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Editorial

A Review of Process Systems Engineering (PSE) Tools for the Design of Ionic Liquids and Integrated Biorefineries

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Over the years, the global process industry is continually improving in product development and process performances. One of the areas is to identify more sustainable products and processes to manufacture products. Process Systems Engineering (PSE) tools have been instrumental in developing optimal processes and identifying better products based on different functions. With the development of novel tools, new sources of chemicals and alternative processing routes for producing products have been identified in the last few decades. Two of the most promising areas that possess the potential to provide optimal products through non-traditional processes are the integrated bio-refineries and ionic liquids. While the potential of these areas are obvious, commercial applications of these areas are still not completely explored, and PSE tools have been instrumental in the transition from the laboratory scale to the industrial scale [1]. Therefore, this Special Issue "Process Systems Engineering (PSE) Tools for the Design of Ionic Liquids and Integrated Biorefineries" makes an effort towards introducing the latest developments in these research areas to the scientific community by inviting research contributions from the top researchers in this field.

Most recently, climate change due to greenhouse gas emissions, especially carbon dioxide (CO_2), has been a major concern of the society. Therefore, various research works have been developed to reduce CO_2. One of the topics of focus is carbon capture, storage, and utilization. To reduce CO_2 from emissions, the number of conventional solvents is currently being used in the absorption systems of CO_2. However, most of these processes suffer from issues such as solvent loss, environmental pollutions, and high energy regeneration, which also contributes to environmental issues. To address this issue, naturally occurring deep eutectic solvent (NADES) constituents have been studied using both experimental and Density Functional Theory [2]. NADES is found to possess most of the desirable attributes needed for CO_2 capture solvents. This work also has the potential to be extended into novel solvent design via NADES for different gases.

On the other hand, it has been recognized that ionic liquids can replace several conventional solvents in the absorption of CO_2 due to their tunability and environmentally benign nature. However, the lack of availability of experimental data and the high cost of ionic liquids are still major challenges to their application in the commercial scale[1]. In addition, the toxicity of ionic liquid is also an important factor to be considered to justify their selection over other conventional solvents. The work by Wang et al. [3] proposed an integrated approach between machine learning and computer-aided molecular design for identifying suitable ionic liquids for various applications. In the proposed approach, machine learning tools such as feedforward neural network (FNN) and support vector machine (SVM) algorithms were used to develop toxicity predictive models. It was found that the FNN-based models have a higher predictive power than SVM-based models. These models can also be incorporated into computer-aided molecular design to identify ionic

Citation: Chemmangattuvalappil, N.G.; Ng, D.K.S. A Review of Process Systems Engineering (PSE) Tools for the Design of Ionic Liquids and Integrated Biorefineries. *Processes* **2022**, *10*, 2244. https://doi.org/10.3390/pr10112244

Received: 10 June 2022
Accepted: 13 July 2022
Published: 1 November 2022

liquids with desirable properties and less toxicity. We highlight that this approach can also illustrate the growing potential and role of machine learning applications in PSE.

Other than focusing on the removal of CO_2 from the end of pipe treatment in stack gas, etc., the replacement of fossil fuels with renewable sources such as biomass can also reduce CO_2 significantly. Biomass, in this work, refers to the organic materials that can be produced from agriculture products (i.e., energy crops) and wastes (i.e., rice husk, palm kernel shell, etc.), and it has been widely recognized as one of the most important renewable energy resources that reduces greenhouse gas emissions. An integrated bio-refinery is a processing facility that can convert biomass into multiple value-added products. It is extremely important to explore the potential of various biomass feedstocks for producing various products via integrated technologies. Said et al. [4] presented the potential of Napier grass to produce syngas through gasification. As reported in Said et al. [4], it was found that this energy crop has comparably high heating values and very high volatile matter, which has high potential for further investigation. Therefore, further exploring the possibility of scale up the gasification technology for practical applications is recommended.

The number of conceptual studies on the potential to produce value-added products in integrated biorefineries has also been explored recently and some of these works covered in this Special Issue. Lee et al. [5] developed a two-stage optimization approach that can identify the optimal product that can be produced from an integrated bio-refinery through a green pathway. A computer-aided molecular design approach is adapted to identify the optimal product, whereas a multi-objective optimization approach considers the economic, environmental, energy, and yield targets for production. It is noted that the bi-oil produced from biomass typically possesses poor properties such as low heating values, high viscosity, and non-homogeneity. To upgrade the bio-oil, one of the cheaper practical approaches is to blend the bio-oil with a solvent. However, the selection of solvent that can be used to upgrade bio-fuel must be based on both the functionalities and also on the cost. There are a number of solvents that have been developed for these purposes in the past. However, such specialty chemicals limit their practical applicability. To render the bio-oil solvent blend suitable for practical applications, a cost model has been integrated within a computer-aided molecular design framework [6]. The identified blends have the best economic potential to be used as fuel for real applications. We note that the final blend must be a homogeneous mixture, and a phase stability analysis was also performed in this work.

Another typical challenge encountered in the management of biomass is to synthesize an optimal supply chain of biomass resources to powerplants that can generate energy from biomass. In this Special Issue, a graphical method has been developed based on an established insight-based approach (Pinch Analysis) for the allocation of biomass to meet the demand of each powerplant [7]. Even though this approach is developed for palm-based biomass, the methodology is also applicable for other types of biomasses. A more complex scenario where the design and comparison of centralized versus decentralized bio-refining options has been performed [8]. This is a critical decision because the bio-refineries are generally small in size and the centralized options are not always the most profitable. The formulation of this optimization problem considerers several objectives such as economic, environmental, and safety aspects. This has been formulated as a multi-objective optimization problem to compare different scenarios for different performance targets. This work also proposes various future research directions that consider a more thorough environmental impact analysis, operational challenges, and uncertainty.

The effect of process intensification is another interesting area to be explored for higher profitability and a reduction in environmental impacts. The integration of both centralized and decentralized bio-refineries with other infrastructures can be considered for additional benefits by applying the concept of industrial symbiosis [8]. It has also been observed that the hydrothermal liquefaction process integrated with kraft mills can significantly mitigate CO_2 emissions [9]. The reduction is due to the replacement of fossil fuels with biofuels and produce biochar for sequestration. With such strategies, significant CO_2 emission reductions can be achieved when compared with the conventional process. An in-depth analysis of the processing conditions may further increase the benefits in these processes. In this issue, a new application of synthesis of integrated flower waste biorefinery is presented [10]. A superstructure approach is adapted to screen process alternatives to valorize flower waste into value added products. Multi-objective optimization approach (fuzzy optimization) is used to trade-off different objectives (maximize economic potential with minimum environmental impacts [10].

Based on the publications in this Special Issue, it can be seen that several promising technologies and novel products have been proposed by the PSE research community. The current work in this area focusses on incorporating more parameters related to cost, environmental impacts, uncertainty, operability, and scaled-up considerations. Considering the enormous interest in this field in the recent years, there is a very high potential for a higher industrial involvement based on the research output in these fields.

Author Contributions: Conceptualization, D.K.S.N. and N.G.C.; methodology, D.K.S.N. and N.G.C.; software, D.K.S.N. and N.G.C.; validation, D.K.S.N.; formal analysis, N.G.C.; investigation, D.K.S.N. and N.G.C.; resources, D.K.S.N. and N.G.C.; data curation, D.K.S.N. and N.G.C.; writing—original draft preparation, N.G.C.; writing—review and editing, D.K.S.N.; visualization, D.K.S.N. and N.G.C.; supervision, D.K.S.N. and N.G.C.; project administration, D.K.S.N. and N.G.C.; funding acquisition, D.K.S.N. and N.G.C. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

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