

Editorial

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Editorial: Perspectives of Chemicals Synthesis as a Green Alternative to Fossil Fuels

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Editorial on the Research Topic

Perspectives of Chemicals Synthesis as a Green Alternative to Fossil Fuels

Renewable energy sources and more efficient and integrated processes are needed to avoid resource depletion and climate change. The production of chemicals, fuels, and materials has to change from a primarily linear synthesis pathway to closed-loop alternatives based on circular economy approaches and rely on green and low carbon synthesis processes while supporting their economic competitiveness in the upcoming years. Green and low-carbon chemicals, fuels, and materials constitute the base for the transition towards a sustainable financial system. Important sectors that need to decrease their dependence on fossil fuels in terms of raw materials and energy consumption are, for instance, plastics, construction, packaging, textile, electronics, batteries, or transport.

Advance towards implementing novel circular approaches and green and low carbon processes urges to move towards techniques that eliminate waste, use renewable sources, or generate fewer emissions (are more efficient) than the overall benchmark processes. Process modeling and assessment stand as powerful tools to evaluate the economic characteristics (business cases) and the environmental benefit of the proposed options. Given the impressive advances in mathematical programming techniques during the last decades, a process systems engineering (PSE) approach is suitable for dealing with synthesis problems, systems analysis, and life cycle analysis (LCA). Besides, the significant advances achieved in solving enormous challenges, particularly for linear and mixed-integer linear programming techniques, offer unique possibilities to deal with this Research Topic.

The focus of this Research Topic is on chemicals, fuels, and materials synthesis processes; circular approaches, green, low carbon, and transitional solutions towards more environmentally friendly options. We look for Original Research, Review, or Mini-Review papers that discuss these issues. Themes of interest include, but are not limited to:

- Techno-economic and life cycle analyses of synthesis of green/low carbon chemicals, fuels, and materials;
- Evaluation, process design, and optimization of new synthesis pathways of chemicals, fuels, and materials;
- Analysis of the implementation of green/low carbon chemicals, fuels, and materials;
- Circular economy, carbon dioxide utilization, and electrochemistry for chemicals synthesis.

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In the following, you will find selected contributions (Original research, Perspectives, and Review) to this research topic. They bring novel solution approaches accompanied by rich case studies and examples of practical interest.

ORIGINAL RESEARCH

The articles in this Special Issue examine different facets of alternative fuels' synthesis from the point of view of fuels as an end product. Contribution by *Antonio Argüelles et al.* should be of interest to the petroleum industry, companies and researchers. It reports a lack of information about the environmental impacts of renewable diesel production. The authors conduct attributional life cycle assessment (LCA) of green diesel obtained by hydrodeoxygenation (HEFA). Results demonstrate that biofuel significantly reduces GHG emissions than its fossil counterpart by about 110%. Renewable diesel (RD) production by HEFA has lower emissions than conventional diesel in the following categories: acidification, ozone layer depletion, and photochemical smog, while in the human toxicity and eutrophication categories, it has a significant environmental impact. Whenever RD has poor cold flow properties, it becomes necessary to mix it with ULSD.

Pacheco-López et al. also analyze the implications of the different end products. They present a techno-economic and environmental comparison of existing liquid fuels and their emerging renewable substitutes from biomass or the chemical recycling of plastic waste. They find that plastic waste pyrolysis oil performs better than diesel in cost (25% reduction) and environmental impacts. Their study also includes assessing bioethanol and ethanol from plastic waste pyrolysis as an alternative to gasoline additives, showing higher costs and variable results regarding the life cycle impacts. Thus, they analyze the effect of these results on gasoline blends and conclude that blends with ethanol from plastic pyrolysis can reduce the impact on human health and ecosystems. In contrast, blends with bioethanol have a lower impact on resource scarcity and better economic profitability.

Conversely, some of the works focus on the processes. Biomass waste used as fuel essentially provides a circular approach, and the following four papers consider organic waste as raw material.

The contribution by *Castro-Amoedo et al.* analyzes different biomass transformation technologies. The authors present a systematic approach for designing, evaluating, and ranking biomass-to-X production strategies under uncertain market conditions. Their framework includes a bi-level mixed-integer linear programming formulation to identify and assess current and promising robustness and resilient designs strategies. After studying the integration of anaerobic digestion of food and green waste biomass in the current Swiss market, they stress energy integration and poly-generation as critical factors for the energy transition.

In a similar light, *Mahmud and Rosentrater* examine the particulars of biomass pretreatment methods. They test low moisture anhydrous ammonia pretreatment to overcome the drawbacks of standard pretreatment methods. Once subjecting Distillers Dried Grains with Solubles, corn gluten feed, corn fiber, and oil palm frond (OPF) with different moisture contents to this

pretreatment process, they find out a decreased lignin content of the materials, increased their percentage of α -cellulose, and improved enzymatic digestibility.

Shafinas and Rosentrater's article reveals the concern of food waste (FW) impacting the environment, societies, and economies, triggering research to find alternative ways to utilize such materials. FW may contain sugars (e.g., glucose) susceptible for conversion into value-added products such as highly demanded ethanol by industries like fuel, beverages, pharmaceuticals, and other industrial applications. To challenge the lower price of ethanol produced from corn, the authors propose an integrated system: a conventional fermentation plant integrated with a novel combined heat and power (CHP) system that reduces utility costs thanks to the recovery of energy from waste (FW). Using techno-economic analysis (TEA), the authors find it more economical and attractive at the commercial scale.

The energy transition needs alternative fuels, more efficient and integrated power plants. The following two papers use solid oxide cells as a technology that can use and provide renewable electricity in a highly efficient manner. From a plant system perspective, in the contribution by *Pérez-Fortes et al.*, the authors apply scenario analysis, and multi-objective optimization to the design of a pilot integrated biomass waste gasifier—solid oxide fuel cell (SOFC) plant. The results in the paper summarize the most optimal operating conditions and provide an optimal plant layout (with anode off-gas recirculation and hot gas cleaning units) and a heat exchanger network. Combined heat and power efficiency can go up to 82%.

From a broader system perspective, the article by *Carbone et al.* evaluates the use of organic waste to power a reversible solid oxide cell (rSOC) via gasification to support the electricity grid. The rSOC system operated in electrolysis mode uses excess renewable electricity to synthesize methane. On the other side, the rSOC system operated in fuel cell mode supplies power when needed by the grid by oxidizing syngas. The paper uses hourly real large-scale energy storage needs and biomass waste generation for the southern Italian peninsula in 2030. The methodology can be of use in other case studies (locations and technologies). For the current situation, the authors calculated the yearly used biomass waste and the yearly electricity storage and generation needs provided by the gasification-rSOC system.

The chemical industry and particularly energy-intensive industries like steel production have inherent CO₂ emissions. Industrial symbiosis, Circular, in essence, industrial symbiosis aims at using waste from an industrial process as feedstock for another one, thus reducing raw materials and resources needs. The article by *Collis et al.* evaluates the potential of using the three flue gases from conventional steel production (blast furnace gas, essential oxygen furnace gas, and coke oven gas, with different ranges of CO, CO₂, and H₂), currently used to produced internal heat and power, as raw material or fuel for other companies. One can extrapolate the applied methodology to other industrial plants and flue gases, and the results compare economic and environmental indicators of the proposed alternatives versus the benchmark situation.

Carbon dioxide may be a potential raw material whose use is, in essence, circular. Existing literature focuses on the potential

environmental benefits while pointing out the technological and economic challenges. CO₂-based products need to be not only competitive with current fossil fuel options, but public acceptance and social willingness to change current behavior are crucial. The social perspective has had less attention, and the work by Simons et al. studies the acceptance of CO₂-based fuels for aviation synthesized *via* Carbon Capture and Utilization (CCU). Here, professionally treated social factors, affective evaluation, and benefit perception of CCU to ultimate consequences: public information and information strategies. A case study of innovative technologies corroborates the interest of this contribution. Here, materials and products manufactured through the reuse of CO₂-based jet fuels in the context of CCU represent an ultimate technological approach receiving increasing attention on the path to meeting climate targets.

PERSPECTIVE

Styring et al.'s considers a systemic approach to using synthetic fuels in a transport energy transition. Using a Theory of Change, the authors show synthetic CO₂-derived fuels to fill the gaps in the shift towards a fully electric vehicle fleet for ground transit. Then, it includes a deep reflection of the pros/cons of the various alternatives considered in the use of Synthetic Fuels in a Transport Transition. Comments on the effects of fossil fuel replacement on air quality showing the importance of atmospheric chemistry consideration as the transition to electric vehicles progresses, concluding on the impact of conventional fuels prohibition on social justice.

REVIEW

Karka et al.'s format also takes rich Encyclopedic background. The authors present relatively mature technological options' current and future potential (e.g., TRL > 6). It looks for greening existing industrial infrastructures in liquid biofuels, which have not yet found actual application at a commercial scale. This context systematically analyses these integration options concerning the present and future opportunities, barriers to overcome, real-world industrial examples, and feasibility to scale up. The material can be used as a reference point for the 2020 status in this research and contribute to coordination and support actions/projects." Otherwise, it can be of substantial interest to decision-makers in industrial practice, as shown through real-world industrial examples.

The Review by Styring et al. analyses the use of dimethyl ether (DME) from sustainable feedstock as a future non-fossil fuel alternative for road transportation, compared to oxymethylene ether and synthetic diesel through Fischer-Tropsch reactions. DME can replace diesel in a compression ignition engine (engines requiring well-known modifications), and it can be produced from CO₂ and carbon-containing waste materials. In its comparison, DME can be produced needing less hydrogen than the other routes. Towards diesel produces lower NO_x,

soot, and particulate matter. The authors conclude that DME can be then one of the fuels used in the future mobility sector.

CONCLUSION

The articles in this Research Topic represent a selected sample of precious contributions to various Perspectives of Chemicals Synthesis as a Green Alternative to Fossil Fuels. The necessary presence of Renewable Diesel in the Petroleum Industry and the need for emerging renewable substitutes of liquid fuels, thus yielding to different biomass transformation technologies. Carbon Capture and Utilization is under examination in the light of novel factors. Food waste novel reevaluation permits the production of competitive ethanol. The techno-economic analysis uncovers more efficient novel combined alternatives recovering energy from waste. A novel Perspective on Fuels in a Transport Transition under examining Theory of Change reveals the impact of conventional fuels prohibition on social justice. A wealthy Review looks for greening existing industrial infrastructures in liquid biofuels, which have not yet found actual application at a commercial scale. Carbon-containing waste as raw material and fuel and more efficient energy conversion and chemical processes are needed towards a net-zero emissions society. And, as a sample of the future community, the current special issue compiles many different greener alternatives; society will require technological options adapted to each specific context.

The authors of this Editorial want it to be of use to its readers and inspiration to many.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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