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Techno-Economic Analysis of 1,3-Butadiene and ε-Caprolactam Production from C6 Sugars

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Abstract : In order to achieve the transition from a fossil to bio-based economy, biomass needs to replace fossil resources in meeting the world's energy and chemical needs. This calls for development of biorefinery systems allowing cost-efficient conversion of biomass to chemicals. In biorefinery systems, feedstock is converted to key intermediates called platforms which are converted to wide range of marketable products. The C6 sugars platform stands out due to its unique versatility as precursor for multiple valuable products. Among the different potential routes from C6 sugars to bio-based chemicals, 1,3-butadiene and ε-caprolactam appear to be of great interest. Butadiene is an important chemical for the production of synthetic rubbers, while caprolactam is used in production of nylon-6. In this study, ex-ante techno-economic performance of 1,3-butadiene and ε-caprolactam routes from C6 sugars were assessed. The aim is to provide insight from an early stage of development into the potential of these new technologies, and the bottlenecks and key cost-drivers. Two cases for each product line were analyzed to take into consideration the effect of possible changes on the overall performance of both butadiene and caprolactam production. Conceptual process design for the processes was developed using Aspen Plus based on currently available data from laboratory experiments. Then, operating and capital costs were estimated and an economic assessment was carried out using Net Present Value (NPV) as indicator. Finally, sensitivity analyses on processing capacity and prices was done to take into account possible variations. Results indicate that both processes perform similarly from an energy intensity point of view ranging between 34-50 MJ per kg of main product. However, in terms of processing yield (kg of product per kg of C6 sugar), caprolactam shows higher yield by a factor 1.6-3.6 compared to butadiene. For butadiene production, with the economic parameters used in this study, for both cases studied, a negative NPV (-642 and -647 M€) was attained indicating economic infeasibility. For the caprolactam production, one of the cases also showed economic infeasibility (-229 M€), but the case with the higher caprolactam yield resulted in a positive NPV (67 M€). Sensitivity analysis indicated that the economic performance of caprolactam production can be improved with the increase in capacity (higher C6 sugars intake) reflecting benefits of the economies of scale. Furthermore, humins valorization for heat and power production was considered and found to have a positive effect. Butadiene production was found sensitive to the price of feedstock C6 sugars and product butadiene. However, even at 100% variation of the two parameters, butadiene production remained economically infeasible. Overall, the caprolactam production line shows higher economic potential in comparison to that of butadiene. The results are useful in guiding experimental research and providing direction for further development of bio-based chemicals.

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