of WH is well explored, the levels of biogas/biomethane vary widely. This study also includes WH collected from different water bodies across India. The elemental and biochemical composition of the whole plant and its individual parts (roots, stem, leaves) differ substantially and the results indicate that WH composition influences digestion behaviour. Samples from different sites exhibit a large variation in BMP (100-220mL CH4/gVS). The different parts of the plant also digest differently, with leaves and stems displaying higher biomethane yields. The utilization of aquatic plants in AD is plausible and recommendations for improved performance are proposed.

Keywords: Aquatic plants, Characterisation, Anaerobic digestion

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### Fundamental studies of lifted and attached jet hydrogen flames in cross-flow

Chengpei Wu<sup>1</sup>, Xiaojun Gu<sup>2</sup>, \*Junfeng Yang<sup>1</sup>

<sup>1</sup> University of Leeds, Leeds, UK, <sup>2</sup> STFC Daresbury Laboratory, Warrington, UK

The increasing demand for clean and efficient energy sources has positioned hydrogen as a promising fuel for various combustion applications, including gas turbines, aerospace propulsion, and industrial safety systems. However, the complex turbulence-chemistry interactions in hydrogen jet flames, particularly in crossflow configurations, present significant challenges in predictive modeling. Understanding flame liftoff, stability, and aerodynamic effects is essential for optimizing hydrogen-based combustion technologies. This study employs computational fluid dynamics (CFD) techniques to investigate hydrogen jet flames in crossflow, utilizing an advanced Reynolds Stress Model (RSM) turbulence closure coupled with a flamelet-based combustion approach.

A major focus of this research is to enhance computational accuracy while minimizing resource consumption. To achieve this, a hydrogen-specific laminar flamelet library is developed and integrated into Code\_Saturne, an open-source CFD platform. The study systematically explores hydrogen jet behavior under varying crosswind conditions, with jet exit velocities of 300 m/s and crossflow velocities of 5 m/s and 10 m/s. Three-dimensional (3D) simulations are performed, incorporating optimized mesh structures and refined boundary conditions to ensure numerical accuracy. Simulation results are validated through dimensionless analysis, benchmarking against experimental JICF data.

Results indicate that crossflow profoundly impacts hydrogen flame dynamics, shifting high-temperature reaction zones downstream and increasing liftoff heights with rising crosswind velocity. Higher crossflow velocities cause increased flame bending, modifying the flame's aerodynamic structure and affecting combustion efficiency. The flame's reaction zone exhibits asymmetric distribution, with stronger turbulent mixing on the leeward side due to enhanced shear-layer interactions. Additionally, the study identifies key controlling parameters for hydrogen JICF stability, including jet-to-crossflow momentum ratios, turbulent Reynolds numbers, and local Damköhler numbers.

While the Reynolds Stress Model (RSM) provides a reasonable representation of turbulence anisotropy, it struggles with fine-scale turbulence structures crucial for capturing complex hydrogen flame behaviors. This limitation motivates the transition to Large Eddy Simulation (LES), which offers improved turbulence resolution at a higher computational cost. Planned future work will focus on LES implementation, involving source code modifications, advanced mesh refinement strategies, and turbulence model calibration. LES will allow for higher-fidelity predictions of hydrogen flame evolution, particularly under extreme operating conditions relevant to gas turbine combustors and hydrogen venting systems.

This research contributes significantly to hydrogen combustion modeling by providing a validated computational approach for predicting hydrogen jet behavior in crossflow environments. The findings offer critical insights for hydrogen energy applications, particularly in optimizing combustion performance, reducing emissions, and mitigating flame instability risks. By integrating advanced turbulence models and flamelet-based combustion techniques, this study bridges the gap between computational efficiency and predictive accuracy, facilitating the development of next-generation hydrogen combustion systems.

Keywords: turbulent, jet flame in cross flow, hydrogen, combustion

Acknowledgement: We extend our appreciation to the University of Leeds for providing access to the ARC4 computer facility, and to the STFC Scientific Computing Department for granting access to the SCARF computer facility.

Size Distribution Measurement of Pneumatically Conveyed Pulverised Fuel in a Square-Shaped Pipe through Acoustic Emission Detection and Electrostatic Sensing

Xingxing Zeng<sup>1</sup>, \*Yong Yan<sup>2</sup>, Xiangchen Qian<sup>1</sup>

<sup>1</sup> North China Electric Power University, Beijing, China <sup>2</sup> Beihang University, Hangzhou, China

On-line measurement of the size distribution of pulverised fuels in square-shaped pneumatic conveying pipes is essential for improving process efficiency and reducing energy consumption. However, existing measurement techniques have difficulties in measuring the size distribution of pulverised fuel because of the complexity of the dynamics of particle flow due to the four sharp corners of a square-shaped pipe. This paper proposes a method that combines acoustic emission (AE) detection and electrostatic sensing to tackle this challenge.

**Sensing system**: A sensing system integrating AE and electrostatic sensors is designed and constructed, as shown in Fig. 1. AE detection is performed by protruding a waveguide into the flow to capture the AE signal generated from the collisions between pulverised fuels and the waveguide. The electrostatic sensors are employed to acquire the particle impact velocity upstream of the waveguide by means of the cross-correlation technique.

**Improved Hertz impact model:** The traditional Hertz theory does not take into account the energy loss during the collisions, which is clearly inconsistent with practical impacts. Therefore, an improved Hertz impact model is proposed to characterise the collisions between pulverised fuels and the waveguide. The improved Hertz model introduces a hysteresis damping factor to describe the energy loss due to inelastic effects during the collisions.

**Novel particle sizing algorithm:** Based on the impact model, a novel particle sizing algorithm incorporating time-frequency sparse coding and peak sound pressure level detection is developed and applied to estimate the particle size distribution.

**Experimental results and discussion:** To assess the effectiveness of this approach, three groups of pulverised fuels with various size distributions (ranging from 78–325  $\mu$ m, 98–407  $\mu$ m and 124–487  $\mu$ m) were selected for experimental tests at particle velocities varying from 10 to 16 m/s and mass flow rates from 7 to 13 kg/h on a laboratory-scale particle flow test rig. The results show that the relative errors of the measured size distributions for the three groups of pulverised fuels are within  $\pm 6.9\%$ ,  $\pm 6.3\%$ , and  $\pm 5.9\%$ , respectively, as shown in Fig. 2. The results demonstrate that the proposed improved Hertz impact model and the novel particle sizing algorithm are effective for the size distribution measurement of pneumatically conveyed pulverised fuels.

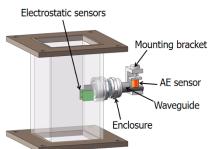


Fig. 1. Structure of the sensing head.

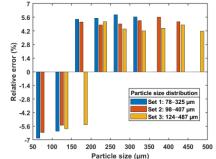


Fig. 2. Errors of the measured size distribution.

*Keywords :* size distribution measurement, pneumatic conveying, pulverised fuel, Square-shaped pipes, acoustic emission detection, electrostatic sensing.

# Co-processing Sargassum with Lignocellulosic Biomass by Hydrothermal Carbonisation: Impacts on Hydrochar Quality

Isabel Smith, Sangeetha Piriya Ramasamy, Andrew Ross

School of Chemical and Process Engineering, Faculty of Engineering and Physical Sciences, University of Leeds

Sargassum is genus of brown seaweed which grows in sub-tropical waters and exists as floating rafts in the upper section of the water column, providing a habitat and source of nutrient dense food for marine life. However, in recent years there an been an astronomical growth in sargassum in the North Atlantic Ocean. The sargassum rafts are then carried by the tides to the Caribbean and Gulf of Mexico, where they wash up on beaches in huge quantities. The resulting overabundance of the seaweed has resulted in a significant waste management problem, as well as threats to biodiversity and public health. While sargassum currently has applications in the food and cosmetics industry due to its bioactive compounds, the overabundant amounts appearing on beaches far exceed the demand for the seaweed. Developing a method of processing this material to produce a valorised product is essential in tackling the waste management problem. Hydrothermal processing presents a strong potential due to its ability to process wet materials that are high in ash. In hydrothermal carbonization (HTC), the feedstock is processed in water at 180-280°C under autogenous pressure. This mimics the natural coalification process to produce an energy dense, hydrophobic char as the primary product. Co-HTC is a method that has gained interest in recent years to mitigate product quality issues when using single feedstocks through co-processing with other available feedstocks.

This study is focused on determining the effectiveness of hydrothermal carbonization of sargassum to produce a high-quality solid fuel. The potential for improving char quality by co-processing with a low ash lignocellulosic feedstock is also evaluated, with the aim to produce an energy dense, low alkali metal hydrochar with ideal properties for combustion. Sugarcane bagasse was selected as the co-feedstock due to its complimentary qualities such as low ash and there being a large resource available in the Caribbean and South America, closely located to where the sargassum resource originates.

**Methodology:** Hydrothermal carbonization was carried out on the single feedstocks (sargassum and sugarcane bagasse) and a series of blend ratios (70:30, 50:50 and 30:70) at two temperatures (200°C and 250°C). HTC experiments were carried out in a 600mL high pressure reactor. The proximate, ultimate and metals content of the hydrochars were determined as well as the ash fusion behaviour. The data for single processed hydrochars was compared to the blended hydrochars to determine the impacts of blending and if additive behaviour was demonstrated.

**Results:** Processed alone the bagasse had a hydrochar yield of 63.8 wt% at 200°C and 46.5 wt% at 250°C, while sargassum was 42.9 wt% at 200°C and 36.8 wt% at 250°C. The hydrochar yield was found to have linear relationship with feedstock blend ratio, making the improvements to solid yield by blending predictable. The metals were found to present non-additive behaviour. Levels of alkali metals (Na and K) were reduced in the hydrochar compared with the raw biomass; however, other metals (particularly Ca) were enriched into the hydrochar. Results indicate sugarcane bagasse is an excellent feedstock for HTC, leading to improvements in co-processed sargassum hydrochar; however, the improvements are limited by the quality of sargassum.

**Keywords:** sargassum, hydrothermal carbonization, sugarcane bagasse, solid fuel.

Acknowledgment: This work has been supported by INIAP (international network on Invasive Aquatic Plants) via the University of Leeds International Strategic funding.

Using carbonate-based nanofluids in an integrated heat pump-thermal energy storage system for providing sustainable domestic heating

Aashir Zaheer<sup>1\*</sup>, Frans Muller<sup>1</sup>, Sven Schroeder<sup>1</sup>, Keeran Ward<sup>1</sup>

School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT, UK1

Domestic heating is a highly carbon-intensive process. In 2017, domestic heating contributed to 14.3% of UK greenhouse gas emissions. To meet the UK's aim of reaching net zero emissions by 2050, it is critical that the domestic heating sector in the UK is decarbonised. Heat pumps are an attractive option for decarbonising domestic heating since it can be solely powered by renewable energy sources; however, renewable energy sources are intermittent and are not a stable energy source. Thermal energy storage materials are well positioned to fill this gap by providing energy during periods of low renewable energy supply.

A novel integrated heat pump-thermal energy system(HP-TES) is proposed. The system buffers heat from renewable electricity and releases this when renewable energy supply is low thus reducing the reliance of the HP-TES system on fossil fuels.

We first developed an Aspen Plus model of a stand-alone heat pump. Fitting the pump performance to literature data revealed that compressor efficiency is key. The model was extended to the integrated heat pump-thermal energy storage system and their performance has been characterised at a range of external conditions and using current time series data for the availability of renewable electricity.

We are evaluating the use of carbonate nanoparticles dispersed in an oil, as a potential medium for thermal energy storage. Dispersing nanoparticles increases the fluid density, potentially resulting in a better volumetric heat capacity (kJ/L.K). Measured thermal properties of the materials have been used with the HP-TES model on Aspen Plus to demonstrate its impact.

Keywords: thermal energy storage, heat pumps

## Structure—Performance—Environment Mapping of Cu-based Catalysts for Green Methanol Synthesis

Xiaodong Liu, Kevin J Hughes, Bill Nimmo

School of Mechanical, Aerospace and Civil Engineering, The University of Sheffield, Sheffield, S3 7RD, United Kingdom

The industrial hydrogenation of CO<sub>2</sub> to methanol offers a viable route toward green methanol synthesis, contributing to the decarbonization of fuel and chemical supply chains. However, catalyst development remains fragmented across performance and environmental domains, complicating efforts to design scalable and sustainable systems. Traditional life cycle assessment (LCA) studies typically focus on isolated catalysts, limiting cross-system comparability. This study proposes an integrated structure-performance-environment (SPE) framework to benchmark Cu-based catalysts for green methanol production. Seven representative catalysts were experimentally assessed for turnover frequency (TOF) and CO<sub>2</sub> conversion, followed by process simulation and validation of the CO<sub>2</sub> hydrogenation to methanol pathway. LCA was conducted using SimaPro with ReCiPe, IPCC, and CML methods to quantify environmental impacts across key categories. The resulting metrics were integrated with catalytic performance data to generate a unified SPE mapping, enabling the identification of trade-offs among activity, efficiency, and environmental burden. Radar plots and heatmaps were employed to visualize comparative trends and support multi-criteria analysis. The framework reveals that while some systems achieve a favourable balance between reactivity and sustainability, others exhibit pronounced trade-offs. This approach facilitates rational catalyst down-selection and provides a transferable methodology for aligning laboratory-scale research with the broader objectives of green methanol synthesis and life-cycle-informed catalyst design.

**Keywords:** CO<sub>2</sub> hydrogenation, green methanol synthesis, Cu-based catalysts, life cycle assessment, process integration, multi-criteria analysis, sustainability benchmarking

Acknowledgement: This work is supported by Energy 2050 Group, School of Mechanical, Aerospace and Civil Engineering, The University of Sheffield, Sheffield, S3 7RD, United Kingdom.

# Production and Optimisation of Oxygenated Biofuel Blend Components via the Butanolysis of Different Lignocellulosic Biomass Feedstocks

Mohamad Anas Nahil<sup>1</sup>, Valerie Dupont<sup>1</sup>, Alison Tomlin<sup>1</sup>, \*Andy Ross<sup>1</sup>

<sup>1</sup> School of Chemical and Process Engineering, University of Leeds, Leeds, UK.

Rapid increases of energy consumption and human dependency on fossil fuels have led to the accumulation of atmospheric greenhouse gases (GHGs) and consequently, climate change. The transport sector emits the highest fraction of greenhouse gases. Decarbonisation of the transportation sector remains a key challenge to meet EU climate goals. One way of achieving this is by the integration of biofuels in road transport. Lignocellulosic biomass can be converted to various high-value chemicals (e.g. alkyl levulinates, sugar, furfural, 5-hydroxymethyl furfural, levulinic acid) by controlled dehydration under various conditions. Alkyl levulinates have been identified as potential biofuel blend components because of their specific physicochemical and combustion properties. This presentation discusses the production of a tailorable advanced biofuel blend (butyl levulinate) from lignocellulosic wastes using acid-catalysed butanolysis. A response surface methodology (RSM) was used to determine optimal process conditions for maximisation of main product yields. The main products are a butyl levulinate and dibutyl ether with some side products including butyl acetate, butyl formate and furfural also being formed during the process.

RSM analysis is employed using the Design Expert software to model the butanolysis of waste corn cob using  $H_2SO_4$  as catalyst. This work investigates the effects of temperature, corn cob loading wt%, corn cob: $H_2SO_4$  mass ratio and reaction time on different responses. Finally, identifying optimum conditions will help tailor the reaction conditions towards the production of useful blend components. The optimum conditions will then be applied in the reaction system using different biomass feedstocks.

The optimal levels of each variable within the design were estimated regarding the demand for a high butyl levulinate yield and low dibutyl ether yield and reaction time. The optimum conditions for our reaction system include a temperature of  $185\,^{\circ}$ C, corn cob loading of 9.52%, corn cob to acid ratio of 10 and reaction time equal 2.16 hour. The optimised conditions predicted a maximum butyl levulinate yield (BL) of 19.80 wt%.

A range of feedstocks were investigated at the optimised conditions including corn cob, rice and wheat straws, rice husk and sugarcane bagasse. The experimental results for corn cob were slightly lower than the predicted values (18.67 wt%) however it exhibited the highest BL yield of the feedstocks investigated. The yield of BL for sugarcane bagasse was slightly lower (17.83wt%), while BL yields produced from rice husk, wheat straw and rice straw were in the range of 12.68 to 16.07 wt%. Dibutyl ether yield for all biomass samples was circa 18 wt%. The results also showed that most of the biomass metal content was retained in the solid residue samples. This will support the potential use of this advanced biofuel blend for the engine applications.

Keywords: Butanolysis, Butyl levulinate, Corn cob, RSM, Homogeneous catalyst, Oxygenates, Biomass Acknowledgement: This work is supported by the Engineering and Physical Sciences Research Council [EP/T033088/1]

A kinetic and mechanistic study of on-purpose renewable propane production via butyric acid hydrothermal decarboxylation over Pt/C

Seyed Emad Hashemnezhad <sup>1</sup>, Jude A. Onwudili <sup>1,2,\*</sup>

Bio-LPG offers a flexible and low-carbon alternative to conventional LPG, with potential applications in off-grid heating, transportation, and industrial sectors. However, current commercial production is largely limited to biopropane co-produced during hydrotreating of vegetable oils and fats, yielding only 5-8% propane by weight. This route is insufficient to meet future Bio-LPG demand and restricts the diversity of feedstocks and production technologies.

To address these limitations, new on-purpose production pathways using renewable, biomass-derived feedstocks are being investigated. Among these, butyric acid, a C<sub>4</sub> fatty acid produced via anaerobic fermentation, has emerged as a particularly attractive intermediate due to its high selectivity toward propane under hydrothermal catalytic conditions. Additionally, recent advances in fermentation have made butyric acid production from lignocellulosic biomass more cost-competitive, reducing its cost to approximately 55% of petrochemically derived equivalents.

In this study, hydrothermal decarboxylation of butyric acid was investigated over a 5 wt% Pt/C catalyst using a batch reactor operated between 513-533 K at an initial acid concentration of 1.1 mol L<sup>-1</sup>. Experiments over 0-60 minutes reaction time confirmed propane as the primary gaseous product, accompanied by CO<sub>2</sub> and trace quantities of CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, and C<sub>4</sub>H<sub>10</sub>. Minor amounts of propanoic acid were observed in the aqueous phase. Reaction conditions were optimised to confirm the absence of mass transport limitations, based on catalyst loading, agitation studies and the Weisz-Prater criterion.

Kinetic modelling was performed using both power-law and Langmuir-Hinshelwood (L-H) expressions. The power-law model suggested a second-order rate law with an apparent activation energy of 118 kJ mol<sup>-1</sup>. The L-H model, which assumes a surface reaction as the rate-determining step, yielded an activation energy of 113 kJ mol<sup>-1</sup> and was found to best fit the data among the three competing formulations, with R<sup>2</sup> values between 0.927 and 0.970. The calculated adsorption enthalpy of -35.14 kJ mol<sup>-1</sup> for butyric acid indicated weak surface binding, consistent with observed reaction behaviour.

The kinetic insights from this work offer a valuable framework for reactor design, modelling, and scale-up of on-purpose biopropane production, supporting broader defossilisation goals across the liquid gas sector.

Keywords: Biopropane, Butyric acid, Hydrothermal decarboxylation, Pt/C catalyst, Reaction kinetics

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<sup>&</sup>lt;sup>1</sup> Energy and Bioproducts Research Institute, Aston University, Birmingham B4 7ET, West Midlands, United Kingdom

<sup>&</sup>lt;sup>2</sup> Department of Chemical Engineering and Biotechnologies, School of Infrastructure and Built Environment, College of Engineering and Physical Sciences, Aston University, Birmingham B4 7ET, West Midlands, United Kingdom

## Modeling of Flue Gas Filters in Energy from Waste Plants to Optimise Surface Particulate Loading

Nicholas Tann\*,1,2, Barry E. Gouldson2, Jane Howarth2 and William Nimmo1

<sup>1</sup> The University of Sheffield, Sheffield, UK, <sup>2</sup> Durham Filtration Ltd, UK

With the UK's commitment to reaching net zero by 2050, bringing the total greenhouse gas emissions of the country to the same level as those being removed from the atmosphere, the EFW industry has become key to the UKs sustainability objective.

EFW plants contribute both to the sustainable disposal of waste and the production of renewable energy, with 16.8Mt of waste being burned to produce 10GWh of electricity in 2024.

In parallel, and complimenting net zero, are ever tighter emissions to atmosphere standards which are part of the UK Government's Clean Air Strategy 2019. The latest round environmental permits under the Waste Incineration Directive (WID) came into force in December 2023.

UK government statistics show that the annual mortality due to human-caused air pollutants is between 28,000 and 36,000. As well as mortality, there are other effects on health such as asthma, lung cancer, heart attack and stroke. This detrimental impact on health is estimated to cost the NHS and social care system £1.6 billion between 2017 and 2025.

Optimisation of pulse jet bag house filtration in the EFW industry is a challenge. There are several factors to consider, though anecdotally many plants primary measures of good operation are;

- Low dP
- Good bag life
- Low emissions

The current work addresses gaps in the understanding of efficient and cost-effective management of filtration systems as deployed in the UK to maximise operational life and minimise outage and maintenance costs. It isn't sufficient to consider dP alone as a sole parameter for decision-making.

The method involves the study of the nature of particulate deposits of filter bag surfaces and how they develop and change with time and use. This will lead to better and more informed choices on pulse-cleaning scheduling and the effect it has on filter loadings and effectiveness. The study involves the application of modelling techniques using MATLAB combined with experimental validation using a Palas filter test unit in the laboratory.

The modelling has shown potential to generate more appropriate setpoint curves which takes account of aging and the dynamics of particulate/filter interactions, and results to date show promising and insightful guidance on how optimum dP setpoints can be obtained and deployed in real plant operating conditions.

Future work will compare data from real plant and from the test rig to further refine the models.

Keywords: Waste to Energy, Particulates, filtration, modeling

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