Integrated Life Cycle Assessment and Techno-economic Analysis for Ionic Liquids-based Biomass Delignification Process

Agusta Samodra Putra[1*], *Yulia* Anita[2]

[1]Research Center for Sustainable Production System and Life Cycle Assessment, National Research and Innovation Agency, KST Prof. BJ Habibie Puspiptek Serpong Banten, Indonesia
[2]Research Center for Chemistry, National Research and Innovation Agency, KST Prof. BJ Habibie Puspiptek Serpong Banten, Indonesia

Abstract. Ionic liquids (ILs) are a sort of green solvent that possess considerable promise for many industrial applications, such as the delignification of biomass. This study conducted an integrated life cycle assessment (LCA) and techno-economic analysis (TEA) of the utilization of 1 g of ILs for the ionosolv delignification process. [bmim][Cl] was selected as a case study. By using the CML 2001 environmental impact analysis method, 1 g of 1-butyl-3-methylimidazolium chloride [bmim][Cl] utilization for the ionosolv delignification process emitted 3.67 g CO_2 eq of GWP100, 0.013 g SO_2 eq of acidification potential, 0.015 g PO_4^{3-} eq of eutrophication potential, and 32.417 g 1,4-DCB eq of HTP 20a.

1 Introduction

Lignocellulosic biomass is a major component in agriculture and forestry waste that has three major components, such as cellulose (30-60%), hemicellulose (14-40%) and lignin (7-25%) [1]. Traditional methods for pretreating biomass encompass a range of techniques, including physical [2], chemical [3], and physicochemical [4] as well as biological [5] pretreatments or their combination [6]. These methods are associated with several drawbacks, such as low efficiency, expensiveness, and environmental safety issues. Hence, alternative, more efficient, cheaper, and environmentally benign methods must be developed.

Ionic liquids (ILs) have garnered considerable interest in recent years for their prospective utilization in biomass delignification processes [7]. The process of delignification is a crucial step in the conversion of lignocellulosic biomass into biofuels, biochemicals, and other value-added products. ILs can be intentionally developed or selected to exhibit selectivity towards lignin, making it possible to target specific lignin fractions or even modify the selectivity based on the desired end-product. ILs typically have low volatility, which means they can be used at relatively low pressures and temperatures. This can reduce energy consumption and minimize the risk of environmental contamination. Some ILs can be generated and reused, which can be economically beneficial in large-scale industrial applications. This can help reduce the overall cost of the delignification process.

* Corresponding author: agus126@brin.go.id

In the pursuit of sustainable and environmentally responsible technologies, the intersection of chemistry, engineering, and ecology has given rise to an innovative field known as integrated life cycle assessment (LCA) and techno-economic analysis (TEA). LCA and TEA are two important tools that can be used to assess the feasibility of biomass delignification technologies. LCA is a holistic approach to assessing the environmental impacts of a product or process over its entire life cycle, from raw material extraction to end-of-life. Meanwhile, TEA is a financial analysis that assesses the costs and benefits of a technology. This includes estimating the capital costs, operating costs, and revenue potential of the technology. By understanding the environmental and economic impacts of these technologies, we can inform about technology development and deployment, and accelerate the adoption of biomass delignification technologies to support a more sustainable future.

Efforts have been made in terms of ionic liquids LCA. For instance, LCA of [Bmim][BF_4] as the solvent for the synthesis of cyclohexane and for the Diels-Alder reaction [8], LCA study of the synthesis of [Bmim][BF_4] and subsequent use as a solvent in the metathesis of 1-octene [9], and cost and environmental LCA of the [C_6MIM][Cl] synthesis and comparison to [C_6Py][Cl] [10]. However, according to the best knowledge of authors, there is still a lack of information for LCA study of the utilization of [bmim][Cl] for biomass delignification (Ionosolv process).

2 Methods

The LCA methodology was based on ISO 14040 to evaluate the environmental impact of ILs utilization for biomass delignification process. In its most complete form, an LCA includes all the environmental impacts from raw material extraction to production, use, and disposal or recycling. According to ISO 14040 guidelines, the LCA methodology consists of four main steps: goal and scope definition, inventory analysis, impact assessment, and interpretation [11].

2.1 System boundary of LCA

In this study, LCA has been conducted on ILs utilization for biomass pretreatment. The ILs production process from cradle-to-gate was analyzed with the functional unit of 1 g of ILs utilization for biomass treatment (Ionosolv process). The system boundary of this LCA study is shown in Fig. 1. [bmim][Cl] was selected as a case study. In the Ionosolv process, the goal is to selectively delignify biomass by dissolving the lignin in an ILs while the cellulose remains undissolved and is not appreciably decrystallized.

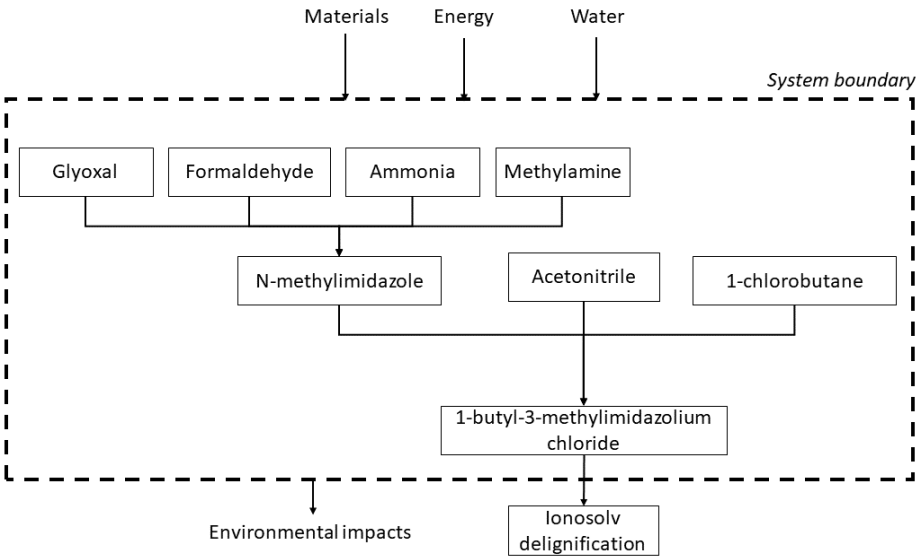

Fig. 1. System boundary of 1 g of [bmim][Cl] utilization for Ionosolv delignification process

2.2 Environmental impact categories

The baseline environmental impact categories, such as global warming potential (GWP100) in kg CO_2 eq unit, acidification potential in kg SO_2 eq unit, eutrophication potential in kg PO_4^{3-} eq unit, and human toxicity potential (HTP 20a) in kg 1,4-DCB eq unit, were quantified. The GWP100 pertains to the emissions of GHG over 100 years. The emission characterization factors associated with GWP100 were determined using the characterization model formulated by the Intergovernmental Panel on Climate Change (IPCC) AR6 [12]. Based on the Regional Air Pollution Information and Simulation (RAINS) model, the acidification potential characterization factors for air emissions were calculated [13]. Eutrophication, which signifies the excessive accumulation of nutrients in aquatic systems, is identified by the rise in nitrogen and phosphorus concentrations, expressed as kg N equivalent and kg PO_4^{3-} equivalent, respectively. Human toxicity potential refers to the harmful impacts of chemicals on human health. The characterization factors for HTP were derived based on the Uniform System for the Evaluation of Substance adapted for LCA purposes (USES-LCA) [14]. Generally, the environmental impacts calculated in this study were following the equation (1).

$$EI = \sum_{i,j=0}^{n} \left(E_i \times f_j\right) \tag{1}$$

Here, E_i is the emission from each material or energy through their life cycle and f_j is characterization factors for each environmental impact category. i is the type of materials or energy emissions, j is the type of emissions factors, and n is the total of types of emissions factors and materials.

2.3 Techno-economic analysis

The economic parameters of ILs utilization for biomass delignification in this study consists of capital costs (Capex), operation costs (Opex), and revenue or income. Total plant cost C_{total} can be calculated as:

$$C_{Total} = C_{Capex} + C_{Opex} \quad (2)$$

The annual earnings parameter was used as a techno-economic performance indicator in the study. The annual earnings were calculated using equation 3.

$$\text{Annual earning} = \text{Annual revenues} - [\text{Opex}+\text{Capex}] \quad (3)$$

3 Results and Discussion

3.1 Life cycle inventory analysis

The life cycle inventory analysis of 1-butyl-3-methylimidazolium chloride production system is described in Table 1. The inventory analysis stage is the most critical and essential to obtaining reliable results. In the production of 1-butyl-3-methylimidazolium chloride, chemicals such as N-methylimidazole, acetonitrile, and 1-chlorobutane were needed.

Table 1. Life cycle inventory analysis of 1 g [bmim][Cl] production system

Input	Amount	Price ($/unit)
Material		
N-methylimidazole	0.523 g	0.001 $/g
Acetonitrile	0.345 mL	0.088 $/mL
1-chlorobutane	0.760 g	2.84 $/g
water	2 L	0.63 $/L
Energy		
Electricity	2.1 kWh	0.087 $/kWh
Product		
[bmim][Cl]	1 g	

3.2 Integrated LCA and TEA

By using CML 2001 environmental impact analysis method, 1 g of 1-butyl-3-methylimidazolium chloride [bmim][Cl] emitted 3.67 g CO_2 eq of GWP100, 0.013 g SO_2 eq of acidification potential, 0.015 g PO_4^{3-} eq of eutrophication potential, and 32.417 g 1,4-DCB eq of HTP 20a. The environmental impact of [bmim][Cl] production depend on the energy consumption of each process as Scope 2 emissions, chemical or reagent used, waste generation, and chemical toxicity. Based on the definition, the Scope 2 emissions are all emissions that occurred from the utilization of energy. In comparison, based on the commercial LCI database (EcoInvent), 1 g of another organic solvent (toluene) emitted 1.5 g CO_2 eq of GWP100, 0.0037 g SO_2 eq of acidification potential, 0.0003 g PO_4^{3-} eq of

eutrophication potential, and 0.14 g 1,4-DCB eq of HTP 20a. The higher environmental impacts of ILs production compared to conventional solvents showed that there is still large of improvement to optimize the IL's production process.

This study took into consideration an IL cost range of $2.5-$50 /kg, which were reasonable given the scale of operation, yet they were still 2-50 times higher than organic solvent costs, such as toluene ($1.02/kg) and acetone ($1.30/kg). The economic performance parameter in the study was the annual earnings. The lifetime of all invested equipment was assumed as 15 years in the study with a 7% bank interest rate. Based on preliminary annual earnings simulation for biomass delignification by using ILs, the positive annual earnings are obtained from third-year production.

4 Conclusion

1-butyl-3-methylimidazolium chloride is a prospective "green solvent" for ionosolv delignification process. ILs have the potential to reduce environmental impact compared to traditional delignification methods that often involve harsh chemicals and generate a significant amount of waste. However, the preliminary results of environmental impacts calculation show that the production of ILs needs improvements.

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