IChemE CAPE SIG Newsletter

COMPUTER AIDED PROCESS ENGINEERING

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INSIDE THIS ISSUE

WELCOME FROM THE CHAIR

Welcome to the Computer-Aided Process Engineering (CAPE) newsletter! As Chair of the Computer Aided Process Engineering (CAPE) Special Interest Group, I am delighted to welcome you to this edition of our newsletter, which focuses on a subject of critical importance: sustainability. In recent years, the intersection of process engineering and sustainability has evolved from being a niche concern to a defining priority for industries and researchers worldwide. Today, CAPE professionals play a pivotal role in driving sustainable innovation, enabling industries to reduce resource consumption, minimize waste, and transition to cleaner, greener systems.

Sustainability is not just an environmental imperative—it's an opportunity to reimagine how we design, optimize, and operate processes to achieve greater efficiency and resilience. From advancements in process modelling for renewable energy systems to the use of AI and machine learning for predictive maintenance and resource optimization, CAPE tools are at the heart of transformative solutions. These innovations empower industries to meet sustainability targets while remaining competitive in an increasingly resource-constrained world.

In this newsletter, you'll find insights into cutting-edge research, case studies, and emerging trends that highlight how CAPE is contributing to a more sustainable future. Whether you're working on carbon-neutral processes, circular economy strategies, or energy efficiency improvements, I hope this issue inspires you to continue pushing the boundaries of what is possible. Let us seize this moment to collaborate, innovate, and lead the way in addressing global sustainability challenges. Together, we can ensure that process engineering remains a driving force for positive change.

Sol Brown
Chair, IChemE CAPE SIG
University of Sheffield

HOT OFF THE PRESS:

A LOOK AT THE LATEST DEVELOPMENTS IN SUSTAINABLE PROCESS ENGINEERING

Witten By Bhavik Mehta

TOWARDS SUSTAINABLE CHEMICAL PROCESS DESIGN: REVISITING THE INTEGRATION OF LIFE CYCLE ASSESSMENT

This review explores the integration of Life-Cycle Assessment (LCA) into model-based chemical process design, emphasizing its importance for sustainability while identifying key gaps. Analysing 53 studies from over 100 articles, it presents 25 metrics to assess LCA integration. The findings reveal that most studies focus on cradle-to-gate phases (74%), neglecting use and end-of-life phases (89%) and rarely defining user functions (92%), limiting the potential for circular strategies and sufficiency measures. Environmental externalities are often excluded, with studies prioritizing economic factors like energy utilities (75%) and material inputs (70%), while emissions (26%) and waste (25%) are frequently overlooked. This narrow focus perpetuates conventional design assumptions and undermines deeper integration of LCA's core features. The review advocates for more comprehensive approaches, including user function perspectives, to enhance end-of-life considerations and support circular process designs. It also provides a classification of computational integrations to assist practitioners in overcoming current challenges in modelling, interpretation, and goal setting. Click here to read the full article.

NEW FRONTIERS IN SUSTAINABLE PROCESS ENGINEERING WITH ADDITIVE MANUFACTURING FOR CONTINUOUS-FLOW APPLICATIONS

The article explores the transformative impact of additive manufacturing (AM) on chemical reactor design, emphasizing its ability to address limitations of traditional manufacturing techniques. AM enables the creation of intricate geometries, such as periodic open cellular structures (POCS), that optimize fluid dynamics, heat transfer, and mass transfer, enhancing reactor efficiency and sustainability. Techniques like Fused Deposition Modelling (FDM), Direct Ink Writing (DIW), and Stereolithography (SLA) are reviewed for their unique benefits, including precision, scalability, and material compatibility. Applications span carbon capture, catalytic reactions, and continuous-flow systems, with 3D-printed structures improving adsorption efficiency, reducing pressure drop, and facilitating uniform reactant distribution. Key challenges include scaling up reactors for industrial use, ensuring material durability under harsh conditions, and addressing flow imbalances. The article underscores the potential of advanced designs, such as MSLA-based systems, to enhance catalytic activity and operational efficiency while lowering production costs. Prospects involve integrating artificial intelligence (AI) and machine learning (ML) to optimize reactor design and performance across diverse chemical processes, presenting opportunities for innovation in environmental and industrial applications. Click here to read the full article.

IMPACT OF 3D MODELLING BEHAVIOUR PATTERNS ON THE CREATIVITY OF SUSTAINABLE BUILDING DESIGN THROUGH PROCESS MINING

This study explores the application of process mining to analyse creativity-driven behaviour patterns in sustainable building design, addressing a gap in research within architecture, engineering, and construction (AEC) industries. Creativity is highlighted as a critical element for green innovation and sustainable development, particularly in the early design stages where computer-aided design (CAD) and building information modelling (BIM) dominate

workflows. Using over 41 million lines of event data from 115 participants in a green building design competition, the study examines four dimensions of creative design behaviour: frequently used commands, frequently used objects, command duration, and tool experience. Artificial neural network models were trained based on these dimensions to evaluate creativity levels in design outputs, demonstrating effective preliminary screening of creative behaviour in large datasets. The integration of process mining, a data-driven approach linking data and process science, is identified as a promising method for uncovering behavioural patterns in 3D modelling processes. This research contributes to the growing use of data-driven technologies in AEC industries, paving the way for innovative approaches to sustainable building design through the analysis of creative design processes. Click here to read the full article.

CHALLENGES AND OPPORTUNITIES FOR COMPUTER-AIDED MOLECULAR AND PROCESS DESIGN APPROACHES IN ADVANCING SUSTAINABLE PHARMACEUTICAL MANUFACTURING

The pharmaceutical industry faces challenges in balancing sustainability, efficiency, and cost while meeting stringent regulatory and safety standards. Current processes for developing new chemical entities (NCEs) generate significant waste, particularly from solvents, with environmental metrics like the E factor (waste per unit of product) showing poor performance compared to other chemical industries. Sustainability efforts must account for solvent impacts across the entire process, including downstream operations, as no solvent is universally "green." Life-cycle assessments (LCAs) and green chemistry principles are valuable but require context-sensitive application. Computer-aided molecular and process design (CAM(P)D) methodologies offer promising solutions by optimizing solvent selection, reaction conditions, and process configurations. These approaches enable integrated decision-making that considers molecular properties, process design, and sustainability metrics. Recent developments, such as model-based frameworks for solvent recycling and crystallization, highlight the potential for reducing waste and emissions while improving efficiency. However, advancing predictive models for critical properties like solubility, kinetics, and transport is necessary for broader adoption. Future directions include integrating process synthesis, route selection, and retrosynthesis into a comprehensive framework to optimize pharmaceutical processes holistically. Combining computational tools with experimental validation can support more sustainable and efficient pharmaceutical development. Click here to read the full article.

A MULTI-STAGE MACHINE LEARNING MODEL TO DESIGN A SUSTAINABLE-RESILIENT-DIGITALIZED PHARMACEUTICAL SUPPLY CHAIN

This study proposes a novel machine learning-based framework to design pharmaceutical supply chains (PSC) that integrate sustainability, resilience, and digitalization—dimensions often neglected in prior research. Motivated by challenges during the COVID-19 pandemic, the framework evaluates suppliers using a Random Forest Regressor (RFR) based on key indicators like delivery time, quality, cost, robustness, and backup availability. A mathematical model incorporating resilience and sustainability is optimized using Fuzzy Lexicographic Multi-Choice Archimedean-Chebyshev Goal Programming (FLMCACGP), with a blockchain-based platform selected for the Information-Sharing System (ISS). Tested on a real-world case study in Iran, the approach demonstrates significant advantages, including reduced environmental impact, improved transparency, and enhanced supply chain robustness during disruptions. The study outperforms traditional methods, highlighting the importance of integrating sustainability, digitalization, and resilience to create efficient, adaptable, and responsible PSCs. It provides actionable insights for optimizing PSCs to meet societal values, regulatory expectations, and the demand for sustainable healthcare systems. Click here to read the full article.

Witten By Manish Aggarwal

DECARBONISING THE SKIES:

THE PROMISE AND CHALLENGES OF SUSTAINABLE AVIATION FUEL

Sustainable Aviation Fuel (SAF) is emerging as a key solution in the aviation industry's pursuit of net-zero emissions by 2050. Capable of reducing lifecycle greenhouse gas emissions by up to 80% compared to conventional jet fuel, SAF offers a significant opportunity to decarbonise air travel [1-2]. However, its widespread adoption faces several barriers. SAF is considerably more expensive than traditional jet fuel due to the limited availability of sustainable feedstocks and the early-stage nature of production technologies. Regulatory constraints also pose limitations: current guidelines allow only a 50% blend of SAF with conventional jet fuel, highlighting the need for further research to support higher blend ratios without compromising safety or engine performance [3]

Blending SAF with traditional fuels is essential for integration into existing aviation infrastructure. As emphasised by the National Renewable Energy Laboratory (NREL) [4], SAF must conform to strict aviation standards and be fully compatible with current aircraft engines and fuel distribution systems. This ensures airlines can adopt SAF without major modifications to fleets or logistics. Beyond emissions reductions, SAF offers socio-economic benefits. It can drive rural economic development through the cultivation of energy crops and the establishment of biorefineries, thereby creating jobs and enhancing energy security. As global air travel demand continues to rise, scaling SAF production becomes critical to balancing growth with sustainability.

Machine learning (ML) is playing an increasingly transformative role in overcoming SAF's challenges. ML models can predict the physicochemical properties of biofuel blends, streamlining the identification of formulations that meet stringent aviation standards [5]. Additionally, ML-driven optimisation of production processes enhances efficiency and lowers costs by uncovering data-driven insights and recommending real-time process improvements.

In conclusion, while SAF presents a viable route to sustainable aviation, its future depends on addressing production, cost, and regulatory challenges. With the support of advanced technologies like machine learning, the path to a low-carbon aviation sector is increasingly within reach.

Feature

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COMMITTEE OVERVIEW

- Sol Brown (Chair)
- Maria Papathanasiou (Secretary)
- Malcolm Woodman (Treasurer)
- Michael Fairweather
- Michael Francis Benjamin
- John Lewis
- Rafael Ventura (Webinar Coordinator)
- Rahul Nabar
- Shoaib Kiyani (Learned Society Officer)
- James Sweeney
- Alberto Saccardo
- Chua Choon Hong (Chair Malaysia chapter)
- Tan Yin Ling
- Vasileios Charitopoulos
- Bhavik Mehta (Newsletter)
- Keeran Ward (Newsletter)
- Irene Chew
- Bishwjeet Binwal
- Sumit Gadwe
- Manish Aggarwal (Newsletter)
- Lazaros Papageorgiou

UPCOMING EVENTS

ESCAPE35 Conference
6-9th July 2025
Leuven, Belgium

The 35th European Symposium on Computer Aided Process Engineering (ESCAPE-35) will be held from July 6–9, 2025, at KU Leuven's Technology Campus Ghent, celebrating KU Leuven's 600th anniversary. Organized with the University of Liège, the conference theme, "Closing the Loop 2.0," focuses on leveraging Process Systems Engineering (PSE), AI, and quantum computing to accelerate progress towards a circular economy across energy, life sciences, and materials sectors. ESCAPE is part of a prestigious annual series supported by the European Federation of Chemical Engineering. For more information, click here.

Advances 2025-IChemE
16-17th October 2025
Manchester, UK

The Advances in Applied Digitalisation of the Process Industries – 2025 conference, hosted by IChemE, will take place on 16–17 October 2025 in Manchester, UK. It will explore how digital technologies like AI, data analytics, and digital twins are transforming process industries. Aimed at engineers, researchers, and technologists, the event will showcase real-world applications, best practices, and future developments to drive innovation, efficiency, and sustainability across sectors like chemicals, energy, and manufacturing. For more information, click here.

AIChE 2025 Annual Meeting
2-6th November 2025
Boston, USA

The 2025 AIChE Annual Meeting, set for November 2–6 in Boston, will bring together academics, researchers, and industry leaders to discuss advancements across chemical engineering fields. It will feature technical sessions, panels, and networking opportunities covering innovations in sustainability, materials, biotechnology, energy, and digitalization. Special focus areas include emerging technologies and interdisciplinary collaboration. The event provides a platform for presenting cutting-edge research and fostering professional growth in chemical engineering. For more information, click here.

NEWS FROM INDUSTRY: SUSTAINABILITY

REVOLUTIONIZING POLYESTER RECYCLING: TURNING TEXTILE WASTE INTO SUSTAINABLE FASHION

Reju, a European startup, has developed a chemical recycling process that transforms used polyester textiles back into high-quality polyester. Unlike traditional methods, Reju's technology employs a catalyst to break down polyester into its monomers at lower temperatures, reducing energy consumption and enabling a closed-loop system. This process addresses the challenges of recycling contaminated fabrics, such as those blended with cotton or containing dyes and additives. Reju's approach offers a scalable solution to the global polyester waste crisis, potentially revolutionizing textile recycling by producing clean, reusable polyester suitable for new garments. Click here to read the full article.

BP'S RECORD PROFITS PROMPT BACKLASH OVER SCALED-BACK EMISSIONS TARGETS

BP announced record annual profits of $27.7 billion for 2022, more than doubling its 2021 earnings, driven by soaring energy prices. However, the company also scaled back its climate targets, reducing its goal to cut oil and gas production by 2030 from 40% to 25%. This move has drawn criticism from environmental groups and political leaders, who argue that BP is prioritizing profits over climate action. In response, BP has committed to investing an additional $8 billion each in oil and gas and in the energy transition, aiming to balance current energy demands with future sustainability goals. Click here to read the full article.

ENAGÁS FAST-TRACKS €2.6 BILLION HYDROGEN NETWORK TO ACCELERATE EUROPE'S GREEN TRANSITION

Enagás, Spain's gas grid operator, is accelerating its 2,600 km hydrogen network project, aiming to commence operations by 2030. As part of the trans-European H2Med corridor, the initiative involves new pipelines and the repurposing of existing gas infrastructure, with an estimated investment of €2.6 billion. Enagás plans to make a final investment decision in 2027 and begin construction in 2028. This move aligns with Spain's green energy goals, leveraging its abundant solar and wind resources to position the country as a European leader in green hydrogen production. Enagás is diversifying from natural gas to hydrogen, ammonia, and CO_2 capture infrastructure. Click here to read the full article.

TOTALENERGIES AND SHELL SCALE BACK ARAMIS CCS INVESTMENT, DUTCH GOVERNMENT STEPS IN

The Dutch government has committed €639 million to support the Aramis carbon capture and storage (CCS) project after TotalEnergies and Shell withdrew from funding the necessary pipeline infrastructure. Despite this, both companies will continue to develop storage sites and provide related services. The Aramis project aims to store up to 22 million tons of CO_2 annually in depleted North Sea gas fields by 2030, contributing to the Netherlands' target of reducing emissions by 55% compared to 1990 levels. The final investment decision is expected in 2026. Click here to read the full article.

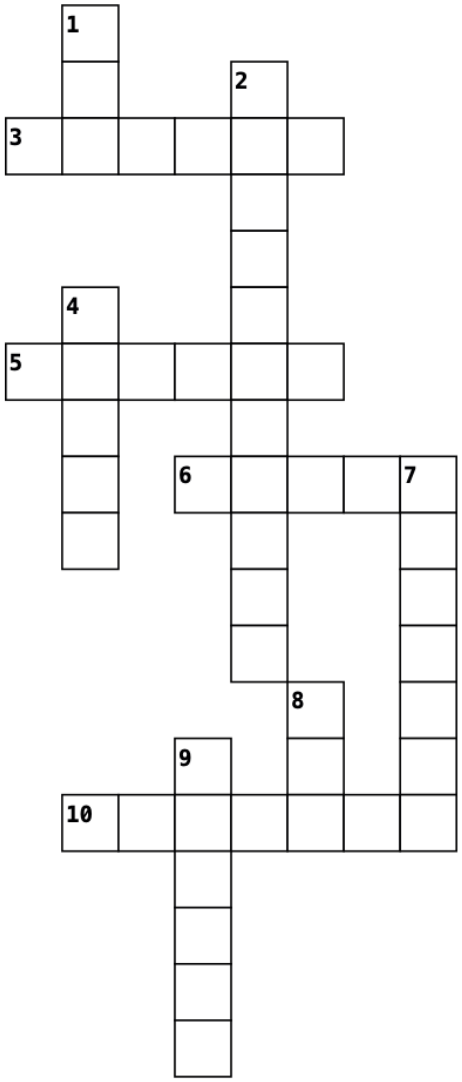
JINKOSOLAR SETS AMBITIOUS NET-ZERO TARGETS WITH SBTI VALIDATION

JinkoSolar, a leading Chinese photovoltaic manufacturer, has become the first in its sector to have its short-term, long-term, and net-zero emission reduction targets validated by the Science Based Targets initiative (SBTi). The company aims to achieve full adoption of renewable energy by 2030 and reduce emissions from purchased goods and services by 58.2% per megawatt of solar-related products produced by 2032. JinkoSolar is also working with its partners to reduce emissions throughout its value chain, embedding greenhouse gas emissions into supplier admission, management, and risk assessment processes to drive supply chain sustainability improvement for the renewable energy industry. Click here to read the full article.

NERD-OUT CROSSWORD

THIS ISSUE'S CROSSWORD IS ALL ABOUT SUSTAINABILITY IN CHEMICAL ENGINEERING

Use the guide below to answer terms used when discussing or assessing Sustainability in the context of Chemical Engineering.



ACROSS

[3] Another word for one of the ''spheres'' of Sustainability
[5] The term given to the start of a product life cycle
[6] The colour assigned to a clean, sustainable source or process
[10] A well-known LCA software

DOWN

[1] The Organisation that created the LCA standard
[2] A principle describing a cradle-to-cradle life cycle.
[4] The term given to the end of a product life cycle
[7] A national strategy that implies 0 carbon footprint
[8] A known LCA impact category linked to carbon footprint
[9] The consequence of the burden derived from a process

CROSSWORD ANSWERS KEY: 1- ISO; 2-CIRCULARITY; 3- DOMAIN; 4-GRAVE; 5-CRADLE; 6-GREEN; 7-NETZERO; 8- GWP; 9- IMPACT, 10-SIMAPRO