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LIFE CYCLE ASSESSMENT OF FORMIC ACID PRODUCTION USING CO_2 FROM PETROCHEMICAL COMPANY EMISSION AND H_2 FROM POWER PLANT ELECTRICITY WITHIN INDUSTRIAL COMPLEX

Yuchan Ahn[1,2] and Jeehoon Han[3,4*]

1 Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, United States

2 Texas A&M Energy Institute, Texas A&M University, College Station, TX, United States

3 School of Semiconductor and Chemical Engineering, Chonbuk National University, Jeonju, Korea (Corresponding Author)

4 School of Chemical Engineering, Chonbuk National University, Jeonju, Korea (Corresponding Author)

ABSTRACT

Many studies have been conducted to illustrate the production of formic acid (FA) utilizing carbon dioxide (CO_2) in an economically viable manner, but the environmental impact has not received much attention. When CO_2 is used to produce FA, greenhouse gas including CO_2 will be reduced although the economics of FA production utilizing CO_2 is lower than that of conventional production using fossil fuel. To achieve a sophisticated understanding of CO_2 utilization, this study focuses on life cycle assessment (LCA) for analyzing the environmental impacts of FA production. Based on new process simulation data for CO_2-based FA production, we compare the environmental impact results of CO_2-based FA to fossil-based FA. LCA has been conducted in consideration of five petrochemical companies located in the industrial complex of Korea to ensure the potential availability of sources.

Keywords: formic acid, CO_2 utilization, life cycle assessment, climate change, fossil depletion, petrochemical company.

NOMENCLATURE

Abbreviations

CC	Climate change
CCU	Carbon capture and utilization
FA	Formic acid
FD	Fossil depletion
LCA	Life cycle assessment

1. INTRODUCTION

As the level of atmospheric carbon dioxide (CO_2) is increased by fossil fuel consumption, alternative methods to reduce CO_2 emission must be found. Several methods have been suggested; here, we focus on carbon capture and utilization (CCU)[1]. CCU is used in many applications by using CO_2 as a carbon feedstock; here, we focus on formic acid (FA) production. FA is produced commercially from CO and methanol by hydrolysis of methyl formate[2]. But, there is an alternative way to produce FA using CO_2, and it leads to lower net CO_2 emission than commercial way. Process economics that utilizes CO_2 to produce FA have been evaluated[2-4], but the environmental impact has not received much attention.

Life cycle assessment (LCA) is generally recommended for assessing the environmental impact of CCU process by all activities from feedstock production to final consumers[2]. Previous studies have analyzed the environmental impact of FA production such as amounts of CO_2 emission[5-8] and from bioelectrochemical system using wastewater[9]. However, to compare with the conventional process, it is necessary to evaluate diverse environmental impacts as well as CO_2 emission. In addition, CO_2 and H_2 produced in the industrial complex (e.g., petrochemical companies or power plants) could be used in the same complex (e.g., production of FA using CO_2 and H_2) and chemical plants (FA consumption). This paper addresses the following issues: (1) the usage of CO_2 and H_2 in petrochemical companies located in a specific boundary; (2) the usage of new process simulation data for CO_2-based FA; (3) application of LCA to evaluate environmental impacts.

We perform LCA to compare the fossil-based FA production with CO_2-based FA production; the goal is to decide which production route is the most environmentally-friendly one. Case studies compare how source variations for producing utilities are influenced on the environmental impacts. Section 2 presents process data and LCA methods. Section 3 describes LCA results. Section 4 presents conclusions.

2. METHODS

2.1 Goal and system boundary of LCA

LCA is implemented in the following four steps: (1) goal and scope definition; (2) inventory analysis; (3) impact assessment; (4) interpretation. The LCA is conducted in consideration of five petrochemical companies located in Jeollanam-do industrial complex in Korea. The region is proper to implement LCA for FA production using CO_2 because it includes the several industrial complexes with high energy consumption and CO_2 emission, and FA consumption in the region has been increased in past two years.

For the feedstock supply, H_2 is produced by electrolysis using electricity generated at a power plant located in the industrial complex, and CO_2 is captured from exhaust gas in petrochemical companies located in the same complex. This study compares CO_2-based FA using CO_2 to fossil-based FA using CO for climate change (CC) and fossil depletion (FD). Using SimaPro LCA software, they are quantified using ReCiPe 1.13 Hierarchist impact category[10]. The main function of the two processes is to produce FA using CO_2 or CO. 1.0 kg of FA is chosen as the functional unit. The overall scheme of this study is shown in Fig 1.

2.2 Fossil-based FA production system

The conventional FA production is selected as a benchmark to compare the results of environmental impacts to the CCU process, and it is divided into the production of electricity, heat, CO, and FA. Considering the hydrolysis of methyl formate, FA is mainly produced using methanol and CO as feedstocks (Eq. 1)[5]. The methyl formate is formed to FA (Eq. 2) in the equimolar conversion of water and methyl formate[5].

$$CH_3OH + CO \rightarrow HCOOCH_3 \quad (1)$$

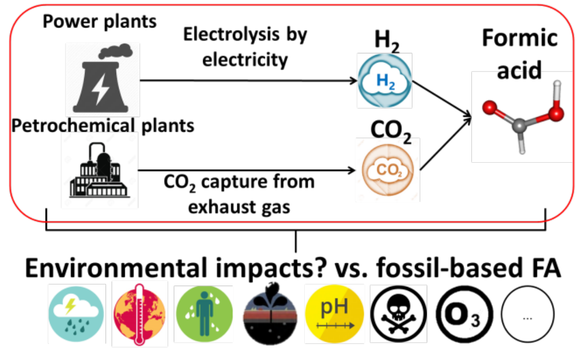

Fig 1 Overall scheme for this study

$$HCOOCH_3 + H_2O \leftrightarrow HCOOH + CH_3OH \quad (2)$$
$$CO + H_2O \leftrightarrow HCOOH \quad (3)$$

The overall net reaction is shown in Eq. 3[5]. The LCA range of fossil-based FA production is as follows: (1) CO emitted from the combustion of heavy oil; (2) electricity generated at the power plant; (3) heat generated at the heat generation plant.

2.3 CO_2-based FA production system

CCU process is to produce FA using triethylamine (NR_3), imidazole ($C_7H_{12}N_2$), CO_2, and H_2[5].

$$CO_2 + H_2 + NR_3 \leftrightarrow HCOOH - NR_3 \quad (4)$$
$$HCOOH - NR_3 + C_7H_{12}N_2 \leftrightarrow HCOOH - C_7H_{12}N_2 + NR_3 \quad (5)$$
$$HCOOH - C_7H_{12}N_2 \leftrightarrow HCOOH + C_7H_{12}N_2 \quad (6)$$
$$CO_2 + H_2 \leftrightarrow HCOOH \quad (7)$$

CO_2-based FA can be obtained using NR_3, which reacts with FA to make the FA-amine-adduct (Eq. 4)[5]. The use of an amine alone is hard to be separated from the amine-FA-adduct. Thus, imidazole is used to separate the amine-FA-adduct. When imidazole is added, NR_3 attached to FA is substituted with imidazole (Eq. 5)[11]. After separation of the imidazole and FA by distillation, the separated imidazole is recycled to remove NR_3 (Eq. 6[11]. The overall net reaction is shown in Eq. 7[5]. The LCA range of CO_2-based FA production is as follows: (1) CO_2 captured from the petrochemical companies; (2) H_2 produced by the electrolysis; (3) electricity generated at the power plant; (4) heat generated at the heat generation plant.

2.4 Utility production systems

Utilities such as electricity and heat (steam) are required to produce FA in two productions (Table 1). Electricity is generated at a power plant by natural gas, and steam is supplied from a heat generation plant using natural gas. Heat and electricity are supplied under the same conditions (e.g., pressure or voltage) for both processes. Also, there are potential sources to produce electricity and heat as follows: feedstocks

Table 1 Input data for LCA of fossil-based and CO_2-based FA productions (values per kg FA)

Process	H_2 (kg)	CO_2 use (kg)	CO use (kg)	Electricity (kWh)	Heat (kWh)	CO_2 emitted (kg)	FA (kg) [purity; %]
Conventional			0.61	0.13	5.35	0.01	1 [98%]
Petrochemical (A)	0.045	0.978		0.207	1.038	0.021	1 [99%]
Petrochemical (B)	0.045	0.978		0.209	0.432	0.021	1 [99%]
Petrochemical (C)	0.045	0.978		0.209	0.471	0.021	1 [99%]
Petrochemical (D)	0.045	0.978		0.206	1.038	0.021	1 [99%]
Petrochemical (E)	0.045	0.978		0.209	1.038	0.021	1 [99%]

(woodchip; oil; hard coal; biogas; blast furnace gas; natural gas) and technologies (wind power; photovoltaic; nuclear; hydropower).

2.5 *Case study*

To analyze the environmental impacts of FA production, it is necessary to select sources to provide the utility requirements in each process. Therefore, this study presents two case studies to illustrate the effects of the sources that produce utilities considering five petrochemical companies. We compare five CCU processes that utilize CO_2 from five petrochemical companies to one conventional FA production process. Five companies use the utilities to produce the main products assigned by each company and use the remaining utilities in the FA production. The amount of CO_2 and H_2 required (input data) is the same (Table 1) because each company uses the same technology of CCU. Case 1 considers that heat is generated from a heat generation plant and electricity is supplied from a power plant; both burn natural gas only. Case 2 uses the most appropriate sources for CC and FD in fossil-based and CO_2-based FA productions. In this study, LCA does not take into account the distance effect because it is within the same industrial area.

3. RESULTS AND DISCUSSION

3.1 *LCA results of FA production*

Including CC and FD, eighteen impacts were evaluated (Fig 2). Specifically, CC value in CO_2-based FA production has similar value (0.098) compared to the results determined by previous studies (0.17 to 2.8 kg CO_2 equivalent per kg FA).[12,13] To compare the environmental impacts in two types of FA production systems, the values of the conventional FA production are set to 100%, and the others calculated as a proportion. Except for water depletion and ozone depletion, all CCU processes obtained lower scores for all environmental impacts (Fig 2).

Fig 3 shows the main contributors of two processes for CC and FD. The environmental impact values

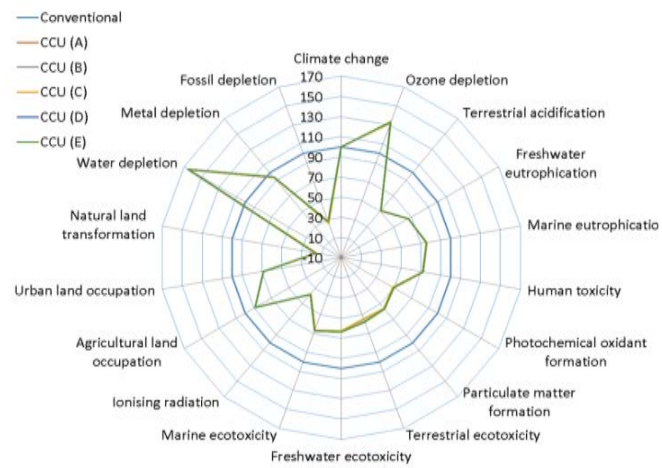

Fig 2 Comparison of environmental impact results

calculated in the conventional process are set to 100%, and that of CCU (A) process is calculated proportionally (Fig 3). The CCU process had low values for CC and FD (i.e., 53.6% CC and 28.3% FD) compared to the conventional process. From these results, CO and H_2 among several contributors is the main contributor of CC and FD in conventional and CCU processes, respectively.

3.2 *Feedstocks/technologies variation to produce FA*

For five petrochemical companies, both electricity and heat are supplied from a power plant using natural gas only. The notable difference in supplying utilities using natural gas is that CC is relatively low in

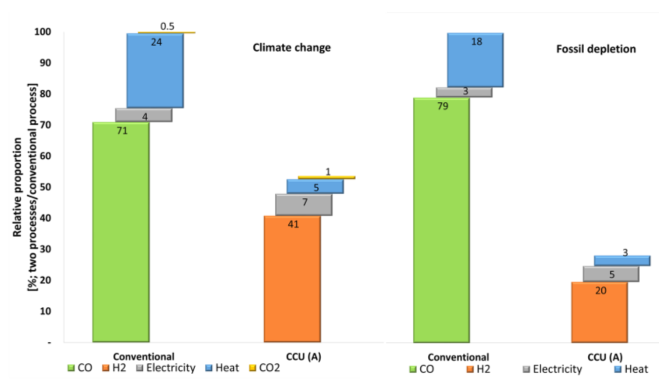

Fig 3 Main contributors for CC and FD between conventioal and CCU (A) processes

companies B and C (Fig 4). The reason for this is because companies B and C supplied the remaining energy after the production of target product in the main process to the FA production process, and the amount of required utilities is relatively small (Table 1).

Among the available potential sources, woodchip (heat) and hydropower (electricity) have the best environmental impact values in this study. Depending on the changes in the sources, it shows a different tendency from the result of using natural gas only (Fig 5). In the results of using natural gas only (Fig 4), B and C companies showed relatively low CC, while woodchip and hydropower cases showed similar values (Fig 5). The reason for this is that the environmental-friendly elements of the woodchip and hydropower do not have a significant impact on CC and FD. If the feedstocks and technologies are changed to the renewable source, then the difference of the required energy to produce FA is less influencing the environmental impact.

4. CONCLUSIONS

This study focuses on LCA to analyze the

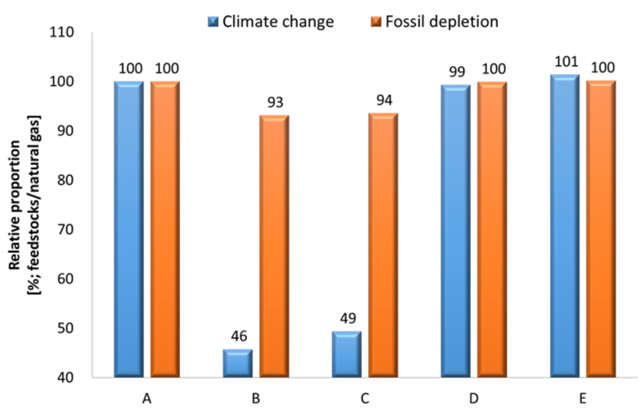

Fig 4 Environmental impacts comparison when use natural gas only

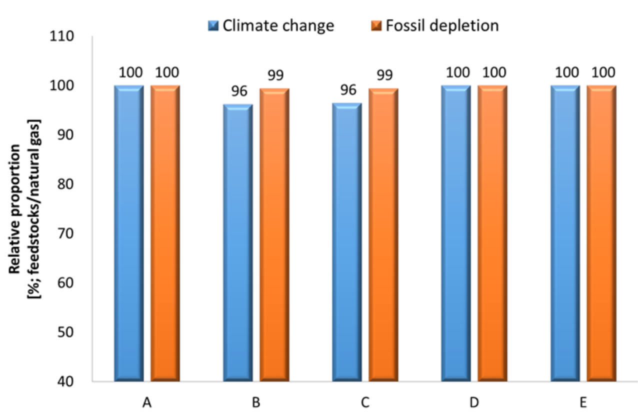

Fig 5 Environmental impact comparison when use hydropower (electricity) and woodchip (heat)

environmental impacts between fossil-based and CO_2-based FA production systems. The LCA has been conducted considering the realistic supply situation of sources in the industrial complex located in Korea. We confirmed that CO_2-based FA produced by CO_2 is more environmental-friendly one than fossil-based FA by CO. When the sources to produce utilities are changed as the renewable energy source, the difference of environmental impacts was decreased although there was the difference of required energy among petrochemical companies.

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