1st SUSTENS Meeting

Advances in Sustainable Engineering Systems

4-5 June 2025

Virtual

H
SUSTENS
B

SUSTainable H
ENgineering U
Systems B




Contents

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Introduction

The **1st SUSTENSHUB Meeting** was held **virtually on June 4–5, 2025**, and was successfully completed with **96 participants**. The organization committee invited all levels of engineers, researchers and industrial practitioners to present their recent advancements and projects through a broad range of Topics, also supporting publication opportunities including this **Book of Abstracts**, **Conference Proceedings** (*proceedings*, MDPI) and a **Special Issue** (*processes*, MDPI).

We are honored by the valuable contribution of distinguished scientists and researchers involved in the **Scientific Committee and Speakers** of the 1st SUSTENSHUB Meeting.

The conference was supported by **51 Scientific Committee members**, **7 Plenary Speakers**, and **8 Invited Speakers** from academia and the private sector.

Moreover, the conference was attended by **72 Presenters**, including **58 Oral and 14 Poster** presentations, as well as **24 attendees** from 17 different countries including: Greece, USA, Sweden, UK, Italy, Belgium, Brazil, Cyprus, Germany, Denmark, India, Qatar, Spain, Finland, France, Iran and Norway.

Conference Chairs

Assistant Professor
Nikolaos A. Diangelakis
School of Chemical and Environmental Engineering, Technical University of Crete, Greece

Associate Professor
Leonidas Matsakas
Division of Chemical Engineering, Luleå University of Technology, Sweden

Professor
Gerasimos Lyberatos
School of Chemical Engineering, National Technical University of Athens, Greece

Conference Sponsors

SUSCHEM GR — European Technology Platform For Sustainable Chemistry

proceedings — an Open Access Journal by MDPI

processes — an Open Access Journal by MDPI

Scientific Committee members

1. **Professor Seferlis Panagiotis**, Resources Institute School of Mechanical Engineering, Aristotle University of Thessaloniki, Greece
2. **Professor Emeritus Spyros G. Pavlostathis**, School of Civil and Environmental Engineering, Georgia Institute of Technology, USA
3. **Professor Mariano Martín**, Department of Chemical Engineering, Universidad de Salamanca, Spain
4. **Professor Apostolis Koutinas**, Department of Food Science and Human Nutrition, Agricultural University of Athens, Greece
5. **Professor Dimitrios Lekkas**, School of the Environment, University of the Aegean, Greece
6. **Professor Sixto Malato**, Energy, Environment & Technology Research Centre, Organismos Públicos de Investigación, Spain
7. **Professor Dimitris Vayenas**, School of Chemical Engineering, University of Patras, Greece
8. **Professor Haralambos Sarimveis**, School of Chemical Engineering, National Technical University of Athens, Greece
9. **Professor Petros Samaras**, Department of Food Science and Technology, International Hellenic University, Greece
10. **Associate Professor Anna Trubetskaya**, Faculty of Biosciences and Aquaculture, Nord University, Norway
11. **Professor Anastasios Zouboulis**, School of Chemistry, Aristotle University of Thessaloniki, Greece
12. **Associate Professor Michael Fountoulakis**, School of Chemical and Environmental Engineering, Technical University of Crete, Greece
13. **Associate Professor Olivia McDermott**, School of Biological & Chemical Science, University of Galway, Ireland
14. **Associate Professor Alessandra Polettini**, Department of Civil and Environmental Engineering, Sapienza University of Rome, Italy
15. **Associate professor Antonopoulou Georgia**, Department of Sustainable Agriculture, University of Patras, Greece
16. **Associate Professor Konstantinos Anastasakis**, Department of Biological and Chemical Engineering, Aarhus University, Denmark
17. **Associate professor Lange Heiko**, Department Of Earth And Environmental Sciences, University of Milano-Bicocca, Italy
18. **Associate Professor Maria Papathanasiou**, Department of Chemical Engineering, Imperial College London, UK
19. **Associate Professor Andreas Yiotis**, School of Mineral Resources Engineering, Technical University of Crete, Greece
20. **Associate Professors George Arampatzis**, School of Production Engineering & Management, Technical University of Crete, Greece

21. **Associate Professor Raffaella Pomi**, Department of Civil and Environmental Engineering, Sapienza University of Rome, Italy
22. **Associate Professor Hariklia N. Gavala**, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Denmark
23. **Associate Professor Katerina Stamatelatou**, Department of Environmental Engineering, Democritus University of Thrace, Greece
24. **Asst. Professor Aurora del Carmen Munguía-López**, University at Buffalo, USA
25. **Assistant Professor Styliani Avraamidou**, Department of Chemical and Biological Engineering, Universtiy of Wisconsin-Madison, USA
26. **Assistant Professor Alexandros D. Kiparissides**, School of Chemical Engineering, Aristotle University of Thessaloniki, Greece
27. **Assistant Professor Vassilis Charitopoulos**, Department of Chemical Engineering, University College London, UK
28. **Assistant Professor Ioanna Ntaikou**, School of Civil Engineering, University of Patras, Greece
29. **Assistant Professor Theodoros Damartzis**, Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece
30. **Assistant Professor Dimitrios Ipsakis**, School of Production Engineering and Management, Technical University of Crete, Greece
31. **Assistant Professor Argyro Tsipa**, Department of Civil and Environmental Engineering, University of Cyprus, Cyprus
32. **Assistant Professor Anestis Vlysidis**, School of Chemical Engineering, National Technica University of Athens, Greece
33. **Assistant Professor Aikaterini Papadaki**, Department of Food Science and Human Nutrition, Agricultural University of Athens, Greece
34. **Assistant Professor Alok Kumar Patel**, Division of Chemical Engineering, Luleå University of Technology, Sweden
35. **Dr. Athanasios I. Papadopoulos**, Chemical Process and Energy Resources Institute, Centre for Research and Technology-Hellas, Greece
36. **Dr. Antonio Del Rio Chanona**, Department of Chemical Engineering, Imperial College London, UK
37. **Dr. Peleka Efrosyni**, Aristotle University of Thessaloniki, Greece
38. **Dr. Linus Stegbauer**, Institute of Nanoscale and Biobased Materials, Technische University Bergakademie Freiberg, Germany
39. **Dr. Konstantinos Moustakas**, School of Chemical Engineering, National Technical University of Athens, Greece
40. **Senior Lecturer Io Antonopoulou**, Division of Chemical Engineering, Luleå University of Technology, Sweden
41. **Dr. Eduard Kerkhoven (Docent)**, Department Life Sciences, Chalmers University of Technology, Sweden

42. **Dr. Payam Ghiaci**, High-throughput Centre, RISE Research Institutes of Sweden, Sweden
43. **Dr. Panagiotis Evangelopoulos**, Thermochemical processes, RISE Research Institutes of Sweden, Sweden
44. **Dr. Konstantina Papadopoulou**, School of Chemical Engineering, National Technical University of Athens, Greece
45. **Dr. Eva Nanaki**, Dep. of New Technologies & Innovation, HELLENiQ ENERGY, Greece
46. **Dr. Carlo Pastore**, Istituto di Ricerca sulle Acque (IRSA-CNR), Consiglio Nazionale delle Ricerche, Italy
47. **Dr. Manuel Salvador de Lara**, Department of Systems Biology, IDENER R&D, Spain
48. **Dr. Krishna Upadhyayula**, Department of Energy Economy & Sustainability, Scania, Sweden
49. **Pantelis Karatzas** (PhD Cand), Software and Machine Learning Department, IQVIA, Greece
50. **Dr Alex Grigoropoulos**, Senior Researcher, Creative Nano, Athens, Greece
51. **Dr. Nikos Tsafantakis**, Senior Researcher, Individual Professional, Greece

Conference Topics

1. **Process design, modeling and optimization**

   Process design, synthesis and optimization; Process and energy integration; Process intensification; Scheduling and control; Supply/Value chain optimization

   Topic Chairs: *Professor Mariano Martín, Universidad de Salamanca, Spai and Asst. Professor Vassilis Charitopoulos, University College London, UK*

2. **Sustainable energy & Circularity**

   Carbon Capture and Storage/Utilization; Circular economy models; Renewable Energy Sources; Energy networks

   Topic Chairs: *Asst. Professor Styliani Avraamidou, University of Wisconsin-Madison, USA and Asst. Professor Aurora del Carmen Munguía-López, University at Buffalo, USA*

3. **Machine Learning**

   Digital Twins; Machine Learning & Artificial Intelligence; Data analysis; Software applications; Data-Driven & Real-Time Optimization

   Topic Chairs: *Assoc Professor Leonidas Matsakas, Division of Chemical Engineering, Luleå University of Technology, Sweden*

4. **Green and innovative chemistries and technologies**

   New products design; Safe and sustainable by Design; Biomass and waste valorization; Bioprocessing; Materials & nanotechnology

   Topic Chairs: *Professor Anastasios Zouboulis, Aristotle University of Thessaloniki, Greece and Dr. Peleka Efrosyni, Aristotle University of Thessaloniki, Greece*

5. **Biotechnology**

   Metabolic engineering tools; Microbial screening and Bioprospecting; Design-Build-Test-Learn

   Topic Chairs: *Donald B. Broughton Professor Costas Maranas, Chemical Engineering Faculty, Pennsylvania State University, USA and Asst. Professor Alok Kumar Patel, Luleå University of Technology, Sweden*

Speakers

Plenary Speakers

- **Prof. Gregory Stephanopoulos**, MIT, USA
- **Prof. Antonis C. Kokossis**, NTUA, Greece
- **Prof. Emeritus Nicolas Kalogerakis**, TUC, Greece
- **Prof. Panagiotis Christofides**, UCLA, USA
- **Prof. Costas Maranas**, PSU, USA
- **Prof. Petros Gikas**, TUC, Greece
- **Prof. Spyros Agathos**, UCLouvain, Belgium

Invited Speakers

- **Prof. Mariano Martin**, USAL, Spain
- **Prof. Anastasios Zouboulis**, AUTH, Greece
- **Prof. Apostolis Koutinas**, AUA, Greece
- **Assoc. Prof. Konstantinos Anastasakis**, Aarhus, Denmark
- **Assoc. Prof. Maria Papathanasiou**, Imperial, UK
- **Dr. Athanasios Papadopoulos**, CERTH, Greece
- **Dr. Manuel Sallvador**, IDENER R&D, Spain
- **Dr. Eduard Kerkhoven**, Chalmers, Sweden

Conference publications

- **16 Extended Abstracts** published in **The 1st SUSTENS Meeting**, *Volume 121, 2025, proceedings, ISSN 2504-3900*
- **55 Short abstracts** published in the Conference **Book of Abstracts**
- **18 Scientific papers** in the Special Issue **1st SUSTENS Meeting: Advances in Sustainable Engineering Systems,** *Processes, ISSN 2227-9717*

Conference awards

Awards for outstanding contributions of authors to the 1st SUSTENSHUB Meeting

- **1st Prize:** ***Varnava, C., Ieropoulos, I., Leontidis, E., Tsipa***, *A. Harnessing Pseudomonas citronellolis 620C for Electro-Bioremediation: Insights from Transcriptional Kinetics and Metabolite Synergy in Microbial Fuel Cells*
- **2nd Prize:** ***Voutetaki, A., Plakas, K.,Seferlis, P., Papadopoulos, A.*** *A Data-driven Approach for Integrated Design and Dynamic Optimization of Renewable Electrodialysis Systems*
- **3rd Prize:** ***Stratis, N., Morbidelli, M., Kipparissides, A.*** *Flux Balance Analysis with Plasmid Integration (FBApi): A novel algorithm to quantify the metabolic burden associated with plasmid replication and expression*

Program

Day-1: Wednesday 4 June 2025

8:30-8:45	**Login to SUSTENS HUB and Entrance to Event Rooms**
8:45-8:55	**Opening the 1st SUSTENSHUB Meeting** Professor Gerasimos Lyberatos, *School of Chemical Engineering, National Technical University of Athens, Greece*
9:00-10:40	**Parallel sessions**
Session: Process design, modeling and integration-1 *Chaired by Asst. Professor Vassilis Charitopoulos, University College London, UK*	
9:00-9:20	**Electrocoagulation as a revived method for industrial wastewater pretreatment** Dimitris V Vayenas, *Christina Vasiliki Lazaratou, Maria Gourniezaki, Maria Kakkou, Stavros Koutroupis, Michael Mageiras, Athanasios Iliopoulos, Alexandros Zolotas*
9:20-9:40	**Bioprocess systems engineering approaches to improve rAAV production for gene therapy applications** Gabriele Mura, *Sarah Fadda, Alexandros Kiparissides*
9:40-10:00	**A Data-driven Approach for Integrated Design and Dynamic Optimization of Renewable Electrodialysis Systems** Alexia Voutetaki, *Konstantinos Plakas, Panos Seferlis, Athanasios Papadopoulos*
10:00-10:20	**Optimization of Residential Energy Systems Design in Distinct Climatic Con-ditions** Rafailia Magdalini Psomiadou, *Nikolaos A. Diangelakis*
10:20-10:40	**Industrial Urban Symbiosis Modelling for Closing the Water Loop** Efthalia Karkou, *George Arampatzis*
Session: Sustainable energy & Circularity-1 *Chaired by Professor Gerasimos Lyberatos, School of Chemical Engineering, National Technical University of Athens, Greece*	
9:00-9:20	**Economic evaluation of novel C-zero processes for the efficient production of energy, chemicals and fuels** D. Ipsakis, *G. Varvoutis, A. Lampropoulos, C. Athanasiou, M. Lykaki, E. Mandela, T. Damartzis, S. Papaefthimiou, M. Konsolakis and G.E. Marnellos*
9:20-9:40	**Assessing the Environmental and Economic Impacts of Shipping: Insights from the Horizon2020 EMERGE (Evaluation, control and Mitigation of the EnviRonmental impacts of shippinG Emissions) Project** Androniki Maragkidou, *Jukka-Pekka Jalkanen, Erik Fridell, Jaakko Kukkone, Jana Moldanova, Leonidas Ntziachristos, Achilleas Grigoriadis, et al.*
9:40-10:00	**Bioprospecting of Oleaginous Microalgal Strains for High Biomass and Lipid Yields under Outdoor Cultivation as a Sustainable Feedstock for Biodiesel Production** Athanasios Karousis, *Theofanis Laskos, Georgia Papapanagiotou, Christina Samara, Alexandros Biziouras, Christos Chatzidoukas*
10:00-10:20	**Optimization of biotrickling filters for biological biogas upgrade to biomethane under mesophilic conditions**

10:20-10:40	*Christina Karyofyllidou, Apostolos Spyridonidis, Vasileios Diamantis, Katerina Stamatelatou*
	CCU Process Design and Evaluation for Methanol Production Using Cement Flue Gases
	Christoforos Siskos, Pantelis Manakas, Lazaros Karaoglanoglou, Anestis Vlysidis
10:40-11:00	**Coffee Break**
11:00-11:50	**Parallel sessions**
Session: Invited Speakers-1	
Chaired by Assistant Professor Nikolaos Diangelakis, Technical University of Crete, Greece	
11:00-11:25	**Systematic Optimal integrated plants for sustainable chemicals production: Multiscale approach for waste valorization**
	Isabel Hernández, Carlos Sanz, Sofía González-Núñez, Jose Enrique Roldan San António, Mariano Martin
11:25-11:50	**A systems engineering approach for novel and sustainable value chains in biopharmaceuticals**
	Associate Professor Maria Papathanasiou, Department of Chemical Engineering, Imperial College London, UK
Session: Invited Speakers-2	
Chaired by Associate Professor Leonidas Matsakas, Luleå University of Technology, Sweden	
11:00-11:25	**Designing Complexity: Methodological Challenges in Engineering Hybrid Bioactive Compounds through Synthetic and Systems Biology**
	Manuel Salvador, IDENER R&D, Spain
11:25-11:50	**Computational models of metabolism as digital shadows of cell factory performance**
	Eduard Kerkhoven, Chalmers University of Technology, Gothenburg, Sweden
12:00-13:00	**Plenary session**
	Chaired by Professor Gerasimos Lyberatos, School of Chemical Engineering, National Technical University of Athens, Greece
12:00-12:30	**Environmental Stewardship Using Evolving Concepts of Biodegradation, Synthetic Microbial Ecology and Bioengineering**
	Professor Emeritus Spiros Agathos, Laboratory of Bioengineering, Earth and Life Institute, Université Catholique de Louvain,Belgium; Laboratory of Marine Bioengineering, Qingdao Innovation & Development Base, Harbin Engineering University, China
12:30-13:00	**Combatting microplastic pollution in the marine environment**
	Professor Emeritus Nicolas Kalogerakis, Professor Emeritus of Biochemical Engineering at the Technical University of Crete
13:00-14:00	**Lunch Break**
14:00-15:40	**Parallel sessions**
Session: Process design, modeling and integration-2	
Chaired by Professor Mariano Martín, Universidad de Salamanca, Spain	
14:00-14:20	**Accelerating innovation in circular composite materials through integration of in-silico design methodologies**
	Panayiota Katsamba
14:20-14:40	**Risk management dashboard for sustainable technologies deployment across water and wastewater processes in chemical industries**

	Anna Trubetskaya, *Colm Gaskin, Ken Stockil*
14:40-15:00	**Rethinking Product and Technology Design Fundamentals: Veolia's Safe and Sustainable by Design Wheel Framework applied for Osmosis Membranes** *Ismahane Remonnay, Natalia Quisel,* Antoine Arnoux, *Daniel Dunet, Hervé Buisson, Pascal Eloy*
15:00-15:20	**Pooling problems under uncertainty: integrating global and robust optimisation algorithms** Asimina Marousi, *Vassilis M Charitopoulos*
15:20-15:40	**Hybrid Modelling Framework for Reactor Model Discovery Using Artificial Neural Networks Classifiers** Emmanuel Agunloye, *Asterios Gavriilidis, Federico Galvanin*
Session: Green and innovative chemistries and technologies-1 *Chaired by Dr. Peleka Efrosyni, Aristotle University of Thessaloniki, Greece*	
14:00-14:20	**An LCA-based evaluation of 'Green' Seaweed-based Bioplastic Production** Christos Nikoloudakis, *Theocharis Tsoutsos*
14:20-14:40	**A circular economy strategy for the management of food waste** Gerasimos Lyberatos, *Konstantina Papadopoulou, George Lytras, Christos Lytras*
14:40-15:00	**Sustainable Engineering Systems: An Accelerator Of The Safe And Sustainable By Design (SSbD) Framework** Lazaros Karaoglanoglou, *Stelios Bikos, Antonis Kokossis*
15:00-15:20	**Laccase-mediated lignin depolymerisation using flow chemistry principles** *Giuseppe Lembo, Marco Orlandi,* Heiko Lange
15:40-16:00	**Coffee Break**
16:00-17:20	**Parallel sessions**
Session: Sustainable energy & Circularity-2 *Chaired by Asst. Professor Styliani Avraamidou, Universtiy of Wisconsin-Madison, USA*	
16:00-16:20	**Dark fermentation vs. electrofermentation for biological H2 production from cheese whey** *Tatiana Zonfa,* Ilaria Laganà, *Marica Falzarano, Alessandra Polettini, Raffaella Pomi, Andreina Rossi*
16:20-16:40	**Innovative Recovery Of Grease From Urban Sewage Sludge: A Sustainable Way To Unlock New Oily Feedstock** Carlo Pastore, *Luigi di Bitonto, Vito Locaputo, Anjie Li Key, Camilla Maria Braguglia, Agata Gallipoli*
16:40-17:00	**Comprehensive Life Cycle Assessment for Circular Polyamide** Caroline Ganzer, *Ann-Joelle Minor, Liisa Rihko-Struckmann, Kai Sundmacher*
17:00-17:20	**Data-driven robust optimisation of hydrogen-led heat decarbonisation pathways to net zero** Vassilis M Charitopoulos
Session: Sustainable energy & Circularity-3 *Chaired by Asst. Professor Aurora del Carmen Munguía-López, University at Buffalo, USA*	

16:00-16:20	**Overview of the use of anaerobic digestion in swine farms and the potential for bioenergy production in Minas Gerais, Brazill** *Marc de Souza Silva*, Sibele Augusta Ferreira, *Brenno Santos Leite*
16:20-16:40	**A novel system dynamics-based framework for modeling circular economy networks – Polyethylene Terephthalate (PET) as a case study** Daniel Pert, *Ana Torres*
16:40-17:00	**Incorporating circular economy policies into product supply chains using bi-level optimization** Paola Alejandra Munoz-Briones, *Meng-Lin Tsai , Styliani Avraamidou*
17:00-17:20	**Integrating Short-Term Operations and Long-Term Planning for Resilient Urban Energy Systems: A Multi-Scale Optimization Framework** Javiera Vergara Zambrano, *Styliani Avraamidou*
17:30-18:30	**Plenary session** *Chaired by Assistant Professor Nikolaos Diangelakis, Technical University of Crete, Greece*
17:30-18:00	**Combining Molecular and Process Systems Engineering (M&PSE) to produce cost-effective liquid fuels from renewable feedstocks** W. H. Dow Professor of Chemical Engineering and Biotechnology Gregory Stephanopoulos, *Department of Chemical Engineering, Massachusetts Institute of Technology (MIT), USA*
18:00-18:30	**Machine Learning in Process Control, Safety and Operations** Distinguished Professor Panagiotis Christofides, *Chemical & Biomolecular Engineering; Electrical & Computer Engineering, University of California, Los Angeles, USA*
18:30	**End of 1st Day**

Day-2: Thursday 5 June 2025

8:30-9:00	**Login to SUSTENS HUB and Entrance to Event Rooms**
9:00-11:00	**Parallel sessions**
Session: Green and innovative chemistries and technologies-2 *Chaired by Professor Anastasios Zouboulis, Aristotle University of Thessaloniki, Greece*	
9:00-9:20	**Valorisation of residual microalgal biomass in broiler feed** Sofie Van Nerom, *Filip Van Immerseel, Johan Robbens, Evelyne Delezie*
9:20-9:40	**Harnessing Pseudomonas citronellolis 620C for Electro-Bioremediation: Insights from Transcriptional Kinetics and Metabolite Synergy in Microbial Fuel Cells** Constantina K. Varnava, *Ioannis Ieropoulos, Epameinondas Leontidis, Argyro Tsipa*
9:40-10:00	**Valorization of microalgal biomass for enhanced methane production during anaerobic digestion of corn stover residues** Anastasia Makri, *Evgenia Politou, Dimitra Matziri, Nikolaos Remmas, Spyridon Ntougias, Paraschos Melidis*
10:00-10:20	**Gas fermentation in a trickle bed reactor with focus on syngas / CO2 biomethanation and variable mass transfer modeling**

	Hariklia N. Gavala, *Sambit Dutta, Ioannis V. Skiadas*
10:20-10:40	**Pilot-scale treatment of flue gas from the cement industry by carbonic anhydrase-promoted CO2 absorption in an aqueous aminoacid amine blend: Benchmarking and techno-economic insights on a 3rd generation hybrid blend**
	Io Antonopoulou, *Álvaro Cabeza Sánche, Ulrika Rova, María López Abelairas, Paul Christakopoulos*
10:40-11:00	**Metal Coatings for Electrocatalytic Applications: towards a Safe and Sustainable by Design Approach**
	Konstantina-Roxani Chatzipanagiotou, *Foteini Petrakli, Joséphine Steck, Elias P. Koumoulos*
Session: Machine Learning	
Chaired by Associate Professor Leonidas Matsakas, Luleå University of Technology, Sweden	
9:00-9:20	**Digital Twins for Circular Economy Optimization: A Framework for Sustainable Engineering Systems**
	Shubham Gupta
9:20-9:40	**Application of Machine Learning Algorithms to Predict Composting Process Performance**
	Vassilis Lyberatos, *Gerasimos Lyberatos*
9:40-10:00	**Prospects of AI and Machine Learning for energy producers: challenges and opportunities for the Oil and Gas industry**
	Athanasios S. Stephanakis, *Dimitra Kolokotsa, Antonis Kokossis*
10:00-10:20	**Machine Learning-Based Prediction of Biomass Composition Using Derivative Thermogravimetric Data**
	Satyajit Pattanayak, *Dipankar Saha, Chanchal Loha, Kush Kumar Dewangan, Io Antonopoulou*
11:00-11:20	**Coffee Break**
11:20-12:10	**Parallel sessions**
Session: Invited Speakers-3	
Chaired by Assistant Professor Nikolaos Diangelakis, Technical University of Crete, Greece	
11:20-11:45	**Engineering of intensified CO2 capture and electrocatalytic reduction systems: From solvent selection to pilot plant testing**
	Athanasios Papadopoulos
11:45-12:10	**Opportunities of coupling hydrothermal liquefaction with wet oxidation: Significance of appropriate thermodynamic model selection in process modeling**
	Konstantinos Anastasakis
Session: Invited Speakers-4	
Chaired by Associate Professor Leonidas Matsakas, Luleå University of Technology, Sweden	
11:20-11:45	**Sustainable production of bio-based chemicals and polymers – The cases of biorefinery electrification and post-consumer bioplastics recycling**
	Apostolis Koutinas
11:45-12:10	**Building a Circular Economy Option through Wastewater Treatment and Resource Recovery Approach**

	Anastasios Zouboulis, *Effrosyni Peleka*
12:30-13:00	**Plenary session** *Chaired by Associate Professor Leonidas Matsakas, Luleå University of Technology, Sweden*
12:30-13:00	**Syngas production from gasification of primary sieved solids** **Konstantinos Tsamoutsoglou, Petros Gikas, School of Chemical and Environmental Engineering, Technical University of Crete, Chania, Greece**
13:00-14:00	**Lunch Break**
14:00-15:00	**Parallel sessions**
Session: Biotechnology-2 *Chaired by Asst. Professor Alok Kumar Patel, Luleå University of Technology, Sweden*	
14:00-14:20	**Fungal-assisted harvesting of the microalga Chlorella sorokiniana using the edible mushroom Pleurotus ostreatus** *Spyridoula Schiza, Eirini Sventzouri, Konstantinos Pispas, Ioanna Petousi, Athanasios Stasinakis, Michael Kornaros,* Michail Fountoulakis
14:20-14:40	**On the impact of plasmid size and transformation method on plasmid DNA productivity in Escherichia coli** Christina Tsiligkaki, *Charitini Nousia, Massimo Morbidelli, Alexandros Kiparissides*
14:40-15:00	**Development of a chemically defined culture medium for high-yield pDNA production in E. coli** Antonia Papadopoulou, *Christina Tsiligkaki, Massimo Morbidelli, Alexandros Kiparissides*
Session: Biotechnology-1 *Chaired by Donald B. Broughton Professor Costas Maranas, Chemical Engineering Faculty, Pennsylvania State University, USA*	
14:00-14:20	**Flux Balance Analysis with Plasmid Integration (FBApi): A novel algorithm to quantify the metabolic burden associated with plasmid replication and expression** Nikolaos Stratis, *Massimo Morbidelli, Alexandros Kipparissides*
14:20-14:40	**Co-Electron Donors Regulate the Patterns of Short and Medium Chain Carboxylic Acids Production by Mixed Culture: Competition Between Electron Donors and Acceptors** Omprakash Sarkar, *Ulrika Rova, Paul Christakopoulos, Leonidas Matsakas*
14:40-15:00	**Zoom in the biosystem to elucidate the missing mechanistic insights in the electro-bioremediation of contaminated waters** Argyro Tsipa, *Sebastia Puig, Luciana Peixoto, Catarina M. Paquete*
15:00-15:30	**Coffee Break**
15:30-16:15	**Poster Session** **Modification of Ornamental Stone Wastes with Terephthalic Acid for Use as an Additive in Drilling Fluids.** *Kelly C. C. S. R. Moreira, Cleocir J. Dalmaschio, Andreas Nascimento* **Assessment of Physicochemical Characteristics and Ecotoxicological Risks of Municipal Biosolids for Agricultural Use.** *IOANNIS GIANNAKIS, Christina Emmanouil, Athanasios Kungolos*

	Ceramic foam structure design with the valorization of fly ash cenospheres: a promising avenue for sustainable bioscaffolds. *Dimitrios Flegkas, Nikos Pagonis, Konstantinos Kountouras, Petros Samaras, Constantinos Tsanaktsidis, Vayos Karayannis* **Stochastically reconstructed 3D heterogeneous microstructures with fined-tuned transport.** Nerantzaki, Lee, Antoniou, Andreas Giotis **Optimizing Inorganic Carbon Utilization in the Autotrophic Cultivation of Microalgae: A Pathway to Enhanced Biomass Productivity and Carbon Sequestration.** *Georgia Papapanagiotou, Athanasios K, Christina Samara, Christos Chatzidoukas* **Preparation of biohybrid organic-inorganic from modified ZrO2 nanocrystals and alginate biopolymer.** *Walter Sperandio Sampaio. Cleocir José Dalmaschio, Anna Trubetskaya* **Technoeconomic and Life Cycle Assessment of ZLD Strategies Towards Sustainability and Resource Recovery.** *Fatima Mansour, Sabla Alnouri, Sabah Solim, Ali Al-Sharshani, Dhabia Almohannadi* **Waste Collection Vehicle Route Optimization: A Case Study at the Hellenic Military Academy.** *Nicholas J. Daras, Paraskevi Divari, Constantinos C. Karamatsoukis, Konstantinos G. Kolovos, Theodore Liolios, Georgia Melagraki, Christos Michalopoulos, Dionysios E. Mouzakis* **Risk Assessment of Bio-Oil Hazards in the MARINES Project** *Nicholas J. Daras, Paraskevi Divari, Constantinos C. Karamatsoukis, Konstantinos G. Kolovos, Theodore Liolios, Georgia Melagraki, Christos Michalopoulos, Dionysios E. Mouzakis* **OPTIMAI: Optimizing Manufacturing Processes through Artificial Intelligence and Virtualization.** *Nikolaos Dimitriou, Dimitrios Oikonomou, Lampros Leontaris* **On the use of Gaussian noise-based data augmentation to improve the performance of hybrid knowledge/data driven growth kinetic models for mammalian cell cultures.** *Aikaterini Sofia Leonida, Evan Claes, Tommy Heck, Alexandros Kiparissides, Jan Schrooten Antleron* **Numerical Investigation of Low Reynolds Number Flow in Double Schwarz-D TPMS Structure.** *Kasimhussen Vhora, Dominique Thévenin, Gábor Janig, Kai Sundmacher*
16:30-17:30	**Plenary session** *Chaired by Professor Gerasimos Lyberatos, School of Chemical Engineering, National Technical University of Athens, Greece*
16:30-17:00	**Using computations to analyze and reshape metabolism for bioproduction** Donald B. Broughton Professor Costas Maranas, *Chemical Engineering Faculty, Pennsylvania State University, USA*

17:00-17:30	**Low-carbon alternative fuels for the maritime industry** Professor Antonis C. Kokossis, *Professor of Process Systems Engineering at the National Technical University of Athens*
17:30-17:45	**Closing the 1st SUSTENSHUB Meeting & Awards announcement** Assistant Professor Nikolaos Diangelakis, *School of Chemical and Environmental Engineering, Technical University of Crete, Greece*
17:45	**End of 2nd Day** **End of 1st SUSTENSHUB Meeting**

Topic 1 - Process design, modeling and optimization

Combining Molecular and Process Systems Engineering (M&PSE) to produce cost-effective liquid fuels from renewable feedstocks

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Abstract
The importance of liquid fuels in transportation is well established, yet, there are presently no viable options for their cost-effective production *at scale* from renewable feedstocks. During the past 15 years we have been engineering the molecular and bioprocess system for the conversion of sugar substrates and gasses to oils and alkanes. Despite achieving near theoretical yields, production of liquid fuels from sugars in not economical, due mainly to the high substrate cost. Mixtures of gasses, on the other hand, like CO_2 and hydrogen (or CO) is more promising using a two-stage system comprising anaerobic fixation of CO_2 and conversion of the CO_2 fixation product (for example, acetate) to lipids. These, in turn, can be used as feedstock for the production of Sustainable Aviation Fuels (SAF), biodiesel and other drop in fuels needed by the shipping and tracking industries. In another application, the CO_2 fixation product is converted to alkanes. This presentation will cover both the molecular engineering of the microbes *and* the development of a process to achieve gas to liquid conversion in prototype systems. These systems are scalable, make no use of land (beyond what is needed for generating renewable electricity for hydrogen production), do not compete with food and are cost competitive based on high level cost analysis and TEA. I will present the essential features of this process in my talk; full details can be found in the 5 papers cited.

References
1. Peng Hu, *et al.*, "Integrated system for biological conversion of gaseous substrates to lipids," *Proceedings of the National Academy of Sciences*, 201516867; DOI: 10.1073/pnas.1516867113 (2016).
2. Jingyang Xu, *et al.*, "Application of metabolic controls for maximization of lipid production in oleaginous yeast," *Proceed. of the National Academy of Sciences*, 114(27): E5308-E5316; DOI: 10.1073/pnas.1703321114 (2017).
3. K.J. Qiao, *et al.*, "Rewiring metabolism to maximize lipid production in *Yarrowia lipolytica,"* *Nature Biotechnology*, 35: 173-177; DOI: 10.1038/nbt.3763 (2017).
4. J.O. Park, *et al*, "Synergistic substrate co-feeding stimulates reductive metabolism," *Nature Metabolism*, 1(6): 643–651; DOI: 10.1038/s42255-019-0077-0 (2019).
5. Li, Jingbo, *et al.*, "Synthesis of High-Titer Alka(e)Nes in *Yarrowia Lipolytica* Is Enabled by a Discovered Mechanism." *Nature Communications*, 11(1): 1-13.DOI: 10.1038/s41467-020-19995-0 (2020).
6. Selected for Editors' Highlights: www.nature.com/collections/idhhgedgigand.

Low-carbon alternative fuels for the maritime industry

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Abstract

The presentation addresses an extensive energy integrated approach with additional considerations of alternative fuels such as H2, methanol, LNG and biofuels as well as options for CCS and CCU on board. Reducing carbon dioxide emissions is crucial to meet short- and long-term climate change mitigation targets. The presentation addresses a comprehensive approach to analyze and compare the environmental impact of alternative fuels used in the shipping industry. The fuels considered include marine diesel oil, liquefied natural gas, methanol, ammonia and hydrogen. The research presented reviews the possibility of using carbon capture, the integration of the ship's energy system, the cruising speed and the origin of each fuel. The work is based on a ROPAX using a Blue Star vessel and a popular route.

An extensive energy integration approach is applied to the ship energy system that is simulated by replacing conventional fuel engines with alternative fuel engines of corresponding power to determine the energy needs of each case under corresponding conditions and then an energy integration methodology is applied to further reduce the energy requirements. The energy analysis is followed by a life cycle analysis from fuel production to combustion emissions (well-to-propeller) is performed using the ReCiPe 2016 Endpoint Hierarchist as the impact assessment method. Important findings are that with energy integration there is potential for energy savings of 10% up to 20%, that with the use of CO2 capture the rate of avoidance of emissions from the whole fuel life cycle ranges from 35% to 76% and the comparison of environmental impact indicators in different impact categories of all fuels.

While, as expected, the most environmentally friendly fuel is renewable hydrogen, the rapid reduction in overall environmental impact from the use of LNG and fuels derived from biomass processing is noteworthy. Finally, the feasibility of implementing carbon capture on board is assessed, based on the constraints of available cargo and storage space, with the use of natural gas being the most realistic, with a strong differentiation from marine diesel and methanol. Carbon capture on board combined with energy integration points to LNG as an exceptionally attractive choice, especially for long routes.

Pooling problems under uncertainty: integrating global and robust optimisation algorithms

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Keywords: Global optimisation, Robust optimisation, non-convex problems, Pooling problem

Abstract

Robust optimisation is extensively applied to identify the worst-case scenario of a problem, either to ensure constraint satisfaction under uncertainty or to serve as a substitute for scenario-based approaches, particularly when statistical data is unavailable [1]. The study of convex problem lies in the core of robust optimisation research, with the two prevailing robust optimisation methods being dual reformulation and robust cutting planes [2,3,4]. However, non-convexities often arise in chemical engineering in the design of reactors, distillation columns, heat-exchanger networks, scheduling and pooling problems among others [5,6,7,8,9,10]. Solving non-convex problems to robust optimality requires the connection of robust and global optimisation methods. The most prevailing approach to achieve this is by deriving the dual reformulation and using either directly or adaptively a global solver to retrieve a solution [9,10]. Recently, different process case studies have been studied using a local linearisation approach based on an iterative random sampling of the uncertain parameters [6]. The non-convex pooling problem under concave uncertainty is addressed in [7] following two solution paths, reformulation and cutting planes. Even though for general convex problems, the comparison of the two methods is inconclusive [11,12], for non-convex problems, it has been observed that using the dual reformulation method can further increase the problem complexity [7]. Existing software that can address non-convex robust problems depends on the use of an external global solver [13,14]. The main disadvantage on relying on a global solver with a robust cutting plane approach is that computational time is spent obtain an optimal solution that is not robustly feasible.

In this work we introduce a novel algorithm that performs a parallel global and robustness search for non-convex quadratically constrained quadratic problems (QCQP). We derive our case studies from benchmark pooling problems with uncertain inlet quality [15]. The proposed algorithm integrates spatial-Branch-and-Bound [16,17] with robust cutting plane algorithms. The main idea lies in the fact that as we search the Branch-and-Bound tree, we evaluate the robustness of the nodes entailing the best-found solutions. For our spatial-Branch-and-Bound algorithm we derive the McCormick envelopes of the bi-linear terms problem resulting in a relaxed convex problem [18]. At each node, the non-convex problem is solved via a local solver. If the acquired solution is as good as the best-found so far, an infeasibility check is performed to evaluate if the obtained solution satisfies feasibility for all uncertainty realisations. If not, then the corresponding cutting planes are added both to the non-convex and convex problems. The algorithm proceeds to the next step once no more violations are detected. The convex problem is solved next, and the solution of this problem is used to decide the most promising variable for branching into two child nodes. With the use of appropriate fathoming criteria, the tree nodes are exhausted, and the robust optimal solution is obtained. The algorithm was tested for various benchmark problems and different types of uncertainty sets showing promising results compared to the-state-of-the-art.

Acknowledgements

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Industrial Urban Symbiosis Modelling for Closing the Water Loop

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Keywords: wastewater treatment; water reuse; industry; simulation; closed loop

Abstract

Population growth, urbanisation and industrialisation intensify the issue of freshwater availability. Freshwater reserves are decreasing and the adoption of the zero liquid discharge concept is now urgent more than ever. The industrial sector accounts for 40% of the total abstracted water in Europe, making the implementation of innovative and efficient technologies and solutions as well as alternative water sources, such as treated wastewater, imperative. Resource-efficient and waste reuse practices for closing the loop in the industrial sector gain attention. The Solvay chemical plant, in Italy, is a water-intensive process industry that exchanges water and treated wastewater within the cross-sectorial symbiotic network among the plant, municipality and a water utility company that has a wastewater reclamation plant. A pilot-scale treatment train (neutralisation, advanced oxidation, membrane bioreactor, granular activated carbon filtration) was deployed in the Solvay chemical plant to treat 10 m3/h of wastewater, which is then sent to the municipality or the water utility depending on the effluent quality. The interrelations among the members of the cross-sectorial symbiotic network are simulated using a non-commercial Process Simulation Modelling and Life Cycle Assessment tool, considering technological, environmental and economic factors. Overall, three closed-loop scenarios were formulated: (1) conventional treatment and discharge to sea; (2) conventional treatment, pilot-scale treatment and discharge to sea; (3) conventional treatment, pilot-scale treatment and direct industrial water reuse within the cross-sectorial symbiotic network. However, there are financial and technological constraints. The water utility sends a maximum of 3.8 million m3/y to the Solvay plant, which pays 1.40 €/m3 and 10.00 €/m3 for secondary and tertiary treatment, respectively. The cost for discharge is zero, on the basis of having treated the industrial wastewater to reach the legislative regulations. Moreover, there are technological challenges since specific water reuse requirements have to be reached through wastewater treatment. The results of this study showed that scenario 1 had the lowest pollutants' removal efficiency and an environmental footprint of 0.93 mPt/m3. Scenario 2 had a higher removal efficiency of pollutants, 91.7% water recovery, 9.5% sludge production and an environmental footprint of 1.12 mPt/m3. Scenario 3 is the best option with zero wastewater discharge and an environmental footprint of 0.72 mPt/m3. The total cost was calculated to be 77 €/h for scenario 1 and 2, while around 84 €/h for scenario 3. However, only scenario 3 that includes the cross-sectorial symbiotic network promoted the circularity and sustainability, allowing the safe water reuse for industrial purposes. In conclusion, the results of this study highlight the importance of cross-sectorial symbiotic networks among industrial and non-industrial actors that are capable of enhancing water circularity, reducing waste generation and environmental footprint.

Accelerating innovation in circular composite materials through integration of in-silico design methodologies

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Keywords: Circular materials, composites, waste valorisation, in-silico design, multi-scale modelling, homogenization

Abstract

Developing the next generation of circular materials requires a deep understanding of their mechanical properties. In this work, we introduce a computational framework for the in-silico design and optimization of AgReCOMPOSITES—sustainable, circular materials made from recycled plastic and biochar sourced from agricultural and livestock waste. Our framework integrates hierarchical homogenization and Finite Element Methods with experimental data to predict the mechanical behavior of biochar-polymer composites, facilitating the optimization of mixing ratios and geometrical configurations for enhanced performance. We highlight the opportunities and challenges of integrating multi-scale modelling, atomistic simulations, numerical homogenization and Uncertainty Quantification in advancing the design of sustainable, circular materials.

A systems engineering approach for novel and sustainable value chains in biopharmaceuticals

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Keywords: modelling, supply chains, biopharmaceuticals

Abstract

Pharmaceutical process and product development rely primarily on time- and cost- intensive experimentation. In recent years, computer-modelling tools have been gaining increasing interest as means to inform, accelerate, and optimise the industrial workflow. In this talk, we will discuss how such tools can enable adaptive process design, sustainable operation and optimal process performance, harnessing the power and economical sustainability of computer-based experiments. We will focus on how model-based tools can: (1) accelerate and inform decisions related to material and process conditions and (2) support decision-making during process scale up to ensure continuous, global supply. Starting from process development, we will present a model-based framework for bioprocess design and optimisation that, beyond the traditional Key Performance Indicators (KPIs), features sustainability metrics. The presented cases studies include biopharmaceutical separation processes, including informed selection of process conditions, as well as a workflow and model-based tools for quantitative comparison of different design options, such as the type of resin.

To complement process development, we will demonstrate a model-based framework that can guide decision-making during scale up. We will showcase how computer-modelling tools can be used and embedded in industrial practices to support manufacturers across the product lifecycle, from clinical trials to commercialisation. In that respect, we will discuss how process uncertainties can be identified quantified and we will illustrate case studies where we evaluate different equipment and scale options with respect to productivity, economic feasibility and environmental sustainability.

Systematic Optimal integrated plants for sustainable chemicals production: Multiscale approach for waste valorization

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Keywords: Circular economy, integrated processes, biowaste valorization, LCA, multiscale approach

Abstract

The sustainable development goals pose a number of challenges to traditional industry requiring a complete transformation of the chemical and consumer goods industry. Chemicals traditionally produced from crude fractions must find substitutes or alternative raw materials and production routes that are renewable and more sustainable as well as avoid intermediates or secondary raw materials coming from fossil resources. Integrated biorefineries that make full use of biowaste and CO2 can be part of the solution to produce the intermediates, the final product as well as interesting byproducts, including biofuels [1]

This work presents the methodology for the integrated production of chemicals from waste by designing integrated biorefineries and its application to obtain sustainable counterparts. A superstructure is formulated, based on models that capture the performance of each transformation. The models are based on first principles but especially surrogate models from experimental data or detailed kinetics [1]. The optimization of the superstructure does not only provide the transformation stages and operating conditions, but also the key economic performance indicators that would allow LCA analysis and a detailed scale up study to evaluate the extension of waste valorization and the biomass design for the proper facility operation. These chemicals such as biopolymers, biosurfactants (APG) or food additives can become the ingredients for performance products, i.e. plastics, food, cleaning products, that will provide reduced environmental impact [2].

The production of APG's uses CO2 and manure to grow algae and produce biogas. Glucose and lipids are obtained from algae and hydrogen from biogas. Next, alcohols are produced via lipids hydrogenation to synthesize the APG's from them and glucose. The production of biopolymer consists of six sections including biogas synthesis from manure wastes, syngas reforming and clean-up, methanol synthesis, algae growing to produce oil and starch, biodiesel synthesis and biopolymer production from the by-product glycerol, sawdust and the algae starch. The production of food additives from jam waste is performed in an integrated process designed to extract phenolic compounds and pectin, producing ethanol, a green solvent, for internal use and/or as a final product. Solid waste can be gasified (GA) or digested (AD) to produce biogas (mainly methane) or syngas (mainly H2 and CO), thermal energy and electricity. These processes are scaled-up developing surrogate models for the investment and production costs to formulate a facility location problem that would allow evaluating the use of waste at regional, national or continental scale to substitute the fossil-based chemicals. For instance, it is possible to substitute up to 51 % of PE with biopolymers from sludge and sawdust in Spain or reduce by 35% the needs for fossil fuels using manure and lignocellulosic residues.

References

1. Roldán-San Antonio JE, Martín-Hernández E, Briones R, Martín M. Sustain Prod Consum. 2021;27:462-470.
2. Taifouris, M., Martín M, Martinez, A., Esquejo, N. (2021). Comp. Chem. Eng. 152, 107384

Bioprocess systems engineering approaches to improve rAAV production for gene therapy applications

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Keywords: Gene therapy, rAAV, Bioprocess optimization, Mathematical modelling, Design space

Abstract

Gene therapies, classified as advanced therapy medicinal products (ATMP), have the potential to revolutionize healthcare by treating genetic diseases through the delivery of a therapeutic gene using viral vectors [1]. Recombinant adeno-associated viruses (rAAV) are the leading platform for the gene delivery [2]. However, current rAAV manufacturing capacity cannot keep up with rapidly growing demand driven by newly approved therapies, highlighting an urgent need for novel and/or more efficient methods to produce viral vectors [1]. Model based approaches enable use of established process systems engineering (PSE) methodologies that can improve process yields at a fraction of the cost compared to purely experimental approaches. The use of mathematical modelling is gaining traction within the scope of Industry 4.0 and the development of Digital Twins as part of the Quality by Design (QbD) framework. PSE approaches have been successfully applied in various bioprocesses, including optimization of mAb production via mammalian cell cultures [3] and porcine growth hormone (pGH) production via E. coli fermentation [4]. Similarly, these tools can play a crucial role in rAAV production by providing a robust framework for understanding and predicting bioprocess dynamics, optimize process conditions and enhancing quality control [5]. The current rAAV production is carried out through transient transfection of human embryonic kidney cells (HEK293) or recombinant baculovirus infection of insect cells from Sf9/Sf21 lines [1]. Due to the different method for the upstream production and the various serotypes employed in the approved therapies [1], downstream purification results in multiple distinct configurations [6]. A model-based approach supports the integration of novel technologies and evaluates the feasibility and productivity of different processes. Herein, we present the development of detailed mechanistic models for each unit operation in a typical rAAV manufacturing process. Developed models are validated through a combination of literature derived data and experimental datasets obtained from partners in the EU consortium GET-IN. Finally, individual unit operation models are integrated into an end-to-end whole bioprocess model implemented in the gPROMS Formulated Products environment. The whole-bioprocess model is used to study the propagation of uncertainty throughout the entire process, define a robust process operating window and identify a multivariable design space within which critical quality attributes (CQAs) are satisfied while ensuring economic robustness. We employed sensitivity analysis to identify critical process parameters (CPPs) that can resolve process bottlenecks and unlock substantial yield improvements. Lastly, we conducted a dynamic optimization to maximize the viral titre. The aim is twofold: (a) to provide a digital tool for bioprocess optimisation and process intensification and (b) to provide a digital decisional tool to assess the viability of novel technologies and/or novel process configurations. Our framework demonstrates the critical role of advanced design tools enabled by mechanistic modelling, to support intensification and optimization of rAAV manufacturing processes.

References

1. Destro, F., Wu, W., Srinivasan, P., Joseph, J., Bal, V., Neufeld, C., Wolfrum, J. M., Manalis, S. R., Sinskey, A. J., Springs, S. L., Barone, P. W., & Braatz, R. D. (2024). The state of technological advancement to address challenges in the manufacture of rAAV gene therapies. Biotechnology Advances, 76, 108433. https://doi.org/10.1016/j.biotechadv.2024.108433
2. Wang, D., Tai, P. W. L., & Gao, G.-P. (2019). Adeno-associated virus vector as a platform for gene therapy delivery. Nature Reviews Drug Discovery, 18(5), 358–378. https://doi.org/10.1038/s41573-019-0012-9

3. Kozorog, M., Caserman, S., Grom, M., Vicente, F. A., Pohar, A., & Likozar, B. (2023). Model-based process optimization for mAb chromatography. Separation and Purification Technology, 305, 122528. https://doi.org/10.1016/j.seppur.2022.122528
4. Kavanagh, J. M., & Barton, G. W. (2008). Productivity improvement of recombinant Escherichia coli fermentation via robust optimization. Bioprocess and Biosystems Engineering, 31(1), 27–35. https://doi.org/10.1007/s00449-007-0156-6
5. Mu'azzam, K., da Silva, F. V. S., Murtagh, J., & Sousa Gallagher, M. J. (2024). A roadmap for model-based bioprocess development. Biotechnology Advances, 73, 108378. https://doi.org/10.1016/j.biotechadv.2024.108378
6. Qu, W., Wang, M., Wu, Y., & Xu, R. (2015). Scalable downstream strategies for purification of recombinant adeno-associated virus vectors in light of the properties. Current Pharmaceutical Biotechnology, 16(8), 684–695. http://dx.doi.org/10.2174/1389201016666150505122228

A Data-driven Approach for Integrated Design and Dynamic Optimization of Renewable Electrodialysis Systems

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Keywords: Electrodialysis, dynamic optimization, process design

Abstract

Electrodialysis (ED) is a suitable technology for the electrochemical removal and/or recovery of ions from dilute streams such as industrial effluents, aquifers, etc. Such streams contain metal cations, sulfur or nitric oxides etc. ED has low capital and maintenance costs, avoids sludge production and enables the use of renewable electricity as it can be connected with photovoltaics (PV), representing an excellent option for both large and small scale applications (e.g. in remote areas). Renewable ED systems are challenged by the fluctuation of renewable energy and the uncertainty of product demand. Meeting the specifications of the ED outlet stream is important, especially in drinking water production where efficient removal of species such as nitrate ions is required due to their harmful health effects. Existing works on optimal ED design and operation mainly propose frameworks where equipment and operational characteristics are designed under nominal settings, while addressing the intermittency of renewable energy generation through batteries (BAT) and/or water tanks. This approach may result in over- or under-designed systems in view of endogenous or exogenous variability and demand uncertainty. There are very few papers that propose dynamic optimization and control as a means of overcoming these challenges. However, they either implement dynamic optimization for a system with fixed equipment sizes or do not address demand uncertainty. Integrated design and dynamic optimization of renewable ED systems with energy storage under demand uncertainty has many advantages as it allows evaluation of all system designs while adjusting system operation to internal or external fluctuations. The lack of such approaches is partly due to the computational challenges arising from the underlying first-principles ED models.

To address the above challenges, we propose for the first time a data-driven approach for the integrated design and dynamic optimization of renewable ED systems. An Artificial Neural Network (ANN) is used as a promising alternative to first-principle ED models, particularly because solutions may be obtained rapidly and accurately given extensive design variable ranges in both equipment capacity and conditions in the temporal dimension. The optimization goal is to design a cost-effective system that treats variable volumes of feed to meet the necessary demand while producing potable water, requiring a minimum of energy from the grid. A first-principles ED model is developed and validated using experimental data. It is then used to train and validate the ANN, also optimizing the number of ANN hidden layers and neurons. The ANN-based ED model is complemented by PV-BAT models and used in Simulated Annealing that handles both system design and optimization of dynamic operation. The system design variables include the PV and BAT numbers. Operating conditions, implemented at intervals of a few minutes within hourly ED batches, include ED stack voltage, flow rate, and feed water volume. Preliminary results indicate improved operating costs compared to an approach where design and operational optimization is performed for values of operating conditions that are fixed for each batch.

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Rethinking Product and Technology Design Fundamentals: Veolia's Safe and Sustainable by Design Wheel Framework applied for Osmosis Membranes

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Keywords: Safe and Sustainable by Design, Osmosis Membranes, eco-design

Abstract

Safe and Sustainable by Design (SSbD) is an innovative approach guiding the design or redesign of the chemicals and materials but also the equipments and technologies. It aims to deliver optimal functionality and performance while minimizing adverse impacts on safety, human health, and the environment. The concept integrates safety, circularity, and functionality aspects of chemicals and materials, emphasizing sustainability throughout their lifecycle to reduce environmental impact and the concept of Right Chemistry.

Veolia has developed the SSbD indicator wheel, a comprehensive framework incorporating specific selection criteria and implementation mechanisms. This wheel is structured around three core criteria: Sustainability (encompassing durability, degradability, environmental footprint, and circularity potential), Market Requirements (including product compliance, performance, transparency, and brand reputation), and Safety (comprising risk assessment, SHE profile, and user protection). Each criterion includes multiple specific indicators for performance evaluation, ensuring a holistic approach to product development.

This study applies the Veolia SSbD wheel framework to a case study on Osmosis membranes, conducted by Chimie ParisTech students under the Design Centre of Veolia Water Technologies' and the Veolia R&D Department supervision. The strength of this approach lies in bridging intergenerational expertise, where future chemists collaborate with Veolia's experienced professionals to foster science-based innovation and unleash creative solutions through their combined knowledge and perspectives.

The 2025 study will address key challenges in membrane technology, including:

– Refining the SSbD Wheel by aligning use, safety, and sustainability criteria
– Developing materials for improved rejection rates, energy efficiency, and durability
– Exploring emerging technologies such as bio-inspired materials
– Membranes/modules end-of-life (management) strategies

The findings will contribute to Veolia Water Technologies' eco-design initiatives, particularly for their TERION equipment - an advanced water treatment solution combining reverse osmosis and continuous electrodeionization for high-quality demineralized water production. As part of the EC marking of TERION equipment under the Machinery Directive (2006/42/EC), Veolia R&D Department conducted an eco-design study and life cycle analysis (development, production, treatment, recycling, and use) in 2020 to identify opportunities for reducing environmental impacts while maintaining technical performance.

This life cycle analysis-based approach will identify opportunities for equipment design improvements, with membrane material optimization as a key focus in implementing SSbD principles in practical water treatment applications. These exploratory and collaborative approaches could serve as key research directions:

– Serve as a comprehensive benchmark for evaluating both current and future product development and technological innovations - extending beyond materials and chemicals - to drive the industrial transformation essential for ecological transition.
– Redefine the fundamental meaning of "Design" to inherently encompass safety and sustainability principles, making the specific term 'Safe and Sustainable by Design' (SSbD) redundant, as these qualities become fundamental to all design processes.

Risk management dashboard for sustainable technologies deployment across water and wastewater processes in chemical industries

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Keywords: wastewater, technology, risk, sustainability, chemical industry, dashboard

Abstract

The increasing regulatory pressures and environmental concerns have necessitated the development of advanced risk management models for water and wastewater technology. The literature lacks comprehensive risk models related to water, possibly because stakeholders perceive water as having less economic value compared to energy and other material costs. This research aims to transform chemical, paper and pulp, and metallurgical industries into sustainable and efficient operations, by integrating advanced water treatment technologies and predicting associated risks. The primary objective is to achieve climate neutrality, sustainability, and competitiveness by 2050, aligning with the EU's key objectives, mainly with respect to water and wastewater life cycle.

The proposed micro-level risk model focuses on identifying and assessing risks associated with the deployment of sustainable water processes at industrial sites in Europe. This model incorporates insights from various technological and environmental risk factors to provide a comprehensive framework for risk management. Key components of the risk model include the integration of smart monitoring technologies, such as affordable and reliable sensors combined with the maturity risk dashboard tool. The monitoring technologies enable real-time data collection and analysis on-site, enhancing the accuracy and efficiency of risk assessments. The micro-level risk dashboard incorporates an intelligent decision support toolkit, which provides a digitally integrated framework for identifying and prioritizing critical risks with the potential to be linked to macro-level risk model. This dashboard tool addresses local catchment and supply chain risks, including environmental regulations, operational parameters, and internal water costs. The biochemical and operational parameters from several industrial sites will be collected and assessed as a part of case studies. The consideration of these parameters within the model will ensure a holistic approach to risk management, promoting the adoption of best practices and more effective mitigation measures on industrial sites. Through prioritizing and weighting risk parameters within integrated assessment tools, the micro-level risk dashboard ensures a robust and reliable framework for risk management.

This micro-level risk dashboard for water and wastewater technology offers a comprehensive and innovative approach to risk management. The dashboard tool facilitates the identification and assessment of critical risks by integrating a maturity risk evaluation framework, promoting the successful deployment of sustainable water processes in European chemical, paper and pulp, and metallurgical industries. Ultimately, this empowers stakeholders to make informed decisions, ensuring the resilience and efficiency of their operations, while offering an opportunity for continuous improvement over the long term.

Stochastically reconstructed 3D heterogeneous microstructures with fined-tuned transport and mixing properties

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Abstract
We develop an integrated methodology for the design of 3D heterogeneous microstructures with fine-tuned transport and mixing properties that can be used as micromixers and catalytic matrices (following appropriate surface coating) in chemical engineering processes. The designed digital domains, while stochastic at the microscale, bear enhanced accurately controlled macroscale transport properties, such permeabilities, hydrodynamic dispersivites and fined-tuned specific interfaces. The designs rely on a stochastic reconstruction algorithm that generates a 3D binary matrix to represent a porous solid using spatial correlation models such as Gaussian or Exponential. A random field is initialized with uniform values and transformed into the frequency domain via a 3D Fast Fourier Transform (FFT). A spectral filter—derived from the Fourier transform of a chosen covariance function—is applied to impose spatial correlation. The decay rate of the covariance function (e.g., Gaussian or Exponential) is governed by the correlation length λ, which influences the continuity of solid structures. Larger λ values lead to smoother, more connected regions; smaller values yield finer, noisier textures. The filtered field is inverse FFT-transformed to real space to obtain spatially correlated values. A threshold based on the target porosity is applied to classify voxels as solid (1) or void (0).
We then employ state-of-the-art 3D printing approaches, based on material jetting and photopolymerization technologies, to fabricate, as a case study, scaled-up replicas of natural sandstones, that are suitable for the study of the scaling between the permeability, the porosity and the mean pore size. The REV- and pore-scale characteristics of the resulting physical micromodels are recovered using a combination of X-ray micro-CT and microfluidic studies. The experimental results are then compared with single-phase flow simulations at pore-scale order to determine the effects of the design parameters on the intrinsic permeability and the spatial correlation of the velocity profile. Our numerical and experimental measurements reveal an excellent match between the properties of the designed and fabricated 3D domains, thus demonstrating the robustness of the proposed methodology for the construction of 3D micromodels with fine-tuned and well-controlled pore-scale characteristics.

Topic 2 - Sustainable energy & Circularity

Technoeconomic and Life Cycle Assessment of ZLD Strategies Towards Sustainability and Resource Recovery

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Keywords: Technoeconomic Assessment, Life Cycle Assessment (LCA), Zero Liquid Discharge (ZLD), Sustainability, Resource Recovery, Environmental Impact Analysis

Abstract
This study conducts an in-depth technoeconomic assessment (TEA) of four different wastewater handling strategies: (1) No Zero Liquid Discharge (No ZLD), (2) Minimal Liquid Discharge (MLD), (3) Near Zero Liquid Discharge (NZLD), and (4) Circular Zero Liquid Discharge (CZLD). The ultimate goal is to identify the most cost-effective and sustainable solutions for industrial wastewater treatment. The analysis explores the trade-offs between operational costs and the potential for resource recovery, focusing on economic viability without compromising environmental goals. While No ZLD and MLD strategies are associated with lower initial costs, they may offer limited resource recovery compared to the more advanced NZLD and CZLD approaches. NZLD and CZLD, though typically higher in cost, have the potential to provide enhanced resource recovery and significant environmental benefits, such as reduced wastewater discharge and a smaller environmental footprint. In order to provide a comprehensive evaluation, a Life Cycle Assessment (LCA) is integrated into the analysis, allowing for a thorough assessment of key environmental indicators, including energy consumption, emissions, and waste generation throughout the entire lifecycle of each strategy. This combined TEA-LCA approach ensures that economic factors are considered alongside sustainability objectives, providing a holistic view of the environmental impact of each strategy. As such, this study offers a robust framework for industries to make informed decisions that prioritize both cost efficiency and long-term sustainability in wastewater management. Moreover, the results are intended to guide industries toward selecting the most efficient and environmentally responsible wastewater treatment strategies, ultimately contributing to the development of more sustainable industrial practices.

Incorporating circular economy policies into product supply chains using bi-level optimization

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Keywords: bi-level optimization, packaging selection, circular economy, circular supply chain, multiple stakeholders

Abstract

Product supply chains are managed by different companies and governmental bodies, which often have competing objectives, making it challenging to effectively navigate economic and environmental interests. Each stakeholder can affect the actions and outcomes of the other stakeholders; for example, a new policy can change the operating behavior and profits of companies within a supply chain. These interconnected stakeholders and their conflicting objectives introduce challenges in the modeling of supply chain operation and decision-making, often requiring game-theoretic approaches to identify optimal decisions for all stakeholders. This study introduces a bi-level optimization model to represent these hierarchical interactions between governmental decision-making (upper level) and industry decision-making (lower level), using a case study on food packaging selection and circular supply chain in the coffee industry.

While food packaging plays a crucial role in facilitating food access and preserving quality of products, the rising volume of packaging waste underscores the need for circular packaging solutions and a sustainable waste management infrastructure. The case study considered here encompasses multiple coffee packaging designs, their production, usage, and multiple pathways for their management at the end of their life. To promote the adoption of sustainable alternative technologies, new policies are often required. This study aims to identify the optimal policy strategies (taxes and/or financial incentives) to encourage companies to adopt sustainable packaging and waste management technologies. The economic impact is evaluated by the cost increase for companies to cover packaging production and waste management costs, while the environmental impact is assessed based on emissions and circularity. The circularity metric considered in this study extends beyond carbon emissions to quantify dimensions including waste generation, natural resource use, and product substitutability.

The bilevel optimization problem formulation includes an upper-level objective function for the governmental body's interest, focusing on maximizing sustainability metrics, including maximizing circularity and minimizing greenhouse gas emissions. The lower-level objective function represents the company's interests, which is to minimize the increase in cost of the packaging. The upper-level problem includes two decision variables: the tax rate on greenhouse gas emissions, and financial incentives provided to companies for selecting circular alternatives. The upper-level problem is constrained by a governmental budget, ensuring that total incentives do not exceed the available budget. The lower-level problem is constrained by companies' technological and operational constraints regarding each packaging production and waste management technologies. The interaction captures the trade-offs between incentivizing circularity, lowering emissions, and maintaining economic feasibility for companies while adhering to government budgetary limits. Two policy scenarios are analyzed: (1) implementing taxes and incentives separately, and (2) combining carbon taxes with incentives to reduce investment costs while penalizing emissions. A sensitivity analysis further examines how varying government budgets affect industrial operations and sustainability outcomes.

Bioprospecting of Oleaginous Microalgal Strains for High Biomass and Lipid Yields under Outdoor Cultivation as a Sustainable Feedstock for Biodiesel Production

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Keywords: Microalgae, Outdoor conditions,2-stage autotrophic cultivation, Biomass composition, Sunlight

Abstract

Microalgae represent a highly advantageous biomass feedstock due to their capacity to harness solar energy through photosynthesis for growth. Among them, several species are classified asoleaginous, exhibiting lipid contents exceeding 20% wt. of their dry weight, which can be further enhanced under stress conditions. This study aims to identify the most suitable strain from the Scenedesmaceae family as feedstock for biodiesel production, by evaluating the biomass productivity and lipid accumulation of four strains under outdoor cultivation conditions.

The microalgal strains investigated included Scenedesmus quadricauda CCAP 276/16, Scenedesmus sp. CCAP 276/66, Tetradesmus obliquus CCAP 276/10, and Tetradesmus obliquus CCAP 276/3A. Experimental cultivations of all strains were conducted simultaneously under outdoor conditions in Thessaloniki, Greece, during Fall 2024. A two-stage cultivation strategy was applied over a 24-day period. The first 16 days were dedicated to biomass accumulation under nitrogen-replete conditions in Bold Basal Medium (BBM).. Subsequently, the cultures were harvested, resuspended in fresh nitrogen-depleted BBM, and cultivated for an additional 8 days to induce lipid overaccumulation. Cultivation was performed in 1 L Duran bottles with working volumes of 500 mL and 400 mL during the first and second stage, respectively. Continuous aeration at 10 L/min was maintained to ensure sufficient culture agitation. Solar intensity and outdoor temperature were continuously monitored and logged, with all experiments conducted in triplicate.

At the end of the first stage, the strain CCAP 276/10 achieved the highest biomass production (3 g/L), followed by CCAP 276/16 (2.3 g/L), while strains CCAP 276/66 and CCAP 276/3A yielded only 1.9 and 1.6 g/L. During the second stage, all strains exhibited a reduced growth rate, , due to nitrogen starvation, with biomass increasing by approximately 250 mg/L. Across this phase, all strains demonstrated a consistent macromolecular composition pattern with, decreasing protein and carbohydrate content and increasing lipid accumulation. At the end of the second stage, lipid content amounted between 25 to 29% wt. for all strains, while protein and carbohydrate contents were between 35 to 45% wt. and 28 to 35% wt., respectively.

All strains successfully grew under real outdoor conditions. Solar intensity reached a peak average of 750 W/m^2 (~1500 μmol photons/$m^2 \cdot s$), with a daily average of 400 W/m^2 and a daylight duration of approximately 10.5 hours. Temperature fluctuated between a maximum of 26.6°C and a minimum of 13.1°C, with an overall average of 19°C. The aftermath of the experiment analysis revealed that Tetradesmus obliquus CCAP 276/10 achieved the highest biomass and lipid accumulation across both cultivation stages, without exhibiting any adverse effects from weather conditions or solar irradiance. Therefore, CCAP 276/10 emerges as a promising candidate for further studies under outdoor conditions and potential scale-up to meet industrial and biorefinery applications.

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Data-driven robust optimisation of hydrogen-led heat decarbonisation pathways to net zero

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Keywords: net-zero, hydrogen-led decarbonization, robust optimization, energy security

Abstract

Given the increasing number of countries committing to a "Net-zero" emissions target by 2050, hydrogen as a low-carbon alternative of natural gas will become a significant player in advancing sustainable decarbonisation pathways. There is a pressing necessity to develop a new hydrogen infrastructure network in the UK and the EU to satisfy the increasing hydrogen demand to meet the ambitious target. Even though the hydrogen infrastructure planning problems on a nationwide scale have been widely explored in the literature[1], they ignore the demand uncertainty inherent to underlying problem, which could bring significant economic loss and even jeopardise the system security. Hence, the uncertainty-resilient schemes are required to alleviate these disadvantages. The common two ways to hedge against the uncertainty in the studies are stochastic programming (SP) and robust optimization (RO) techniques[2]. However, often it can be challenging to get the probability distribution of uncertainties required in SP. On top of that, even if the stochastic process governing the uncertainty is fully or partially recoverable, the number of scenarios needed for its accurate representation tend to computationally intractable problems even for systems of moderate size. Thus, robust optimisation as an effective alternative offers a practical trade-off between feasibility and computational tractability.

In this work, we focus on the spatially-explicit hydrogen infrastructure planning problem with 5-year steps 2035-2050 and hourly resolution to elucidate the trade-off between operational and strategic decisions. This kind of complex energy-planning model typically involves representative days to alleviate the computational complexity considering their multi-scale nature. The issue of systematically accounting for the uncertainty introduced through the deployment of representative days within the planning models remains largely unexplored. To this end, we employ a data-driven adaptive robust mixed-integer linear programming optimization framework, where the demand uncertainty is captured through the introduction of uncertain representative days[3] and polyhedral uncertainty sets. In the two-stage adaptive robust optimization (ARO, min-max-min problem), decisions are made on the "wait and see" basis, where the operational decisions like the hydrogen transmission flowrates across regions can be adjusted after the uncertainty realizations. This problem is NP-hard and cannot not be solved directly using off-the-shelf solvers. Therefore, we propose a new hybrid decomposition algorithm based on the column and constraint generation algorithm and block coordinate descent methods to handle it, which avoids the introduction of big-M linearizations, and can achieve a higher computing efficiency. Numerical results illustrate the effectiveness of the proposed framework and method with reductions in computational time exceeding 65% compared to monolithic approaches that are largely employed in the literature. Using as case study the decarbonisation of the heat sector in Great Britain, we further compare the two-stage ARO with the single-level static RO where decisions are made "here and now" without uncertainty feedback. The results show that ARO can lead to a lower system cost, and verify the advantages on controlling conservatism of ARO whilst allowing us to elucidate the added value of different flexibility options.

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Optimizing Inorganic Carbon Utilization in the Autotrophic Cultivation of Microalgae: A Pathway to Enhanced Biomass Productivity and Carbon Sequestration

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Keywords: Microalgae cultivation, CO_2 sequestration, bicarbonate supplementation, biomass productivity, photobioreactors

Abstract

Autotrophic microalgae cultivation embodies a promising biological system for CO_2 sequestration, effectively coupling carbon capture with sustainable biomass production. However, CO_2 conversion in microalgal cultures remains inefficient, with a significant portion of the supplied inorganic carbon being released into the environment rather than assimilated by the cells. This study investigates the effects of diverse inorganic carbon supplementation strategies on the growth and carbon capture performance of Chlorella sorokiniana, including scalable approaches suitable for large-scale open pond cultivation systems. A total of four 8-day cultivation trials were conducted. Three trials employed isocarbonic conditions using $NaHCO_3$, CO_2, or a combination of both as inorganic carbon sources, while one control trial relied solely on atmospheric CO_2. All trials were performed in a 5L stirred-tank photobioreactor (F1, Bionet, Spain), containing 3L of Bold Basal Medium inoculated with a fresh cell population of 100 mg L^{-1} (dry cell weight-DCW). The cultures were exposed to artificial illumination of 250 μmol m^{-2} s^{-1} intensity, following a16:8 h light-dark photoperiod, with continuous agitation at 300 rpm, aeration at 0.8 L min^{-1}, and a constant temperature of 25°C. Biomass production and sodium nitrate concentration were monitored daily, with nitrogen supplementation provided as necessary to maintain sufficient availability. Additionally, exhaust gas composition (oxygen and CO_2) was continuously measured and logged to evaluate carbon assimilation efficiency.

The cultivation trials performed were:

T1. Continuous $NaHCO_3$ supplementation during the daily photosynthetic period at a rate of 13.4 mg C L-1 h-1, with continuous pH regulation to neutrality.

T2. Simultaneous $NaHCO_3$ and CO_2 supplementation (each at 6.7 mg C L^{-1} h^{-1}) during the photosynthetic period, with continuous pH regulation to neutrality.

T3. Continuous CO_2 supply during the photoperiod at a rate of 13.4 mg C L-1 h-1 with continuous pH regulation to neutrality.

T4. Control trial, relying solely on atmospheric air, with continuous pH regulation to neutrality.

Among the trials, T3 exhibited the highest biomass production, achieving 1.89 g L^{-1}, closely followed by bicarbonate-based strategies T2 and T1, which reached final biomass concentrations of 1.66 and 1.64 g L^{-1}, respectively. The control trial (T4), relying solely on atmospheric CO_2, attained a significantly lower biomass of 0.62 g L^{-1}. Gaseous CO_2 supplementation (T3) demonstrated superior performance regarding total biomass accumulation. However, bicarbonate-based strategies (T1 and T2) also showed considerable productivity, underscoring their potential as scalable and efficient alternatives, particularly in open pond systems where minimized CO_2 degassing losses are critical. Additionally, lipid accumulation was notably highest in T1 and progressively decreased in the other trials. These findings highlight the potential for optimizing bicarbonate supplementation strategies to significantly enhance microalgal biomass productivity, lipid accumulation, and carbon capture efficiency in large-scale open pond cultivation systems.

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Comprehensive Life Cycle Assessment for Circular Polyamide

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Keywords: circular economy, life cycle assessment, recycling, carbon capture and utilization

Abstract

Conventional polymer production and disposal contribute to climate change and other environmental burdens. Circular economy aims at transforming the existing routes by replacing raw materials with residual or waste materials, and closing the cycle of disposal and production. Several options exist to supply polymers to the economy sustainably. They include mechanical recycling, chemical recycling, bio-based synthesis, and derivation from captured carbon. Combinations of synthesis, recycling, and end-of-life options differ in cost, carbon and water footprint, land use, as well as overall sustainability.

In this work, we conduct life cycle assessment (LCA) for polyamide 6 (nylon 6) synthesis, recycling, disposal, and combinations thereof. The use phase is excluded, as it is identical for all routes. We include as primary production the synthesis from fossil benzene (Herps, 2020), two bio-based pathways via γ-valerolactone (Han, 2017) and 1,6-hexanediol (Thaore et al., 2018), and CO2-based synthesis via direct air capture (DAC), methanol synthesis, and methanol-to-aromatics. Recycling options are mechanical recycling, chemical recycling back to caprolactam by hydrolysis using phosphoric acid (Minor et al., 2023), as well as recycling via carbon capture and utilization (CCU). Incineration with and without carbon capture and sequestration (CCS) (Tang & You, 2018), and landfill are considered as end-of-life treatment for the amount of PA-6 which is not recycled. We gather LCAs and techno-economic assessments (TEAs) from literature for the individual processes, and perform LCA using ECOINVENT 3.10 in Brightway2-ActivityBrowser. We apply the concept of the planetary boundaries (Sala et al., 2020), analyzing which pathways transgress the safe operating space for PA-6.

We calculate the carbon intensity and other LCA indicators including resource depletion, ecotoxicity, and eutrophication for combinations of primary production, recycling, and disposal. We estimate which mitigation strategies can move impacts below the planetary boundaries, and quantify burden-shifting between LCA categories. Further, we vary the recycling quota to evaluate how the impacts may evolve over time if ambitions for circularity in plastics are realized, and estimate the lowest possible environmental impact PA utilization could have. Our results suggest a high mitigation potential for bio-based routes, although some burden-shifting is present. Unless burden-free electricity is available, DAC- and CCU-based systems are unlikely to lead to a reduction in environmental impacts due to the high demand for electrolytic hydrogen for methanol synthesis. Several planetary boundaries appear difficult not to transgress, even at high recycling rates.

References

1. Han. ACS Sust Chem & Eng, 5(2): 1892–1898, 2017.
2. Herps. PhD thesis, Utrecht University, 2020.
3. Minor et al. Chem Eng J, 474: 145333, 2023.
4. Sala et al., J Env Mgmt, 269:110686, 2020.
5. Tang & You. ACS Sust Chem & Eng, 6(1):937–956, 2018.
6. Thaore et al. Chem Eng Res & Design, 135:140–152, 2018.

Assessment of Physicochemical Characteristics and Ecotoxicological Risks of Municipal Biosolids for Agricultural Use

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Keywords: Biosolids, circular economy, soil amendments, metals

Abstract
Biosolids are rich in organic matter, nutrients, and micronutrients, which can improve soil structure, enhance water retention, and increase nutrient availability. However, their application also carries potential risks, including contamination with heavy metals, pathogens, and organic pollutants. To ensure their safe environmental use, thorough characterization is necessary. This study evaluates the environmental impact of biosolids in soil through ecotoxicity testing and chemical analysis. Specifically, toxic metals were analyzed in biosolids from three different Wastewater Treatment Plants, both in the solid material and their leachates. Additionally, the ecotoxicological effects were assessed using indicator organisms.

Syngas production from gasification of primary sieved solids

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Keywords: WWTPs, waste to energy, gasification

Abstract

Conventional wastewater treatment is widely recognized for its high energy consump-tion (Tsamoutsoglou et al., 2025). Biosolids are a by-product of wastewater treatment that require additional processing. Conventional biosolids treatment and disposal methods are inadequate given the current demanding standards (Manali et al., 2024) and immediate future targets (2024/3019, EU Directive). The removed Primary Sieved Solids (PSS) have high solids content between 35-45% and HHV between 23.5- 24.4 MJ/kg, and thus they are ideal for gasification. A novel integrated process (Figure 1) for the man-agement of PSS along with energy production was installed at the Wastewater Treatment Plant (WWTP) of Rethymno, Crete, Greece. The industrial-scale pilot plant consists of a microsieve (with capacity of about 5000 m3/d of raw wastewater) followed by drying, gasification and production of electric energy through an internal combustion co-generation engine. The system utilizes the heat energy of the flue gas for drying the PSS.

From November 2023 to December 2024, gasification trials were conducted at the Rethymno WWTP using three different feedstocks: wood, PSS, and dried secondary sludge. Specifically, three mixtures were tested. Mixture I comprised of 10% dried secondary sludge and 90% PSS, mixture II consisted of 20% dried secondary sludge and 80% PSS, and mixture III contained equal proportions of 50% dried secondary sludge and 50% PSS. Wood served as the initial feedstock for the gasifier to assess the system's operability. Dried secondary sewage sludge was obtained from the WWTP of Rethymno and uti-lized to enhance syngas quality in conjunction with PSS. The produced dry syngas was analyzed for its gas composition (i.e., H2, CO, CO2, CH4) using automated syngas analyz-ers installed in the pilot unit. The gasifier operated alongside the internal combustion engine for a total of 1,856 hours during the study. The average gasification temperature was 658 °C, and air was used as the oxidizing agent. Figure 2 illustrates the average monthly syngas quality from different feedstocks.

During the initial operation of the pilot plant, the feedstock occasionally contained high-er moisture or impurities, which likely led to increased CO_2 production due to enhanced gas-phase reactions. As the operation of the pilot unit was optimized, syngas quality im-proved and stabilized over time. The syngas produced from the mixtures of PSS and dried secondary sludge consistently maintained high quality, suitable for both electrical and thermal energy generation. The average syngas composition derived from PSS, as the gasification feedstock was found to be 15.5% H2, 16.4% CO, 3.3% CH4, and 7.5% CO2, respectively. The average maximum value of electrical energy was calculated equal to 9 kW from January to December 2024.

References

1. Manali, A., Pothoulaki, A., Gikas, P., 2024. The state of the art in biosolids gasification. J.Environ.Manage. 364, 121385.
2. 2024/3019, EU Directive of the European Parliament and of the Council, of 27 November 2024, Concerning urban wastewater treatment, Official Journal of the European Union.
3. Tsamoutsoglou, K., Kechagias, A., Katzourakis, V.E., Chrysikopoulos, C. V, Gikas, P., 2025. Investigation and efficiency estimation of a hydrocyclone for the treatment of primary municipal wastewater. J.Environ.Manage. 380, 125134.

Assessing the Environmental and Economic Impacts of Shipping: Insights from the Horizon2020 EMERGE (Evaluation, control and Mitigation of the EnviRonmental impacts of shippinG Emissions) Project

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Keywords: Ship emissions, exhaust gas cleaning systems (EGCS), sulfur regulations, marine pollution, atmospheric modeling, ecotoxicology, alternative fuels, maritime policy, sustainability, risk assessment

Abstract

The implementation of strict global regulations on January 1, 2020, significantly affected maritime emissions, mandating a reduction from 3.5% to 0.5% in fuel sulfur content. In Sulfur Emission Control Areas (SECAs), restrictions have been progressively tightened, from 1.5% in 2006 to 0.1% in 2015. The compliance options available to shipowners were low sulfur fuels, liquefied natural gas (LNG), or exhaust gas cleaning systems (EGCS). While EGCS effectively reduce sulfur oxides (SOx) emissions, their effluent discharges release pollutants including polycyclic aromatic hydrocarbons (PAHs) and heavy metals, which increase the environmental risk to marine ecosystems.

EMERGE provided a comprehensive assessment of the atmospheric and marine impacts of shipping emissions by utilizing real-world case studies that included onboard measurements and modeling along main shipping routes and in five ecologically sensitive areas in Europe. The project systematically examined the interactions between emission control technologies, pollutant environmental fate, and impacts, evaluating the effectiveness and cost-efficiency of different abatement strategies.

Advanced emissions, atmospheric and marine modeling tools were adapted to quantify the environmental impacts of baseline (2018) and future shipping emissions and discharges on the selected EU regions and the European domain under various environmental conditions. Shipping emissions contributed on average 28% of SO2, 19% of NOx, and 6% of PM2.5 to baseline pollution in the five case study regions.

The project also developed eight future scenarios for year 2050, considering factors such as alternative fuels, emission control technologies, and potential EGCS discharge restrictions.

Scenario analyses for the year 2050 projected substantial increases in EGCS discharge volumes, particularly in the Baltic and Mediterranean Seas, with potential contamination risks extending up to 10-30 km from major shipping lanes. The project also identified high risks for near-shore and archipelagic ecosystems due to the proximity of shipping lanes to these sensitive coastal environments. Air quality model results showed that shipping significantly impacts port and coastal communities of the case study areas. In the Mediterranean NECA

scenario, EGCS use effectively reduced NO_2, while both Mediterranean NECA and alternative fuels effectively controlled PM2.5 and SO_2.

Ecotoxicological experiments conducted across European research institutions revealed that EGCS effluents pose substantial risks to key species in marine food webs. The study demonstrated that even at extreme dilution levels (1:1,000,000), EGCS effluents resulted in diminished egg production, deformations, and abnormal development of the larvae of these species. Quantitative risk assessments utilizing Predicted No Effect Concentration (PNEC) values and Quantitative Structure–Activity Relationship (QSAR) models highlighted the significant toxicity contribution of alkylated polycyclic aromatic hydrocarbons (alkyl-PAHs), which remain unregulated under current environmental policies.

Economic evaluations indicated that over 95% of EGCS-equipped ships recovered investment costs within five years, reinforcing the continued use of high-sulfur fuels and hindering the transition to more sustainable alternatives. To support policy development, EMERGE introduced a web-based decision support tool, integrating emission and environmental impact assessments to facilitate strategic decision-making aligned with sustainable development goals.

EMERGE findings emphasize the necessity of holistic emission control strategies, advocating for stricter EGCS discharge regulations, and a transition towards inherently cleaner fuels to safeguard marine ecosystems.

Innovative recovery of grease from urban sewage sludge: a sustainable way to unlock new oily feedstock

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Keywords: Sustainable processes; Grease Recovery; Sewage Sludge Treatment; Biorefinery; Circular Economy

Abstract

A novel solvent-free process for the recovery of lipids from municipal sewage sludge was developed and investigated. The process consists in a well-defined sequence of simple unit-operations which allow an efficient recovery of grease from sewage sludge. Thickened municipal sewage sludge was centrifuged, acidified, treated with hydrogen peroxide, heated to 70 °C and immediately centrifugated again. This approach was first tested on a laboratory scale using different acids, in particular formic acid (HCOOH) and hydrochloric acid (HCl), evaluating the synergistic effect of the addition of hydrogen peroxide (H2O2) in terms of lipid recovery. The process was then scaled up to a pilot stage, processing two cubic meters of thickened sewage sludge per hour. The lipid recovery yield depended primarily on the original composition of the sewage sludge, with the yield reaching 73.3% for samples containing 66.2 g of lipid per kg of dewatered sludge. In addition to the high-purity lipid fraction (with a free fatty acid content of 90-92%), two main by-products were obtained: an acidic aqueous phase and a solid cake. The potential for sustainable integration of this technology into various wastewater treatment plants, both with and without anaerobic digesters, was explored and validated. It was found that the co-generated by-products were found to be digestible under anaerobic conditions and lead to higher biomethane production than expected based on the initial biomethane potential of the sewage sludge. The relevant kinetics of biomethane production confirmed that no inhibitory compounds were formed. On the contrary, the reactive steps had a positive effect on the digestibility of the starting sewage sludge. In addition, the residual cakes could be dried efficiently, resulting in a high calorific residue that can generate the electrical and thermal energy required to operate the solvent-free process. These experimental results pose this new process as a sustainable method for processing urban sewage sludge while recovering valuable resources, in coherence with the Circular Economy principles.

A novel system dynamics-based framework for modeling circular economy networks - Polyethylene Terephthalate (PET) as a case study

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Keywords: Circular Economy, System Dynamics, Plastic Recycling, Supply Chains

Abstract
The transition to a circular economy (CE) requires agents in circular supply chain (SC) networks to take a variety of different initiatives, many of which are dynamic in nature. However, there is a lack of generic mathematical models for circular initiatives that incorporate the time dimension, and their combined effects on different agents and overall SC circularity is not well understood. We use a system dynamics (SD)-based approach to develop a generic framework for dynamic modeling of CE networks and use it to model the supply chain for Polyethylene Terephthalate (PET) plastic packaging, a significant contributor to pollution in landfills and waterways. Novel contributions include generic quantitative models for material quality loss and a model for a consumer that includes both continuous and discrete product reuse.

We propose a prototypical circular SC network by combining dynamic models for five agents: a manufacturer, consumer, material recovery facility (MRF), recycling facility, and the Earth. We use the planetary boundaries framework to quantify the absolute environmental sustainability of the network while accounting for feedback effects between different Earth-system processes. We apply this framework to the case study of the PET SC by considering different scenarios over a 65-year time horizon in the US, including both "slow-down-the-loop" initiatives (i.e., those that extend product use time through demand reduction or reuse) and "close-the-loop" initiatives (i.e., those that reintroduce product to the supply chain through recycling) by the consumer, as well as capacity expansion of the MRF and recycling facilities.

We find that given the current recycling infrastructure in the U.S., "slow-down-the-loop" initiatives are more effective than "close-the-loop" initiatives, which require capacity expansion to accommodate the increased recycle rate and an associated time delay. However, combining the two eliminates the need for capacity expansion and leads to the highest circularity. Sensitivity analyses are performed to analyze the effect of consumer behavior on network circularity. As the consumer recycle rate increases, circularity increases until reaching a plateau. This plateau may be due to recycling capacity limitations or quality loss due to the mechanical recycling process; above this plateau, there may be a trade-off between circularity and sustainability. Overall, we conclude that although chemical recycling technologies have the potential to eliminate quality loss and may be promising long-term solutions, such technologies have a significantly higher cost and environmental impact than mechanical recycling and are not currently widespread in the U.S. Thus, in the short term, "slow-down-the-loop" initiatives are more promising solutions for a CE transition.

Dark fermentation vs. electrofermentation for biological H2 production from cheese whey

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Keywords: Biofuel; organic waste, dark fermentation; electrofermentation; biohydrogen

Abstract

Even if H2 is in principle recognized as a renewable and low-carbon energy vector that could play a pivotal role towards decarbonisation, in 2022 H2 still covered less than 2% of the EU overall energy consumption [1]. Moreover, the H2 production processes exhibited a non-negligible carbon footprint resulting from the use of fossil fuels (e.g., natural gas). Thus, in order to fulfil the decarbonization targets, the REPowerEU strategy stated that "by 2050, renewable hydrogen is to cover around 10% of the EU's energy needs, significantly decarbonising energy intensive industrial processes and the transport sector", where "renewable hydrogen is produced through the process of electrolysis, using renewable electricity to split water into hydrogen and oxygen and is therefore a Renewable Fuel of Non-Biological Origin' (RFNBO)". Keeping in mind the targets set at EU level and the proposed strategy to reach them, it is worth asking whether alternative routes may be integrated to RFNBO production and play a role in decarbonizing the energy sector. For example, it is well known that H2 can be produced via biochemical processes such as photofermentation and dark fermentation, or via bioelectrochemical systems such as bioelectrofermentation reactors, microbial electrolysis cells and microbial fuel cells. If organic waste of municipal or industrial origin is used as the substrate of the biological process, bioH2 production may represent a valid option for organic waste valorization. According to Eurostat [2], over 59 million tons of organic waste were produced in 2022, 46% of which were generated upwards in the food supply chain. Thus, dark fermentation of organic waste (e.g., anaerobic digestion controlled so as to produce H2) may represent a very promising strategy for attaining both organic waste valorization and green H2 production, due to the possibility of integrating the fermenter into the already existing anaerobic digestion plants; in fact, the digestate from dark fermentation may be fed to the conventional anaerobic digester to complete the conversion into CH4.

In the present study cheese whey from mozzarella production, a very abundant effluent from dairy industry [3], was tested in an automatically controlled fermenter under batch conditions. The H2 yields and kinetics, as well as the metabolite evolution over time (VFAs, lactic acid and ethanol) were compared with those observed integrating the process with electrofermentation. Different voltages were tested, spamming from 1 to 0.2 V, and the preliminary results demonstrated a better performance of the electrofermentation process compared to the sole dark fermentation.

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Engineering of intensified CO2 capture and electrocatalytic reduction systems: From solvent selection to pilot plant testing

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Keywords: Solvents, Electrocatalytic reduction, CO2 capture

Abstract
Electrocatalytic CO2 reduction (CO2R) enables the transformation of CO2 into chemicals or fuels, using renewable energy. Conventionally CO2R makes use of CO2 that has been captured through a separate process, such as solvent-based absorption/desorption, and the use of H2 that has been produced separately through water electrolysis. Several pieces of equipment are needed (absorption and desorption columns, electrolyser and CO2R cell) with detrimental impacts on capital and operational costs. Converting the CO2 into products either directly from its gaseous phase or through dissolution into water, has detrimental effects on conversion efficiency and energy consumption. In recent years there has been a growing trend towards integrated CO2 absorption-CO2R processes. Instead of using thermal CO2 desorption, the solvent-bound CO2 may be fed into the CO2R cell directly from the absorber of the capture system. The aqueous mixtures of amine solvents or of inorganic bases and salts used in CO2 absorption provide a source of hydrogen which may react in situ with CO2-derived activated species on an electrode surface toward the desired product, whereas the solvent may be recycled to the absorber. The high CO2 solubility in such solvents avails higher CO2 quantities in the cell, with beneficial effects on their efficiency and the associated energy costs. Despite the potential of this approach, very few solvents have been investigated to date, with all of them selected arbitrarily and based on prior knowledge regarding their suitability as CO2 absorption media. No criteria have been proposed to enable solvent selection by accounting for the interactions of CO2 absorption and reduction systems, making existing solvent options unsuitable for such systems.
In this work, we elaborate for the first time on the properties that a solvent should have in order to promote both CO2 absorption and reduction and we explain the underlying mechanisms. We propose criteria for solvent selection that include the solvent CO2 solubility, kinetic constant, ionic conductivity, and concentration of the bicarbonate, carbamate and solvent cation in the CO2-loaded solution. Additional criteria include sustainability performance during solvent production and solvent use in such systems. They are implemented for solvent selection (a) from novel, aqueous mixtures of MCA (N-methylcyclohexylamine) with PZ (piperazine), AMP (2-amino-2-methyl-1-propanol), KOH (potassium hydroxide) and KCl (potassium chloride), and (b) from aqueous MEA (monoethanolamine), AMP, KOH, MCA and PZ solutions. Versions of a modified Kent-Eisenberg model for strong bases, carbamate and non-carbamate forming amine solutions are developed and parameterized through experimental equilibrium measurements. Experimental results from a pilot CO2R setup are presented for solutions of KOH and MCA+KOH, as these indicate desired trade-offs for CO2 absorption and reduction.

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Integrating Short-Term Operations and Long-Term Planning for Resilient Urban Energy Systems: A Multi-Scale Optimization Framework

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Keywords: urban energy systems, multi-scale, MILP

Abstract

Over the last 150 years, global energy demand has increased unprecedentedly due to the rapid growth of population and industrial development. This escalating demand presents a critical challenge: building resilient and sustainable energy infrastructure. Addressing this requires a comprehensive transformation of energy systems, including advancements in storage technologies, grid management, policy frameworks, assessments of resource availability, economic feasibility, and environmental impact. Urban areas, as major energy consumers, need to effectively integrate and optimize multi-energy systems to enhance energy efficiency, sustainability, and resilience. Effective infrastructure planning is essential to navigating this complex transition and ensuring a reliable energy future.

Existing mathematical models and tools for urban energy systems focus on either long-term infrastructure planning or short-term operational management, often lacking the resolution necessary to capture the variability of intermittent energy sources and the interdependence of multi-energy systems. This research addresses this gap by introducing a multi-scale mixed-integer linear programming (MILP) optimization framework for the infrastructure expansion planning of urban energy systems. The framework integrates electricity, heating, and cooling demands while considering short-term operational and long-term planning decisions. It employs a dual resolution, with hourly resolution for operational decisions and yearly resolution for capacity expansion planning decisions. This hybrid approach accurately represents the system's performance over time and provides actionable insights for energy planners and policymakers, supporting the transition to more resilient, efficient, and sustainable energy systems. Additionally, this study expands the environmental analysis by considering the life-cycle emissions of energy generation technologies, accounting for emissions beyond operational phases.

The proposed framework is applied to a case study that considers the energy transition in a university campus, with the model solved hourly over a 25-year horizon, incorporating a pre-processing step to reduce computational complexity and improve problem tractability. This step involves generating future weather data using ARIMA and LSTM models to then estimate the energy production of weather-dependent technologies, such as solar panels and wind turbines, over the entire planning horizon. The results underscore the importance of temporal granularity in effective energy planning, offering valuable insights into infrastructure design, system operations, and strategies to enhance local energy production integration and demand-side management in urban growth. The framework developed is designed to serve as a decision-making tool for different stakeholders, allowing the exploration of different budget scenarios, estimation of economic and environmental impacts, and exploring their trade-offs, ultimately informing more balanced energy strategies. Furthermore, the model could simulate the impacts of subsidies, taxes, or incentives for specific technologies.

CCU Process Design and Evaluation for Methanol Production Using Cement Flue Gases

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Keywords: Process design, Carbon footprint reduction, Methanol production, Techno-economic analysis

Abstract

Climate change driven by atmospheric CO2 accumulation from human activities presents a critical environmental challenge. The cement industry alone accounts for approximately 8% of global CO2 emissions, underscoring the urgency of reducing its carbon footprint. This study addresses this challenge by designing and evaluating a carbon capture and utilization (CCU) process using Aspen Plus V11 software. The process consists of two main units: (1) a CO 2 capture unit utilizing monoethanolamine to treat cement production flue gases, and (2) a CO 2 utilization unit for methanol production via direct hydrogenation. A comprehensive techno- economic analysis was performed, along with a carbon footprint assessment of alternative process configurations. For unit capacities of 627 ktons CO 2 /year and 445 ktons methanol/year, the capital expenditures were estimated at €118 million for the capture unit and €301 million for the combined capture and utilization process. The production costs were calculated at €110 per ton of CO 2 captured and €1,467 per ton of methanol produced. Economic feasibility analysis revealed that the capture process would become marginally profitable at a carbon tax of €151 per ton of CO 2 , while the full CCU process would require a carbon tax of €637 per ton of CO2. Key cost drivers identified include green hydrogen feedstock, fixed capital investment, steam, and electricity. A sensitivity analysis was conducted to evaluate strategic cost reductions. Under an optimized scenario with hydrogen priced at €1.94/kg and a 35% reduction in capital investment, methanol production costs decreased by 43% to €836 per ton, while the break-even carbon tax dropped to €292 per ton of CO 2 . An environmental assessment, conducted in compliance with ISO 14040 and 14044 standards using SimaPro 9.1, quantified the global warming potential over 100 years. Compared to a "Do Nothing" scenario, the carbon footprint for the capture-only process presented "positive" impact due to the CO2 uptake and reduced by 96.7% for the CCU process. Although not yet economically viable, the proposed technologies demonstrate clear environmental benefits and represent a promising pathway for mitigating emissions from the cement industry.

Optimization of biotrickling filters for biological biogas upgrade to biomethane under mesophilic conditions

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Keywords: biogas upgrade, biomethane, mesophilic hydrogenotrophic methanogenesis, Trickle Bed Reactor, ex-situ

Abstract

Biomethane is a gas mixture primarily composed of methane (over 95%) and serves as an alternative to natural gas. It is generally produced from biogas by removing carbon dioxide using physicochemical methods, which are established but can be energy-intensive. A promising alternative method involves utilizing the ability of hydrogenotrophic methanogens to convert carbon dioxide into methane in the presence of hydrogen. This process can lead to increased methane production, making it suitable for energy storage, especially when green hydrogen (derived from surplus renewable energy) is used.

The most favorable conditions for productivity and efficiency are found in ex-situ hydrogenotrophic methanogenesis using Trickle Bed Reactors (TBRs) at thermophilic temperatures, which can achieve very low Gas Retention Times (GRTs) of less than one hour. However, mesophilic hydrogenotrophic methanogenesis has been less extensively studied.

In this study, we thoroughly investigated mesophilic biogas upgrading in two 1-liter TBRs operating in parallel at a temperature of 39±1°C for over 500 days. The TBRs were filled with polyethylene rings (Kaldnes K1) as packing material, providing a specific surface area of 800 m^2/m^3. The feeding gas consisted of 60-68% v/v H_2, 15-23% v/v CH_4, and 17% v/v CO_2 and was introduced from the bottom of the reactors. Diluted anaerobic digestate served as the nutrient medium, trickled from the top to the bottom of the TBRs, and recirculated at a rate of 3 L/L/d.

The GRT was reduced to 1.8 days, and the TBRs could produce biomethane with over 94% CH_4 content. When the headspace of one TBR was connected to a 1-meter high water column, creating an overpressure of 0.1 bar, the GRT dropped to 1 hour without compromising efficiency (94%), compared to 84% efficiency at 1 hour GRT under atmospheric pressure. It was also observed that the ammonia level in the nutrient medium should be maintained above 20 mg/L, achieving a biomethane content of 97.0±1.9% methane at a GRT of 2.2 hours. However, when the ammonia nitrogen concentration fell below 10 mg/L, the biomethane content decreased to 93.0±3.3% CH_4.

Moreover, the recirculation rate impacted the efficiency; the methane content in the gas outlet was found to be 97.3±3.0%, 95.3±2.7%, and 93.4±3.1% under recirculation rates of 3, 2, and 1.5 L/L/d, respectively, all at the same GRT of 2.2 hours. Long-term operation demonstrated the competitiveness of this process under mesophilic conditions, as it maintained high CH_4 proportions (94%) at low GRTs (1 hour) under slight overpressure (0.1 bar) while levels of volatile fatty acids (VFAs) remained low (30-170 mg/L), even under overloading conditions.

Topic 3 - Machine Learning

Machine Learning-Based Prediction of Biomass Composition Using Derivative Thermogravimetric Data

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Keywords: machine learning, biomass composition, thermogravimetric data

Abstract

The current trend towards biomass as a renewable energy source requires efficient and accurate methods for assessing the composition of biomass. Standard approaches that utilize, for example, wet chemistry or spectroscopic methods are generally laborious, time-consuming, and invasive, and therefore not applicable in large-scale industrial scenarios. In this study, we propose a novel method for predicting bamboo biomass composition (cellulose, hemicellulose, and lignin) through the application of advanced machine learning (ML) models to derivative thermogravimetric (DTG) data.

The model that performed best among the models evaluated was the Extreme Gradient Boosting (XGB) Regressor, which involved the least prediction error and gave high predictive accuracy with near perfect R^2 values of 1.00 for cellulose and 0.99 for both hemicellulose and lignin. Additionally, the model showed exceptional error metrics and thus reliably and robustly processed the complex thermal decomposition profiles characteristic of DTG data. This method obviates the requirement of invasive, or laborious, spectroscopic calibrations or wet chemistry, providing a rapid and nondestructive method for the analysis of biomass.

To interpret model predictions and explain the connection between particular DTG temperature intervals and biomass composition, the study also utilizes Shapley Additive Explanations (SHAP). Important temperature ranges (DTG_80 and DTG_280 for cellulose, DTG_400 for hemicellulose, and DTG_60 for lignin) were identified to be necessary for good prediction. These results match known thermal degradation phases, which add to the interpretation and application of the interest value of the findings.

This innovative methodology greatly advances the field of biomass characterization and is a hopeful prescription for validating biomass databases to the point where reliable process simulations would be possible. This allows for rapid, precise predictions without requiring traditional laboratory-based methods or promotion of large-scale bioenergy production. The approach is shown to be adaptable to biomass types and scalable to enable the applications of the methods to a wide range of types, especially with the addition of other data sources including spectroscopy. This research establishes a new benchmark for optimizing biofuel production by conducting machine learning on DTG data and integrating that with the existing process.

The XGB model in this work significantly outperformed traditional methods and other machine learning techniques (compared to other recent studies). Results demonstrate the potential to transform the use of DTG data with state-of-the-art ML techniques in unmatched levels of accuracy and efficiency. This study, while focused on bamboo biomass, opens the way for future study of the applicability of this methodology to other feedstocks through transfer learning and hybrid data integration.

This study concludes by proposing a robust, scalable framework for biomass compositional analysis that circumvents the pitfalls of traditional analysis methods and offers the potential to propel renewable energy production. The integration of DTG data and machine learning is a major advancement in developing sustainable

strategies for the use of biomass resources while presenting an innovative practical solution to bioenergy optimization problems.

Machine Learning in Process Control, Safety and Operations

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Keywords: Machine learning, process control, reactor operation, reactor control, nonlinear processes

Abstract
Machine learning is creating new paradigms and opportunities in the design of advanced process control systems for chemical processes. Traditionally, model predictive control (MPC), a constrained optimization-based control problem formulation that is the gold standard employed in advanced control of chemical processes, is formulated with linear data-based empirical models and is used to compute control actions to maintain optimal process operation while accounting for process and control actuator constraints. However, chemical processes are inherently nonlinear and often require nonlinear models in order to be controlled efficiently. Nonlinear first-principles process modeling provides a direct way for accounting for nonlinear process behavior in the control system design but it may be cumbersome and difficult to implement in complex industrial processes which are not well-understood. Machine learning tools like recurrent neural networks and ensemble learning provide an efficient way to build nonlinear dynamic models from data that can be used in the model predictive control system, thereby improving control system performance, process operational safety and process operation. In addition to revealing nonlinear dynamic process relationships from data, machine learning tools can address classification problems such that the ones arising in diagnosing process faults and cyber-attacks, thus providing a broad array of topics where machine learning can make an impact.
In this talk, we will primarily present our research work on the use of machine-learning tools in developing nonlinear model predictive control methods that ensure optimal control system performance and process operational safety, as well as establishing cybersecurity for nonlinear processes. Specifically, we will present: a) a machine-learning-based predictive control framework that integrates recurrent neural networks within MPC and utilizes ensemble learning and parallel computing for enhanced prediction accuracy and computational efficiency, b) machine-learning-based MPC structures for nonlinear processes, which address simultaneously closed-loop stability and performance, and ensure process operational safety in the sense of guaranteed avoidance of unsafe operating conditions, and c) a two-tier detector-controller architecture that uses a machine learning-based classification detector to ensure process robustness with respect to a broad set of cyber-attacks. Throughout the talk, we will present applications of our methods to chemical processes of industrial interest to demonstrate their applicability and performance in meeting next-generation industrial goals related to improving process economics, safety and cyber-security. We will conclude the presentation by discussing the use of machine learning for data reduction and real-time operational decision making in deposition processes, additive manufacturing and an experimental electrochemical reactor.

OPTIMAI: Optimizing Manufacturing Processes through Artificial Intelligence and Virtualization

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Keywords: Artificial Intelligence, Digital Twins, Augmented Reality

Abstract

The OPTIMAI project, funded under the European Commission's Horizon 2020 program (GA: 958264), represents a transformative initiative aimed at enhancing the competitiveness of European manufacturing by integrating cutting-edge Industry 4.0 technologies such as Artificial Intelligence (AI), Digital Twins (DT), Augmented Reality (AR), and blockchain. Over 36 months, OPTIMAI addressed critical industrial challenges—defect reduction, productivity optimization, workforce training, and sustainability—by developing a comprehensive ecosystem of innovative tools validated across pilot sites in Greece (KLEEMANN), Spain (TELEVES), and the UK (Microchip).

At its core, OPTIMAI leverages AI-driven methodologies to redefine traditional manufacturing trade-offs between speed, cost, and reliability. Advanced techniques, including Computer Vision (CV) for real-time visual inspection, Generative Adversarial Networks (GANs) for DT creation, and Reinforcement Learning (RL) for dynamic process optimization, enable predictive maintenance, early fault detection, and automated calibration. These AI systems are integrated with DTs, which virtualize production lines to simulate and monitor processes, reducing pre-production ramp-up times and minimizing material waste through zero-defect strategies.

OPTIMAI integrates a Decision Support System (DSS) to provide actionable insights for optimizing production processes and improving resource allocation. The DSS empowers decision-makers with real-time data analysis and recommendations, enhancing operational efficiency. An Active Learning (AL) approach is integrated with DSS to address data scarcity challenges. AL dynamically selects the most informative data points for AI training, ensuring adaptability to evolving shop-floor conditions and improving the accuracy of predictive models. Additionally, the project adopts human-centric approaches to enhance workforce efficiency and collaboration. Augmented Reality (AR) tools offer real-time guidance and training to operators, reducing errors and improving accuracy. By prioritizing human-centric design, OPTIMAI ensures that advanced technologies complement and empower workers rather than replace them.

A standout innovation is the MAIAR subsystem, an AR platform featuring smart glasses equipped with gesture recognition and X-ray vision capabilities. This tool enhances human-machine collaboration by enabling workers to inspect machinery in hard-to-reach areas, reconfigure systems in real time, and perform quality checks with augmented situational awareness. Pilot end-users reported significant improvements in decision-making speed and defect inspection accuracy, highlighting the system's user-friendly interface and operational efficiency.

To ensure data integrity, OPTIMAI employs a blockchain-based traceability system utilizing Ethereum networks with Proof of Authority (PoA). This system securely records sensor data, defect logs, and AI parameters via smart contracts, fostering transparency and trust across supply chains.

The project's environmental impact is significant: AI-optimized processes greatly reduce production scrap, predictive maintenance minimizes unplanned downtime, and automated resource-efficient calibration minimizes ramp-up times. These advancements align with circular economy principles, as demonstrated by the Intelligent Marketplace, a platform for reusing defective components.

In conclusion, OPTIMAI – this work was also supported by the European Commission through Project ENCIRCLE funded by the European Union H2020 programme under Grant 101178230 – successfully bridges technological innovation with industrial practicality, achieving, as demonstrated in controlled environments carried out through project pilots, a 20% increase in equipment productivity, a 15% reduction in time-to-market, a defect detection rate exceeding 80% across multiple use-case scenarios, and enhanced workforce competency through AR training. By integrating AI, virtualization, and human-centric design, the project establishes a scalable blueprint for sustainable, high-quality manufacturing, reinforcing Europe's position in the global

industrial landscape. The outcomes of the OPTIMAI project are being further extended and supported under the ongoing ENCIRCLE project (GA: 101178230).

On the use of Gaussian noise-based data augmentation to improve the performance of hybrid knowledge/data driven growth kinetic models for mammalian cell cultures

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Keywords: Data augmentation, Hybrid model, Mammalian cells, HEK293

Abstract

Mammalian cells are vital for producing complex biological medicines, such as recombinant monoclonal antibodies or viral vector-based therapies. However, the high cost of these therapies is driven by low yields and large dose requirements (Fu et al., 2023). Process model-based methods offer valuable strategies to reduce production costs and time while optimizing key biomanufacturing steps. The adoption of hybrid models, which offer greater robustness and improved predictive accuracy, has further advanced the application of digital twins in process modeling (Tsopanoglou and Del Val, 2021). Hybrid models integrate data-driven and mechanistic models with the aim of combining their strengths. One of the primary requirements in data-driven modelling is the availability of extensive high-quality data to effectively train the model (Wen et al., 2021). However, obtaining sufficient experimental data, especially for biological processes, is often too costly and time-consuming. Data augmentation, which is the generation of synthetic data samples from real data, is a common method to ensure the availability of sufficient data. For time series datasets this method comes with unique challenges, as one should be careful not to affect the dependencies within the data which could impact the model's training and predictive accuracy (Wen et al., 2021). By adding Gaussian noise based on the mean and standard deviation of the available experimental data, synthetic datasets can be created while maintaining the correlation between the model inputs.

Herein, we present the development of a hybrid model of HEK293 growth kinetics. A data-driven approach is employed to derive relevant kinetic rates which are subsequently integrated in a mechanistic model based on dynamic mass balances. The hybrid model is used to predict the macroscopic behavior of key state variables, such as viable cell density, glucose and lactate concentration. The developed model was used to predict HEK293 cell expansion in a proprietary fixed bed bioreactor. The hybrid model was trained both on real and augmented datasets. To evaluate the impact of data augmentation, Normalized Root Mean Squared Error (NRMSE) values were calculated for models trained with both datasets. The results indicate that models trained on the Gaussian noise-based augmented dataset exhibit lower variability and achieve lower NRMSE across various experimental conditions compared to models trained on a real, but sparse, experimental dataset. In conclusion, the integration of Gaussian noise for data augmentation in hybrid models proves to be a valuable strategy to improve model performance by overcoming the challenge of limited experimental data availability.

References:

1. Fu, Q., Polanco A., Lee Y. S., & Yoon S. (2023). Critical challenges and advances in recombinant adeno-associated virus (rAAV) biomanufacturing. Biotechnology and Bioengineering, 120(9), 2601–2621. https://doi.org/10.1002/bit.28412
2. Tsopanoglou A. & Del Val I. J. (2021). Moving towards an era of hybrid modelling: advantages and challenges of coupling mechanistic and data-driven models for upstream pharmaceutical bioprocesses. Current Opinion in Chemical Engineering, 32, 100691. https://doi.org/10.1016/j.coche.2021.100691
3. Wen Q., Sun L.,Song X., Gao J., Wang X.,& Xu H. (2021). Time series data augmentation for deep learning:A survey. Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence (IJCAI-2021), 4653–4660. International

Topic 4 - Green and innovative chemistries and technologies

Combatting microplastic pollution in the marine environment

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Abstract
Plastic debris represents a significant problem among the various pollution problems facing the marine environment. Several studies have been conducted on the fate and weathering of plastics in the marine environment including the generation and fate of microplastics. Sorption of toxic substances present in seawater by microplastics represents an additional environmental concern. Laboratory results on the biodegradation of plastics show great variability. An important question, which remains unanswered, is what is the level of weathering that makes the common plastics, in particular those with a C-C backbone, biodegradable at a reasonably fast rate. Is Natural Attenuation a potential biodegradation route that allows us to hope for clean oceans? In this presentation, we focus on the determination of biodegradation and fragmentation rates of polystyrene and polyethylene films naturally weathered on beach sand as well as polypropylene films weathered in seawater mesocosms. Results from 300-day long field experiments in Souda Bay (Crete, Greece) are also presented. Our findings are very encouraging pointing to new challenges that need to be addressed for a successful biodegradation of plastics in the marine environment as well as significant advances in the context of circular economy.

Pilot-scale treatment of flue gas from the cement industry by carbonic anhydrase-promoted CO2 absorption in an aqueous aminoacid amine blend: Benchmarking and techno-economic insights on a 3rd generation hybrid blend

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Keywords: amine, carbonic anhydrase, CCUS, MDEA, aminoacid amine blend

Abstract

Conventional CO2 absorption processes are based on amine solvents. The current state-of-the-art for CO2 capture is the primary amine MEA that is highly reactive and shows high absorption rates. However in turn, this results in high desorption temperatures (120-140oC) due to formation of carbamates, requiring high energy consumption for solvent regeneration. On the contrary, tertiary amines, such as MDEA, form bicarbonates requiring lower regeneration temperatures but suffer from significantly lower absorption rates. Blending amines and ionic liquids in aqueous solutions have shown promising results coupling advantages of both sorbents. In particular, introducing an amino functional group in ionic liquids by the use of an amino acid generates so called amino acid ionic liquids which, when blended with MDEA, have shown increased CO2 absorption rates maintaining the good desorption properties of both solvents.

The enzyme carbonic anhydrase (CA) is one of the fastest enzymes known and catalyzes the hydration of CO2. Although CA is known to improve CO2 absorption rates in aqueous methyldiethanolamine (MDEA) solvents, its use in industrial settings is often limited. High temperature and inhibitors forming and accumulating in the solvent during continuous CO2 capture processes lead to degradation and/or inactivation. The development of a thermostable carbonic anhydrase with enhanced tolerance to off gas inhibitors and reusability potential is critical for the economical use of this efficient enzyme in conventional amine scrubbers.

Aim of this work was the pilot treatment of flue gas from a cement industry in an automated absorption column (1 m) employing a hybrid blend comprising of 5% PEHA prolinate: 20% MDEA: CA. The absorption conditions (temperature, L/G ratio) were optimized in terms of highest absorption rate and absorption efficiency under steady state conditions and under solvent recirculation. A technoeconomic analysis was performed based on the experimental data to provide an insight on bottlenecks and a benchmarking compared to primary amine MEA.

Gas fermentation in a trickle bed reactor with focus on syngas / CO2 biomethanation and variable mass transfer modeling

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Keywords: Gas fermentation technology, syngas, trickle bed reactor, mass transfer

Abstract

The increasing demand for efficient and sustainable industrial processes has accelerated research for green alternatives. Gas fermentation technology, i.e. biological processing of syngas generated via gasification or pyrolysis and CO2 found in the off gas of industrial activities together with renewable H2, presents great potential for enhancing the transition of our society to a sustainable era and alleviating the climate crisis (Gavala et al., 2021). Scalability, robustness and economic viability are decisive factors for successfully bringing emerging technologies on a commercial scale. Compared to traditional liquid phase fermentation, gas fermentation comes with additional challenges, that mainly stem from gas-liquid mass transfer limitations.

Over the last 10 years, at DTU Chemical and Biochemical Engineering, we have developed gas fermentation technology based on Trickle Bed Reactor (TBR) configuration to alleviate mass transfer challenges (Asimakopoulos et al., 2021), and a thermodynamics-assisted methodology for tailoring microbial enrichments specialized for gas fermentations (Grimalt-Alemany et al., 2018, 2020). A TBR offers the dual benefit of high surface area, thus facilitating mass transfer, as well as high density of microbes that results in enhanced production rates. Dynamic modelling of both microbial growth and mass transfer is a powerful tool for optimal up scaling and offers reliable predictions that can be tailored to specific cases in terms of scale and products.

The presentation will summarize the status of gas fermentation technology and will subsequently focus on syngas and CO2 biomethanation from lab-scale to pilot-scale. We will show how the scale and different reactor geometry and operating conditions affected the efficiency of syngas biomethanation, and how modelling of variable volumetric mass transfer coefficient allows optimal up-scaling of a rather complex reactor system (Dutta et al., 2024a, b).

Predicting and controlling the volumetric mass transfer coefficient is valuable, not only for maximizing the mass transfer rate, but equally importantly, for preventing inhibition phenomena. Temperature, pressure, reactor geometry and gas and liquid flow rates can be adjusted to secure maximum efficiency of the gas fermentation process. As this approach and modelling tool can be adjusted to different reactors and microbial systems, it can be very useful for designing new and re-visiting established processes in the field.

References:

1. Gavala HN, Grimalt-Alemany A, Asimakopoulos K and Skiadas IV (2021) Gas biological conversions: the potential of Syngas and Carbon Dioxide as production platforms, https://doi.org/10.1007/s12649-020-01332-7
2. Asimakopoulos K, Kaufmann-Elfang M, Lundholm-Hoeffner C, Rasmussen, NBK, Grimalt-Alemany A, Gavala HN and Skiadas IV (2021) Scale-up study of a thermophilic trickle bed reactor performing syngas biomethanation, https://doi.org/10.1016/j.apenergy.2021.116771
3. Grimalt-Alemany A, Łężyk M, Kennes-Veiga DM, Skiadas IV and Gavala HN (2020) Enrichment of mesophilic and thermophilic mixed microbial consortia for syngas biomethanation: the role of kinetic and thermodynamic competition . Waste and Biomass Valorization, 11, 465-481.
4. Dutta S, Krikeli M, Gavala HN and Skiadas IV (2024a) Dynamic tank-in-series modelling and simulation of gas-liquid interaction in trickle bed reactor resigned for gas fermentation. https://doi.org/10.1016/j.jclepro.2024.143433

5. Dutta S, Gavala HN, Skiadas IV (2024b) Scaling up Trickle Bed Reactor for gas fermentation technology: the effect of temperature and reactor characteristics on mass transfer, https://doi.org/10.3390/fermentation10120623

A circular economy strategy for the management of food waste

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Keywords: Food waste, waste prevention, waste valorization, circular economy

Abstract

Food waste management represents one of the most challenging environmental problems in our times. It is estimated that one third of the food produced worldwide is lost or wasted with significant social, economic and environmental consequences. Food is lost or wasted along the entire value chain: during harvesting on the farm, after leaving the farm for handling, storage, and transportation, during industrial or domestic processing and/or packaging, during distribution to markets (wholesale and retail), during consumption in hotels, restaurants and cacfeterias and finally in households. Food loss and waste prevention is the best option from a hierarchical point of view. However, food surplus is always unavoidably generated and it is best managed by redistribution and upcycling practices.

The food that cannot be saved or utilized for human or animal consumption ends up as food waste. While its disposal to landfills is responsible for the emissions of potent greenhouse gases, such as methane, to the atmosphere, if separately collected, it may be exploited to produce added value products. Our experiences with food waste valorization are presented. Source separated and collected Food Waste is dried and shredded, generating product we named FORBI (Food Residue Biomass) with the following advantages: (a) It has 1/4 the weight of food waste, implying reduced transportation costs, (b) It has low-moisture (less than 10%) and may be stored for prolonged periods of time without deterioration, (c) It is homogeneous, (d) It does not emit odors, (e) It may be valorized in several different ways for the production of: Gaseous Biofuels (Methane, Hydrogen, Hythane). Liquid Biofuels (Bioethanol), Compost, Solid biofuels (pellets), Alternative fuel for the cement industry, Direct production of electricity via microbial fuel cell technology, Adsorbent for wastewater purification and as Animal Feed. The most promising ones are (a) biogas production, (b) use as fuel in the cement industry and (c) production of compost.

Biogas produced from food waste may be upgraded to bioCNG (biological origin compacted natural gas) and used to fuel collection trucks, a perfect example of circular economy. as the vehicles that collect food waste are fueled by a fuel generated from them! Biogas may be alternately used in a combined heat and power process (CHP) or injected into the natural gas network. The second option consists of using FORBI as an alternative fuel for the cement industry, where the replacement of fossil fuels is highly desirable as it leads to: (a) Reduction of energy costs, (b) Saving of natural resources and (c) Reduction of CO2 emissions. It turns out that FORBI may be used as it is as an alternative fuel for the cement industry! Finally, FORBI may be used as a compost enhancer, since its readily degradable organic content helps speed up significantly the composting process of prunings, that would otherwise take months to achieve. It is proved that separate collection and valorization of food waste, along with the other recyclables, leads to diversion of more than 80% of municipal solid waste from landfilling.

Valorization of microalgal biomass for enhanced methane production during anaerobic digestion of corn stover residues

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Keywords: Agricultural residues, microalgal, digestate utilization, anaerobic digestion, methane production.

Abstract

Agricultural residues exhibit a significant potential for biogas production through anaerobic digestion, due to their abundance and low cost. Regarding anaerobic digestion of residual agricultural biomass, large quantities of digestate are generated, requiring proper management. The sustainable use of digestate offers both economic and environmental benefits, although its valorization is a challenging issue, since plant growth stage, soil type, stabilization level, and the presence of pollutants influence digestate applicability. These limitations indicate the need for alternative waste management solutions to permit a safe and a more sustainable use of digestate. In this context, the liquid fraction of digestate, rich in both micro- and macronutrients, can be valorized as a culture medium for microalgae growth. Specifically, co-digestion of microalgal biomass with agricultural residues offers several advantages, including a higher C/N ratio and improved buffer capacity. It also leads to the dilution of inhibitory compounds and provides a better nutrient balance, which can enhance organic matter availability and digestibility, thereby improving biogas yield. Thus, the present study examines the potential of liquid digestate derived from corn stover residues to be utilized in microalgal cultivation, with the subsequent use of the produced microalgal biomass in anaerobic co-digestion of corn stover residues. Microalgae from freshwater were initially enriched and then introduced into a batch reactor, which operated under optimal conditions. The liquid digestate derived from the anaerobic digestion of corn stover residues in the presence of rumen microorganisms served as the growth medium for the microalgal inoculum. Subsequently, the microalgal biomass was introduced into the anaerobic digester to enhance methane production during anaerobic digestion of corn stover residues. The efficiency of this process was initially assessed in Biochemical Methane Potential (BMP) test and then evaluated in continuous stirred-tank reactors (CSTR). In batch reactors, the use of liquid digestate increased microalgal biomass production by 84% compared to the reference batch reactor, where an inorganic nutrient solution was used for microalgal growth. Moreover, the anaerobic co-digestion of corn stover residues with microalgal biomass enhanced methane production by 3.11-fold compared to the anaerobic digestion of corn stover alone. The addition of rumen fluid (5% w/v) during co-digestion of corn stover and microalgae biomass further increased methane yield by 4.84-fold.

An accelerator of the safe and sustainable by design (SSbD) framework

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Keywords: SSbD, systems engineering

Abstract

Sustainable engineering systems focus on designing and operating processes that integrate environmental, economic, and social considerations. By optimizing resource use, minimizing environmental impact, and enhancing societal well-being, these systems contribute positively to economic development while ensuring sustainability throughout a product or process lifecycle.

Sustainable engineering applies engineering principles to resource harvesting, conversion, and utilization, promoting environmentally responsible technological advancements. This holistic approach ensures engineering activities support economic progress and improved living standards with minimal environmental harm [1]. Additionally, it integrates social, environmental, and economic considerations into product, process, and energy system designs, emphasizing lifecycle impacts to maximize sustainability benefits [2].

The European Commission's Safe and Sustainable by Design (SSbD) framework, introduced on December 8, 2022, is a voluntary initiative guiding sustainable innovation in chemicals and materials. Its objectives include:

- Promoting a green industrial transition.
- Reducing or eliminating substances of concern in compliance with regulatory standards.
- Minimizing health, climate, and environmental impacts across sourcing, production, use, and end-of-life stages.

The framework consists of two key phases:

1. (Re-)Design Phase – Establishing goals, scope, and system boundaries for sustainable material assessment.
2. Assessment Phase – Evaluating safety and sustainability through hazard assessment, worker exposure, user exposure, and life-cycle assessment.

The Joint Research Centre (JRC) has developed a Methodological Guidance document to facilitate SSbD implementation, addressing common challenges faced by users [3]. However, stakeholders have highlighted data availability as a significant challenge in adopting the framework, as discussed in several workshops organized by EU projects IRISS [4] and PARC [5].

These two projects aim to engage industry stakeholders to identify critical data, tools, and training needs. The PARC project, in particular, has been developing a computational toolbox aligned with sustainable engineering objectives, supporting:

1. Predicting chemical properties and behaviors.
2. Defining material specifications for optimal efficiency, safety, and minimal environmental impact.

This study underscores the role of sustainable engineering systems in facilitating broader adoption of the SSbD framework within the EU and globally. Furthermore, the role is addressed of the SusChem Technology Platform, founded in 2004 as a response of EU (Bio)Chemical Industry and Professionals to the encouragement of Horizon2020, in enhancing the interaction between sustainable engineering and SSbD. As the European Technology Platform for Sustainable Chemistry, SusChem ETP along with its National Technology Platform Network foster collaboration among industry, academia, policymakers, and society to drive sustainable innovation in processes and products [6].

Through training programs and dissemination efforts, SusChem promotes a shared vision for sustainable chemical production, supporting industry leaders, SMEs, and policymakers. SMEs, as key drivers of future innovation, require targeted support to ensure feasibility and sustainability in adopting SSbD principles.

Strengthening sustainable supply chains and fostering collaborative networks will be crucial for a competitive and sustainable future in chemical production.

References

1. Rosen M., Engineering Sustainability: A Technical Approach to Sustainability; Sustainability 2012, 4, 2270-2292;
2. Glavic, P. Updated Principles of Sustainable Engineering. Processes 2022, 10, 870
3. Caldeira, C., et al.; doi:10.2760/487955, JRC128591
4. https://iriss-ssbd.eu/
5. https://www.eu-parc.eu/
6. https://suschem-gr.org/

Laccase-mediated lignin depolymerisation using flow chemistry principles

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Keywords: polysaccharides, polyphenols, borax, hydrogels, characterisation

Abstract

Lignin represents the most abundant aromatic biopolymer on earth; it exhibits a great potential to replace oil-based products. The molecular structure of lignin is complex, and depends on the botanical species and the employed fractionation process. The depolymerization of lignin can be a promising first and fundamental step towards valorization. The potential of ligninolytic enzymes such as laccases and peroxidases has been extensively investigated for this purpose. By generating phenoxy radical species from phenolic endgroups, they can induce oxidative coupling, leading to lignin depolymerization, and lignin oxidation at the C-α position in the β-O-4' bonding of terminal phenolic units. Flow chemistry and continuous processing, initially developed in the context of synthetic chemistry, offers superior control of reaction conditions, mixing, , and potential automation, etc. The combination of these two research fields, i.e., the use of enzymes as biocatalysts for lignin depolymerisation and flow chemistryallows for the development of more efficient and environmentally friendly biocatalytic processes in the biorefinery area.

Aim of our research was the development of a continuous flow process for the biocatalytic conversion of lignins using laccase immobilized laccase (EC.1.10.3.2) in combination with a mediator. Immobilised laccase and the lignin were packed in column reactors, with the lignin being followed by a pad of celite. The mediator was dissolved in the aqueous buffer system circulating in the reactor set-up. Products of the continuous flow reactor set-up were analyzed using state-of-the-art techniques in the field of polyphenol research: the laccase-mediator oxidation in continuous flow generated various monomeric compounds from the, in the aqueous phase insoluble lignin, such as vanillin, 4-hydroxy benzaldehyde, and 4'-hydroxy acetophenone. Repolymerisation is suppressed using the advantages offered by the continuous processing.

Valorisation of residual microalgal biomass in broiler feed

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Keywords: Broiler, Chlorella vulgaris, feed additive, protein source, digestibility

Abstract

Microalgae are emerging as a valuable production system for high-quality compounds in various sectors, including chemical and pharmaceutical industries. Within a bio-circular and zero-waste approach, the residual biomass remaining after extraction of high-value components can be repurposed, such as for animal feed. Microalgae offer both nutritional and health benefits, as they are rich in proteins, lipids, and bioactive compounds, including polyunsaturated fatty acids (PUFAs) and antioxidants like phenolics, flavonoids, and carotenoids. This research is conducted within the framework of the GeneBEcon project.

Our first study evaluated the potential of microalgal biomass as a health-promoting feed additive. Pulsed electric field (PEF) treatment of Chlorella vulgaris achieved up to 80% cell disruption efficiency, improving digestibility, particularly for autotrophic C. vulgaris. Digestibility trials showed that PEF-treated algae were more digestible than untreated cells. However, the feed digestibility of crude protein, fat, and ash did not differ significantly between feeds supplemented with processed and non-processed algae.

In another study, broilers received diets containing 2% C. vulgaris (both autotrophic and heterotrophic) under a coccidiosis challenge. The inclusion had minimal impact on growth performance, health, and meat quality. No significant differences were observed in feed intake, daily gain, or feed conversion ratio, although a slight trend suggested reduced feed efficiency with algae supplementation. Welfare assessments indicated slight improvements in litter quality and footpad condition in broilers fed heterotrophic algae. However, ovotransferrin levels suggested a potential increase in gut leakage, while antioxidant capacity in the blood was enhanced with heterotrophic algae. No significant differences in intestinal morphology were observed. Meat quality analyses revealed that heterotrophic algae-fed broilers had darker, redder, and more yellow breast meat, likely due to pigment absorption, but also exhibited more cases of wooden breast and white striping. Overall, while C. vulgaris had slight effects on welfare and meat quality, its impact on performance was negligible, and no major health effects were observed.

A subsequent study investigated the digestibility of autotrophic C. vulgaris as a protein source, comparing non-processed and PEF-treated algae at inclusion levels up to 20%. Higher inclusion levels negatively affected the digestibility of crude protein, crude fat, gross energy, and crude ash. However, PEF processing mitigated these effects, leading to a less steep decline in digestibility. Based on these findings, inclusion levels should not exceed 10% to prevent substantial reductions in nutrient digestibility. Even at this level, digestibility of crude ash and crude protein remained lower compared to soybean meal, even when using PEF-treated algae.

The trials conducted so far indicate that C. vulgaris has potential as a protein source, but inclusion should remain below 10% due to its impact on digestibility. Further research is needed to optimize processing and formulation techniques. As a feed additive, low inclusion levels appear feasible, as they do not significantly impact performance or health. This suggests that residual biomass could be incorporated into poultry diets in limited amounts without adverse effects.

An LCA-based evaluation of 'Green' Seaweed-based Bioplastic Production

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Keywords: LCA, macroalgae, sustainable production, bioplastic

Abstract

Plastic waste is a growing environmental concern in recent years. The emergence of bioplastics is proposed as an alternative to fossil-based plastics, offering an attractive solution to the plastic pollution problem[1]. They have the beneficial material characteristics of petrochemical plastics while giving the field for a transition towards circular economy practices, reducing fossil resources depletion and potentially reducing environmental burdens at their end of life[2]. Under this concept, a product from Blue Economy has emerged; seaweed-based bioplastic. Macroalgae, or more commonly seaweed, can replace terrestrial biomass feedstocks in biorefineries, to produce sustainable bioenergy, high-value products, and biomaterials[3]. In addition, unlike terrestrial crops, seaweed does not require arable land or fresh water and has the potential to sequester carbon and nutrients, reducing emissions and eutrophication in marine waters while providing a natural habitat for marine organisms[4].

Seaweed-based bioplastics have the potential to improve the bioplastics market and contribute to the blue economy, but challenges remain as production methods are still in their "infancy" and further research is needed to scale them up from low TRL levels to industrial TRL levels[5]. This study aims to perform an LCA to compare green production methods of seaweed-based bioplastics quantitatively.

This study builds on an earlier review of green production methods, which compared them qualitatively[6]. Listed methods, along with their sources, are utilized to perform a life cycle assessment of the production methods and assess the impact of the final products, used for the production of bioplastic films. Seaweed species can be divided into 3 general categories, brown, green, and red, each of which produces different products due to the different polysaccharides they are composed of. The functional unit was defined as "production of 1 kg of bioplastic film". From the review, a total of 6 production methods were selected for further investigation employing LCA. Due to data limitations, the life cycle was examined from a gate-to-gate perspective. Input-output data were retrieved from the sources contained within, which were mainly derived from lab-scale experiments rather than pilot-scale applications. Therefore, it was necessary to upscale these data to produce the required amount of biopolymer used to produce 1 kg of bioplastic. Special interest and focus has been given to the enzyme-assisted extraction methods among the 6 methods. Regarding impact assessment methodology, ReCiPe2016 was used to assess impact across 18 midpoint and 3 endpoint categories. The results of the preliminary analysis of the 6 green production methods showcase advantages such as reduced solvent requirements, lower energy consumption, and improved extraction yields compared to conventional chemical extraction methods. Especially enzyme-assisted extraction methods have the advantage of high extraction yields, sustainability and high chemical selectivity. Although, several challenges remain for these technologies compared to conventional methods because of high equipment costs, long processing times and expensive enzyme costs[6]. Another concerning issue is the seasonal variation of macroalgae composition. Environmental assessment of these production methods through LCA will provide clearer guidance for industries and researchers seeking to prioritize sustainable bioplastic production technologies and advance the scale-up of seaweed-based bioplastics.

References

1. D. Ita-Nagy, I. Vázquez-Rowe, R. Kahhat, G. Chinga-Carrasco, and I. Quispe, "Reviewing environmental life cycle impacts of biobased polymers: current trends and methodological challenges," The International Journal of Life Cycle Assessment, vol. 25, no. 11, pp. 2169–2189, Oct. 2020, doi: 10.1007/s11367-020-01829-2
2. G. Bishop, D. Styles, and P. N. L. Lens, "Environmental performance comparison of bioplastics and petrochemical plastics: A review of life cycle assessment (LCA) methodological decisions," Resources Conservation and Recycling, vol. 168, p. 105451, Feb. 2021, doi: 10.1016/j.resconrec.2021.105451
3. A. Pantis, C. Nikoloudakis, and T. Tsoutsos, "A Critical Review of Macroalgae Exploitation Pathways Implemented under the Scope of Life Cycle Assessment," ChemEngineering, vol. 8, no. 4, p. 74, Jul. 2024, doi: 10.3390/chemengineering8040074
4. M. Ayala, N. Goosen, L. Michalak, M. Thomsen, and M. Pizzol, "Prospective LCA of brown seaweed-based bioplastic: Upscaling from pilot to industrial scale," Sustainable Production and Consumption, vol. 52, pp. 416–426, Nov. 2024, doi: 10.1016/j.spc.2024.11.020
5. M. Ayala, M. Thomsen, and M. Pizzol, "Life Cycle Assessment of pilot scale production of seaweed-based bioplastic," Algal Research, vol. 71, p. 103036, Mar. 2023, doi: 10.1016/j.algal.2023.103036
6. C. Lim, S. Yusoff, C. G. Ng, P. E. Lim, and Y. C. Ching, "Bioplastic made from seaweed polysaccharides with green production methods," Journal of Environmental Chemical Engineering, vol. 9, no. 5, p. 105895, Jun. 2021, doi: 10.1016/j.jece.2021.105895

Preparation of biohybrid organic-inorganic from modified ZrO2 nanocrystals and alginate biopolymer

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Keywords: Nanocomposite, polymer, nanoparticles, cross-linking, hydrogel

Abstract

Hybrid materials represent a class of materials with diverse applications, ranging from biomedical fields to engineering solutions. Their unique properties and functionalities arise from their molecular structure, composition, and intermolecular interactions with surrounding media. By combining nanoparticle interface effects with polymer gel structures through chemical crosslinking, it is possible to enhance their properties or introduce additional functionalities, such as altering rheological and filtration characteristics. This work aims to develop a nanocomposite hydrogel using sodium alginate biopolymer and surface-modified zirconia nanocrystals (NCs). The ligand exchange procedure was employed to modify ~4 nm ZrO_2 NCs with amino groups using APTES, rendering them colloidally stable in acidic aqueous solutions, electrically charged, and chemically reactive.

This study investigates both chemical crosslinking reactions, facilitated by the EDC/NHS coupling agent, and physical crosslinking through electrostatic interactions between the biopolymer and the nanocrystals. Various reagent concentrations and pH values were explored to optimize nanocomposite formation and synthesis conditions. The modified nanocrystals were characterized using XRD and TEM to analyze the inorganic core, while FTIR spectroscopy confirmed the success of the ligand exchange procedure. Elemental analysis and thermogravimetry were conducted to quantify the number of amino groups on the modified ZrO_2 NCs, enabling a rational approach to reaction conditions with carboxyl groups from alginate.Particle size distribution analysis using DLS revealed that ZrO_2@APTES is well-dispersed at pH values below 7, with sizes around to 15 nm. When mixed with alginate, the particle size distribution exhibited three major peaks: 48.9 nm (19% volume), 1050 nm (5% volume), and 5590 nm (76% volume). For chemically crosslinked nanocomposites using a low amount of coupling agent, a dual peak size distribution was observed, with peaks at 90.6 nm (53% volume) and 602 nm (47% volume). Increasing the amount of coupling agent resulted in three peak distributions: 88 nm (7.0% volume), 820 nm (13% volume), and 5130 nm (80% volume).Further analysis is required to investigate the chemical reaction yield and other characteristics to determine the extent of the reaction and the behavior of the nanocomposite.

We conclude that the optimal pH range for chemical crosslinking is between 6.5 and 7.5. Additionally, a high number of amino groups on the modified nanocrystals can cause alginate aggregation before synthesis. Moreover, electrostatic interactions increase the size of the aggregated nanocomposite, which must be minimized to improve the coupling reaction yield. This work paves the way for the development of advanced engineering materials that require tailored surface charges and polymeric structures.

Production of Recombinant Cellulase Enzyme from Engineered Penicillium funiculosum for Efficient Biomass Hydrolysis

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Keywords: Cellulase, Biomass hydrolysis, β-glucosidase, Second-generation biofuels

Abstract
This study explores the production of recombinant cellulase enzymes using an engineered strain of Penicillium funiculosum, focusing on optimizing biomass hydrolysis for second-generation biofuel applications. The research employs media optimization to enhance cellulase and β-glucosidase enzyme production, leveraging modifications that exclude trace elements to mitigate inhibitory effects. Comparative fermentation analyses in a 20L bioreactor assessed the cellulose utilization dynamics and the enzymatic yield under varied conditions. The findings indicated significant improvements in enzyme activity, with the highest productivity observed in modified media formulations. The purification of β-glucosidase using a Ni-NTA system yielded high-purity enzymes with increased specific activity, suitable for synergistic applications with cellulase. Biomass hydrolysis trials using a cocktail of these enzymes demonstrated superior lignocellulose degradation efficiency and higher glucose release than commercial enzyme formulations. The optimized enzymatic cocktail exhibited resilience to inhibitory byproducts, enhancing the hydrolysis of pre-treated rice straw. This research contributes to cost-effective, scalable strategies for lignocellulosic biomass conversion by integrating process optimization with high-efficiency enzyme systems. These advancements support the development of sustainable biofuel production technologies, aligning with global energy security and environmental sustainability goals.

Harnessing Pseudomonas citronellolis 620C for Electro-Bioremediation: Insights from Transcriptional Kinetics and Metabolite Synergy in Microbial Fuel Cells

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Keywords: electro-bioremediation, transcriptional kinetics, metabolites, biofilm, microbial electrochemical technologies

Abstract

Microbial fuel cells (MFCs) harness the capabilities of electrochemically active microorganisms for bioremediation and electricity generation. While Geobacter sp. and Shewanella sp. have been extensively studied, Pseudomonas citronellolis 620C, a novel strain isolated in 2020 [1], has demonstrated remarkable electrochemical activity [2]. This strain not only produces significant bioelectricity but also efficiently degrades highly toxic oily wastewater, facilitated by biofilm formation and the production of the electron shuttle pyocyanin [2]. Moreover, it synthesizes biosurfactants (BSFs) [3], which enhance extracellular electron transfer (EET) and synergistically support biodegradation.

This study investigates P. citronellolis 620C in a dual-chamber MFC, focusing on BSF production, hydrocarbons and fatty acids degradation, and accumulation of other added-value products, such as polyhydroxyalkanoates (PHA). BSF production was confirmed through surface tension kinetics and GC-MS analysis [3], while PHAs and pyocyanin were identified using UV-Vis and GC/MS. Biodegradation efficiency was assessed via COD and GC/MS, alongside continuous bioelectricity monitoring. Transcriptional kinetics were also employed to monitor key metabolic processes, including hydrocarbons and fatty acids biodegradation; PHAs, BSF, pyocyanin and biofilm formation; quorum sensing; and metabolic shifts during starvation periods (feed interruption). The results demonstrated the rapid and simultaneous production of pyocyanin and lipopeptide BSF, the swift initiation of biodegradation, and the influence of PHAs, biofilm formation, and quorum sensing on electro-bioremediation. This study highlights the importance of understanding microbial behavior under MFC conditions, including the production of added-value metabolites and the role of transcriptional kinetics as biomarkers for mechanistic insights, paving the way for enhanced microbial electrochemical technologies (METs) that integrate bioremediation, bioelectricity generation, and valuable bioproduct synthesis.

Topic 5 - Biotechnology

Environmental Stewardship Using Evolving Concepts of Biodegradation, Synthetic Microbial Ecology and Bioengineering

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Keywords: Environmental bioengineering; Biodegradation; Microbial Consortia; Ecological Water Management

Abstract

A dominant aspect of environmental stewardship concerns the restoration of natural habitats, including water and soils, after many decades of accumulated pollution from toxic contaminants such as persistent organic pollutants released by mining, industrial, agricultural, and urban activities. Biotechnology provides concepts and tools for the effective clean-up of contaminated sites via microorganisms that can oxidize/reduce, bind, immobilize, volatilize, or transform contaminants. Despite the progress achieved by bioremediation, its application to clean up contaminated sites can be variable. Therefore, there is a need to critically reassess current concepts and assumptions for the estimation of biodegradation rates and extents. Furthermore, biotic (e.g., occurrence of specific degrader microorganisms) and abiotic factors (e.g., local transport limitations and transient conditions) may be useful in understanding the processes affecting biodegradation and in rationally intervening to enhance its application. Combining new subsurface oxidoreduction sensors with DNA and RNA sequencing-based microbiome analysis could help elucidate the processes of biostimulation in contaminated soils in relation to active microbial communities. Additional concepts from microbial physiology and molecular microbial ecology offer promise for the sustainable management of low-concentration contaminants such as micropollutants. Finally, through ecological bioengineering, a given microbial community, first natural and eventually synthetic, can be manipulated in engineered, open ecosystems and serve to generate rules for the future precision engineering of sustainable microbial waste management systems.

Fungal-assisted harvesting of the microalga Chlorella sorokiniana using the edible mushroom Pleurotus ostreatus

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Keywords: microalgae, pelletization, bio-flocculation, harvesting, digestate

Abstract
Harvesting microalgal biomass is a crucial step in its utilization, significantly impacting overall production costs. Various harvesting techniques, including centrifugation, flocculation, coagulation, filtration, and flotation, have been explored (Zhang et al., 2023). Among these, flocculation has emerged as the most efficient and cost-effective method (Luo et al., 2019). Different types of flocculants are widely used in this process, including inorganic flocculants such as aluminum sulfate, ferric chloride, and ferric sulfate, as well as organic alternatives like chitosan, cationic starches, modified tannins, and polyacrylamides. However, inorganic flocculants often negatively affect the quality of the harvested biomass, while organic flocculants require large quantities, making them economically unfeasible for full-scale applications.

A recent advancement in flocculation technology is the use of bio-flocculants. Microbially assisted flocculation, known as bio-flocculation, involves the use of bacteria, fungi, or their polymeric compounds and is commonly applied in wastewater treatment systems (Ummalyma et al., 2017). In this study, we investigated the harvesting efficiency of Chlorella sorokiniana using bio-flocculation with fungal pellets produced by the edible fungus Pleurotus ostreatus. Specifically, we examined the formation of fungal pellets under different cultivation times and pH conditions, as well as the effects of fungal pellet size, fungi-microalgae contact duration, and pH on the harvesting process. Additionally, the composition of the harvested microalgal-fungal biomass was analyzed.

The results showed that the highest harvesting efficiency (74%) was achieved at pH 4.5 using large fungal pellets (formed after 9 days) with an extended contact time of 24 hours. At pH 5.5, the highest efficiencies (68–69%) were observed with medium-sized fungal pellets (formed after 7 days) after 6 hours of contact time, or with small-sized fungal pellets (formed after 5 days) after 24 hours of contact time. The composition of the harvested biomass varied slightly between pH 4.5 and 5.5, with protein content ranging from 40–45%, carbohydrate content from 33–36%, and fatty acid content around 4–5%.

Overall, the use of fungal pellets produced by P. ostreatus presents a promising approach for harvesting fungal-algal biomass, with potential applications in food and animal feed production

References
1. Luo S, Wu X, Jiang H, et al Edible fungi-assisted harvesting system for efficient microalgae bio-flocculation. Bioresource Technology, 2019, 282, 325–330.
2. Ummalyma SB, Gnansounou E, Sukumaran RK, et al. Bioflocculation: An alternative strategy for harvesting of microalgae – An overview. Bioresource Technology, 2017, 242, 227–235.
3. Zhang J, Li Y, Shao E, et al. Feasibility and constraints of edible fungi bio-flocculating microalgae. Algal Research, 2023, 70, 103004.

Designing Complexity: Methodological Challenges in Engineering Hybrid Bioactive Compounds through Synthetic and Systems Biology

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Keywords: Databases integration, Cheminformatics, Systems Biology, Synthetic Biology.

Abstract
Efforts to design hybrid bioactive compounds—such as biosurfactants and siderophores tailored for industrial application—are increasingly framed within the broader promises of synthetic and systems biology. Yet, translating these interdisciplinary toolsets into reliable workflows has proven more complex than anticipated. While genome mining, metabolic modeling, and machine learning-based predictions offer a compelling blueprint for rational strain engineering, their implementation has revealed per-sistent technical and epistemological challenges that merit critical reflection.

One of the most significant, and perhaps underestimated, obstacles lies in the fragmentation of available data. Functional, structural, and genomic repositories often diverge in their formats, nomenclatures, and scope, impeding cross-referencing and integration. Public databases may differ not only in coverage but also in their handling of experimental metadata, such as phys-icochemical properties, strain origin, or biosynthetic context. In many cases, essential information remains buried within un-structured text across scattered literature. These discontinuities constrain the predictive capacity of computational models and complicate empirical reproducibility, particularly in early-stage retrosynthetic design.

A parallel source of complexity arises from the construction of quantitative structure-activity/property relationship (QSA(P)R) models. These are frequently invoked as a means of inferring molecular functionality—e.g., surface activity or metal-binding potential—based solely on structure. However, in the context of complex natural products, the paucity of experimentally validated data introduces a high degree of uncertainty. Models trained on limited or chemically narrow datasets are susceptible to overfit-ting and may struggle to generalize beyond familiar scaffolds, raising concerns about their reliability in exploratory design con-texts.

Metabolic retrosynthesis compounds these challenges. While progress has been made in reaction rule mining and scaffold de-composition, defining the boundaries between core and accessory genes within biosynthetic gene clusters (BGCs) remains an open question. Accessory elements, often overlooked or ambiguously annotated, are precisely those that drive the functional variability sought in engineered compounds. Several strategies have been proposed to distinguish these, including ribosomal flow models and comparative genomic context, though their integration into automated design platforms is still at an early stage.

Meanwhile, the pace of genome sequencing has far outstripped our capacity for interpretive analysis. Although newer machine learning approaches show promise in identifying cryptic or non-canonical BGCs, they raise concerns regarding interpretability and validation. Tensions persist between rule-based detection tools—such as AntiSMASH—and more recent data-driven frameworks. Reconciling these outputs and understanding their respective biases is critical for reliable genome mining.

This presentation will reflect on strategies adopted to navigate these layered challenges, drawing from a multidisciplinary effort aimed at designing novel microbial amphiphilic molecules. Rather than offering a linear success narrative, the discussion will highlight the interplay between algorithmic inference and experimental validation, emphasizing the need for flexible, iterative methodologies. Ultimately, advancing the rational design of complex bioactive molecules will depend not only on technological sophistication but also on how the field conceptualizes and manages biological complexity itself.

Computational models of metabolism as digital shadows of cell factory performance

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Keywords: Metabolic model; constraint-based; computational metabolic engineering; systems biology

Abstract

When microbes act as cell factories in bioprocesses, there is value in knowing how their metabolic networks function during bioreactor cultivations. Technological challenges make it infeasible to get detailed direct measurements on intracellular metabolic fluxes, which render black box models considering in- and outflow from the bioreactor as the only possible strategy. Genome-scale constraint-based models of metabolism are able to describe the black box interior, but the complexity and size of the metabolic network render them unable to for high confident determination of intracellular fluxes. Instead, consideration of enzyme efficiencies and protein levels can provide realistic condition-specific constraints on the cellular capabilities, resulting in realistic and feasible estimation of internal flux distributions.

To address the challenge of available enzyme activity (kcat) measurements, we have developed a deep learning algorithm (DLKcat) that is able to predict kcat value, solely based on amino acid sequence and chemical structure of the substrate. When complemented with condition-specific proteomics data, these models are digital shadows of cell factories during bioreactor cultivation, yielding realistic intracellular flux distributions. One of the current challenges is to accommodate for the environmental, genetic and phenotypical heterogeneity encountered during bioreactor cultivations.

Development of a chemically defined culture medium for high-yield pDNA production in E. coli

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Keywords: Process design; plasmid DNA; high cell density; chemically defined medium; scale up

Abstract

The increasing prevalence of new modalities that rely on high quality plasmid DNA (pDNA) for their manufacture, such as mRNA vaccines and cell therapies, has led to a substantial surge in pDNA demand. Traditional methods of pDNA production suffer from low yields and batch-to-batch variability[1]. The latter is primarily due to the use of rich culture media which contains microbial and/or animal derived ingredients. Chemically defined synthetic culture media can significantly improve reproducibility[2], reduce manufacturing costs[3] and ensure compliance within a dynamically evolving regulatory landscape due to the volume of new therapies receiving regulatory approval. However, the development of such a medium is non-trivial due to the underlying complexity of the biological process that can vary due to plasmid size[4], plasmid design[5], culture mode[5] and host organism[4].

Herein, we experimentally explore this complex process design landscape following a formalized experimental design approach. The aim is twofold: (i) to determine the effect of different media components, including carbon source and the C/N ratio, and (ii) to identify the impact of plasmid size, culture mode and host cell selection on pDNA titre and quality. Initial screening experiments were conducted in microwell plates and Erlenmeyer flasks. Successive design of experiments (DoE) rounds were conducted in Erlenmeyer flasks, while the final optimization round was conducted in a 3.7L benchtop bioreactor. Optical density, dry cell weight, pDNA concentration and percentage of supercoiled pDNA were measured hourly in triplicate. The performance of the final optimized medium formulation was evaluated across 2 different cell lines, 2 different transformation methods (electroporation and chemical transformation) and 3 different plasmid sizes (ranging from 2.7 to 13.8 kbp). Ongoing research aims to extend these findings by evaluating how switching to a continuous cultivation mode might further impact pDNA production efficiency.

References

1. Kopp, J., Slouka, C., Spadiut, O. and Herwig, C. (2019). The Rocky Road From Fed-Batch to Continuous Processing With E. coli. Frontiers in Bioengineering and Biotechnology, 7. doi:https://doi.org/10.3389/fbioe.2019.00328.
2. Gąciarz, A., Khatri, N.K., Velez-Suberbie, M.L., Saaranen, M.J., Uchida, Y., Keshavarz-Moore, E. and Ruddock, L.W. (2017). Efficient soluble expression of disulfide bonded proteins in the cytoplasm of Escherichia coli in fed-batch fermentations on chemically defined minimal media. Microbial Cell Factories, 16(1). doi:https://doi.org/10.1186/s12934-017-0721-x.
3. Rozkov, A., Larsson, B., Björnestedt, R., Strömberg, P., Lindqvist, F. and Schweikart, F. (2006). Cost-effective production of labeled recombinant proteins in E. coli using minimal medium. Microbial Cell Factories, 5(Suppl 1), p.P44. doi:https://doi.org/10.1186/1475-2859-5-s1-p44.
4. Yau, S.Y., Keshavarz-Moore, E. and Ward, J. (2008). Host strain influences on supercoiled plasmid DNA production in Escherichia coli: Implications for efficient design of large-scale processes. Biotechnology and Bioengineering, 101(3), pp.529–544. doi:https://doi.org/10.1002/bit.21915.
5. Islas-Lugo, F., Vega-Estrada, J., Alvis, C.A., Ortega-López, J. and del Carmen Montes-Horcasitas, M. (2016). Developing strategies to increase plasmid DNA production in Escherichia coli DH5α using batch culture. Journal of Biotechnology, 233, pp.66–73. doi:https://doi.org/10.1016/j.jbiotec.2016.06.025.

Using computations to analyze and reshape metabolism for bioproduction

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Keywords: metabolism, bioproduction, retrosynthesis, machine learning, protein design

Abstract

Metabolism is defined as the full complement of chemical transformations in living systems. Our group has previously introduced a variety of computational tools (i.e., OptKnock, OptForce) for shaping host native metabolism towards various overproduction goals. However, in many cases the native metabolic repertoire needs to be expanded upon. To support this goal, we will discuss computational tools for constructing thermodynamically feasible, carbon and energy efficient synthesis pathways. Protein engineering, either through de novo design or directed evolution, can expand upon the parts-list available for constructing pathways by re-designing existing enzymes to carry out novel conversions. Leveraging these capabilities, we have developed retrosynthesis tools which allow for seamlessly blending known biochemical reactions with de novo steps to construct atom and energy balanced synthesis pathways. Machine learning methods will be introduced for predicting novel enzymes' kinetics coupled with the deployment of kinetic models with a genome-wide coverage for assessing the efficacy of identified designs. Insight and lessons gained from the application of these tools on a variety of bioproduction challenges as members of the bioenergy centers CBI and CABBI as well as the NSF AI retrosynthesis institute MMLI will be provided.

Optimizing Hyaluronic Acid Production in Recombinant Pichia pastoris: A Metabolic Flux Analysis Approach

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Keywords: Hyaluronic acid; recombinant Pichia pastoris; Flux balance analysis; Metabolic flux analysis; Culture medium optimization

Abstract
Hyaluronic acid (HA) is a common glycosaminoglycan that can consist of several thousand units. Units of this biopolymer consist of two parts: UDP-glucuronic acid (UDP-GlcA) and N-Acetyl-D-glucosamine (UDP-GlcNAc), which are expressed at a concentration and molecular weight (MW) that varies in different tissues. It is vital for various physiological functions in the body and has wide applications in the medical and pharmaceutical industries. HA can be extracted from vertebrate tissues. Rooster combs and human umbilical cords are some of the richest sources of HA. However, due to high expenses, potential risk of viruses, low yields, and low-scale production of animal-derived products, synthesizing with bacteria is preferred over extracting it from animals. However, some bacteria are pathogenic, which reduces safety. Additionally, the low flux rate of HA remains a major challenge. This study aims to optimize the production of HA in recombinant Pichia pastoris using flux balance analysis (FBA). We used the iMT1026 genome-scale metabolic model containing 2240 reactions and 1708 unique metabolites with added HA synthesis genes hasA and hasB. iMT1026 is superior because of more annotated genes. Then, we simulated various culture conditions to maximize HA yield. The model for predicting HA production flux rate was first validated with experimental HA production data from the literature. Adding effective amino acids to Pichia pastoris medium could enhance the HA production flux rate. This study showed that glutamine was the most effective simulated amino acid in HA production pathway. Furthermore, the effects of co-utilization of methanol and glycerol with glucose in the induction phase were investigated. The effects of glycerol feeding rate were also investigated, demonstrating that a mixed feeding strategy of glycerol with methanol can increase the HA expression flux rate. These findings have practical implications for optimizing HA production processes, potentially leading to increased productivity and cost-effectiveness.

Co-Electron Donors Regulate the Patterns of Short and Medium Chain Carboxylic Acids Production by Mixed Culture: Competition Between Electron Donors and Acceptors.

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Keywords: Microbial Chain Elongation; Medium Chain Carboxylic Acids; Acidogenic Fermentation; Electron Donor.

Abstract

Chain elongation is an innovative biological technology that offers an environmentally sustainable method for converting organic waste materials into medium-chain carboxylic acids (MCCAs). Among the produced MCCAs, caproic (C6), enanthic (C7), and caprylic acid (C8) hold particular significance due to their various market uses. In addition to being utilized in biofuel production, the versatility of MCCAs spans multiple sectors, such as pharmaceuticals, food and beverage, and cosmetics. The central mechanism of this process is the reverse-β oxidation that produces MCCAs. In this process, ethanol and lactate act as electron donors, while the fermentation broth rich in fatty acids derived from organic waste serves as the electron acceptor.

Ethanol and lactic acid have been recognised as effective electron donors in the process of chain elongation, leading to the production of MCCAs, such as caproic acid and caprylic acid. Ethanol is oxidised to generate acetaldehyde, which is then converted into acetyl-CoA, with roughly 5/6 of its being involved in reverse β-oxidation. Lactic acid is partially oxidised to yield pyruvate, which further transforms into acetyl-CoA while releasing CO2. Additionally, some of the acetyl-CoA also participates in reverse β-oxidation. Moreover, a fraction of the lactate is converted into propionate, employing lactyl-CoA, acrylic-CoA, and propionyl-CoA as intermediate compounds. To date, the majority of research has concentrated on employing single electron donors, such as ethanol, methanol, or lactic acid, for the production of MCCA.

This study focused on the production of short-chain carboxylic acids (SCCA) and MCCA through the fermentation of brewery spent grains (BSG) using a mixed microbial culture. The study aimed to assess the impact of varying ratios of co-electron donors, specifically ethanol and lactic acid, at concentrations of 1:1, 2:1, 3:1, 1:3, and 1:2. Additionally, the study explored the interactions—both synergistic and competitive—between the two electron donors and their effects on the production of SCCA and MCCA by the mixed culture. Co-electron donor supplementation significantly enhances the production of MCCAs, particularly when utilised at a ratio of 2:1. Under a 1:1 electron donor ratio, the production of acetic and butyric acids was higher; however, MCCA production was limited to caproic acid. In contrast, at the 2:1 ratio, there was an increased production of butyric and valeric acids, with all MCCAs produced exceeding 2 g/L. Specifically, the production levels reached 4.5 gCOD/L for caproic acid, followed by 3.1 gCOD/L for valeric acid and 2.7 gCOD/L for hexanoic acid. The experimental results indicate that while a single electron can effectively lead to the production of chain-elongated MCCA, the presence of multiple electron donors in the fermenting medium is essential for achieving improved and targeted MCCA in mixed cultures that utilise waste as feedstock. Additionally, this study will investigate the microbial diversity within the mixed culture to identify the dominant and key producers of SCCA and MCCAs under various experimental conditions.

Zoom in the biosystem to elucidate the missing mechanistic insights in the electro-bioremediation of contaminated waters

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Keywords: Wastewater treatment, Genes of electro-assisted biodegradation, Enzymes of electro-assisted biodegradation, Metabolites of electro-assisted biodegradation, Extracellular electron transfer genetic mechanisms

Abstract

Electro-bioremediation of contaminated waters has been validated as a proof of concept at the technology readiness level (TRL) of 3, with specific cases where the technology has progressed to TRL 5 (Technology validated in relevant environment). The use of mixed cultures in electro-bioremediation is beneficial, but it hinders the evaluation of gene regulation, and enzymatic and protein steps involved in the process. For instance, although biodegradation of pollutants may result in electron transfer events, the enzymatic steps of pollutant biodegradation are typically unidentified. Furthermore, even though extracellular electron transfer takes place, the metabolic pathways involved are still unknown. This information can only take place by studying pure cultures of microorganisms at micro-scale level. Following this step, the knowledge can be transferred to the microbial community leading to better understanding of the microbial interactions and the metabolic pathways involved in electro-biodegradation of pollutants.

This presentation will review the studies performed with pure cultures, in the bio-electrochemical degradation of several pollutants, including of nitrogenous, phosphorous, and sulphurous compounds, hydrocarbons, metals, and azo dyes. This will be crucial to define the rate limiting steps in these processes, and start developing strategies to improve this technology towards their practical implementation.

Among the six major categories of pollutants studied, only 40 studies have been performed with pure cultures, including studies where the dominant genus/species in a mixed culture have been identified. Among them, only a few describe the genes, enzymes, proteins and metabolites involved in the electro-assisted biodegradation of these exemplary water pollutants. This presentation acknowledges this gap in knowledge in microbial electrochemical technologies (METs) used for electro-bioremediation, opening new perspectives and strategies to increase its TRL. In addition, strategies towards this direction are suggested such as next generation sequencing, omics techniques and molecular biology. Specific steps are suggested towards optimization including mathematical modelling and synthetic biology.

We believe that only through understanding of the metabolic capabilities of the biodegraders and electroactive microorganisms, these technologies will be advanced and become sustainable.

Flux Balance Analysis with Plasmid Integration (FBApi): A novel algorithm to quantify the metabolic burden associated with plasmid replication and expression

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Keywords: Flux Balance Analysis, Design Space Identification, Plasmid, Recombinant Expression, PCA

Abstract

Detailed understanding of plasmid-host physiological interactions and recombinant protein expression is crucial for the design of multiple biotechnological applications. The integration of plasmids carrying exogenous DNA inside a host-cell organism incurs a 'metabolic burden' due to the metabolic costs required for plasmid replication and recombinant protein expression. The extent of this response is both host-cell and plasmid dependent[1] and usually involves a quantifiable reduction in cellular specific growth rate[1], increased metabolic resource cycling (ATP/ADP, NAD/NADH, NADP/NADPH)[1] and in some cases even modification of nutrient uptake and metabolite secretion rates[1,2]. This results in a Pareto-like balance between plasmid efficiency (expression & replication) and cellular growth that is non-trivial to navigate during process development.

Herein we present a novel computational algorithm based on Flux Balance Analysis (FBA), that can account for the metabolic burden associated with the integration of plasmids in host-cells as a function of plasmid copy number, plasmid size and recombinant gene expression efficiency. The aim is to provide a computational tool to assist the decision-making process during plasmid design and cell-line development. Initially, FASTA files for the plasmid and any included recombinant proteins are parsed to derive the resource costs in terms of required nucleotide and amino acid building blocks as well as in terms of energy (ATP/ADP) metabolites. Subsequently, bespoke stoichiometric reactions for the synthesis of the plasmid (if/when applicable), the selection marker protein (usually some form of Antibiotic Resistance) as well as any other recombinant protein are developed based on the required metabolic costs computed in the previous step. Finally, by employing the recently developed Design Space Identification (DSI)[3] method from Papathanasiou and coworkers, the effect of heterologous gene expression intensity and selected growth rate on the flexibility and robustness of the process operating window is quantified.

We compared the metabolic profiles of E. coli BL21 cells transformed with the pORI1 and pORI2 plasmids using FBApi. Since the expression level of the plasmid encoded genes and the heterologous protein fractional contribution to the biomass vary across different strains and organisms, we created multiple models that cover the range of these parameters.

The solution space of the resulting models was sampled using the Artificial Centering Hit and Run (ACHR) algorithm and the retrieved samples were anonymized and randomly scrambled to eliminate any potential bias. Principal Component Analysis (PCA) was then applied[4] to the mixed samples to identify whether any differences in metabolic configuration could be identified and whether said differences could be a factor of plasmid size. PCA was able to discriminate the metabolic states of the cells containing plasmids and to effectively select reactions/subsystems affected in the metabolic network.

The proposed algorithm was able to quantify the productivity of plasmids, mRNA, and recombinant proteins by considering their structural characteristics, such as size and nucleotide/amino acid sequences, along with the tradeoff between growth rate and plasmid-associated reactions. This makes it a robust and versatile tool well-suited for a wide range of biotechnological applications.

References

1. Heyland, J., Blank, L. M., & Schmid, A. (2011). *Quantification of metabolic limitations during recombinant protein production in Escherichia coli*. Journal of Biotechnology, 155(2), 178–184. https://doi.org/10.1016/j.jbiotec.2011.06.016
2. Gotsmy, M., Strobl, F., Weiß, F., Gruber, P., Kraus, B., Mairhofer, J., & Zanghellini, J. (2023). *Sulfate limitation increases specific plasmid DNA yield and productivity in E. coli fed-batch processes*. Microbial Cell Factories, 22, Article 242. https://doi.org/10.1186/s12934-023-02248-2
3. Sachio, S., Likozar, B., Kontoravdi, C., & Papathanasiou, M. M. (2024). *Computer-aided design space identification for screening of Protein A affinity chromatography resins*. Journal of Chromatography A, 1722, 464890. https://doi.org/10.1016/j.chroma.2024.464890
4. Luginsland, M., Kontoravdi, C., Racher, A., Jaques, C., & Kiparissides, A. (2024). *Elucidating lactate metabolism in industrial CHO cultures through the combined use of flux balance and principal component analyses*. Biochemical Engineering Journal, 202, 109184. https://doi.org/10.1016/j.bej.2023.109184

On the impact of plasmid size and transformation method on plasmid DNA productivity in Escherichia coli

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Keywords: *Escherichia coli*, pDNA production, transformation

Abstract

In recent years, the use of plasmid DNA (pDNA) in novel clinical applications, such as DNA/RNA-based vaccines, cancer therapies and/or gene therapies, has lead to a substantially increased demand for fast and efficient methods to produce large quantities of pDNA [1]. Regulatory authorities place strict requirements on pharmaceutical grade pDNA for clinical applications in terms of high product purity, stability and integrity [2]. The U.S. Federal Drug Administration (FDA) in particular recommends that plasmids used for clinical applications have >80% content in the supercoiled conformation to avoid mutations [2]. In order to meet the ever increasing demand for pharmaceutical grade pDNA, technological breakthroughs are required throughout the entire biomanufacturing process not only upstream and downstream but also in terms of host cell line development and plasmid design [3]. However, the availability of information surrounding the interplay between plasmid size (and design), host cell line and transformation methods for intensified pDNA manufacturing is currently limited [3].

Towards that end, we present herein a comprehensive comparison of two state-of-the-art *Escherichia coli* strains and their derivatives (DH5a and JM109), two transformation methods ($CaCl_2$/heatshock treatment and electroporation) and three plasmids of varying size. Specifically, the plasmids evaluated in the present study were: (i) mEGFP-N1 (4. 7 kb) which expresses the fluorescent protein EGFP, (ii) pcDNA3_SARS-CoV-Spike [SARS-CoV-2 RBD] (9.2 kb) which expresses the chimeric SARS-CoV spike with the SARS-CoV-2 receptor binding domain, and (iii) pCHMWS_eGFP_T2A_Fluc-IRES-Puro (13.8 kb) which is a lentiviral transfer plasmid expressing EGFP and luciferase proteins. DH5a strains (DSMZ, DSM 6897) were made chemically- and electro- competent with $CaCl_2$ and electroporation treatment respectively in house and compared against commercially available chemically (MAX Efficiency DH5a, Thermo Fisher Scientific, Cat. No. 18258012) and electro- competent (ElectroMAX Stbl4, Thermo Fisher Scientific, Cat. No. 11635018) strains. Both commercial and in-house chemically competent cells were transformed with the heat shock method to load each of the three plasmids. Similarly both commercial and in-house electro-competent cells were transformed via electroporation to load each of the three plasmids. Transformed cells as well as parental strains were grown in triplicate on Luria Bertani (LB) media in orbitally shaken Erlenmeyer flasks for up to 12 hours. Biomass concentration (via optical density measurements), pDNA productivity (via nanodrop) and pDNA quality (via agarose gel electrophoresis) were evaluated hourly throughout all cultures.

References

1. Nguyen, T. T., Bui, L. M., Byun, J. Y., Cho, B. K., & Kim, S. C. (2023). Exploring the Potential of a Genome-Reduced Escherichia coli Strain for Plasmid DNA Production. International journal of molecular sciences, 24(14), 11749.
2. Hassan, S., Keshavarz-Moore, E., & Ward, J. (2016). A cell engineering strategy to enhance supercoiled plasmid DNA production for gene therapy. Biotechnology and Bioengineering, 113(9), 2064–2071.
3. Selas Castiñeiras, T., Williams, S. G., Hitchcock, A. G., & Smith, D. C. (2018). E. coli strain engineering for the production of advanced biopharmaceutical products. FEMS microbiology letters, 365(15).

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