

Sustainability and Economic Analysis of Propylene Carbonate and Polypropylene Carbonate Production Processes Using CO₂ and Propylene Oxide

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Abstract

Currently, the industrially important polycarbonates are synthesized from bisphenol A and diphenyl carbonate, which are highly toxic and hence other feasible alternatives are preferable. Following the considerable advances on the catalyst for the synthesis of carbonates from CO₂ and propylene oxide (PO), industrial scale processes for the productions of propylene carbonate (PC) and polypropylene carbonate (PPC) have been designed and simulated with sustainability and economic analyses. The CO₂ is supplied by a nearby bioethanol plant, while the PO from a petrochemical process. The first part of the study is for the production of 200 million lb/year cyclic PC by using 9990 lb/hr of CO₂. Ionic liquid-1-n-ethyl-3-methylimidazolium chloride is used as a catalyst. The net CO₂ emission reduction is around -0.318 lb CO₂/lb PC, while the net cost of duty (heating+cooling) is around \$1.92×10⁻³/lb PC. The second part is for the production of 261 million lb/year PPC by using 14523.2 lb/hr CO₂. The process uses (salen) Cr(III) complex as catalyst. The net CO₂ emission reduction is around -0.342 lb CO₂/lb PPC, while the net cost of duty/lb PPC is around \$7.978×10⁻³/lb PPC. Economic analyses show that the feasibility of the both production plants depends on the selling price of PC and PPC. Both the production plants for PC and PPC are sustainable as they use CO₂ and avoid toxic feedstock. Beside the engineering economics, a focused sustainability analysis should also be considered in the feasibility evaluation of chemical process technologies.

Keywords: Polypropylene carbonate; Cyclohexylene; Economic analysis; Polycarbonates; Sustainability

Introduction

We add around 3500 million tonnes CO₂ worldwide annually, while the usage of CO₂ as feedstock is only around 3% [1,2]. Production of various chemicals from CO₂ can have a limited yet positive impact on the global carbon balance [3], provided that that the process can be carried out without resulting in a net increase in CO₂ emissions [4].

There is a growing interest in developing effective processes for harnessing CO₂ for the production of cyclic carbonate [5-8] and polycarbonates [9-12], which have a large worldwide consumption annually. Currently, the industrially important polycarbonates are synthesized from bisphenol A and diphenyl carbonate, which are highly toxic [13] and hence other feasible alternatives are preferable. The copolymerization of CO₂ and epoxides was first demonstrated by Inoue and co-workers [14] in 1969 using a heterogeneous catalyst derived from diethyl zinc and water. Since then, the synthesis of cyclic carbonates-propylene carbonate (PC) and polycarbonates, such as poly(propylene) carbonate (PPC), poly(cyclohexylene) carbonate, poly(trimethylene) carbonate from CO₂ and epoxides has been widely studied [9]. Cyclic PC has the IUPAC name of 4-methyl-1,3-dioxolan-2-one with molecular formula C₄H₆O₃, density of 1.205 g/ml, melting point of -67°F, boiling point of 464°F, and flash point of 270°F PC is an important intermediate in a number of different processes for instance as the replacement of highly toxic phosgene as carbonating agents in processes such as the production of isocyanates or polycarbonates. PC is aprotic polar solvent, which does not donate protons to the dissolved substances, and is used extensively as intermediate in the production of drugs and pesticides [15]. Due to its high dielectric constant of 64, it is frequently used as a high-permittivity component of electrolytes in lithium batteries, usually together with a low-viscosity solvent [15]. PPC is soluble in polar solvents, while insoluble in ethyl alcohol, ethylene glycols, water, and aliphatic hydrocarbons. Glass transition temperature (T_g) is 100.4°F, thermal degradation temperature (T_d) is at 486°F, and

density is 1.27 g/cm³ at 77°F. It has 1.9 GPa Young's modulus and 29 MPa tensile strength. With these properties, PPC may have potential applications in industry as binder resins, substitutes of thermoplastic polymers (e.g., polyethylene and polystyrene), and hydrolytically and/or biologically degradable polymers [16,17]. The physical properties of a polymer are strongly dependent on the size or length of the polymer chain. The use of biodegradable polymers includes orthopedic fixation devices, drug delivery, tissue engineering, and some medical devices. Composites of PPC and starch can be used as biodegradable plastics. PPC is also used in applications where diffusion of oxygen through the structure is required [17].

The purpose of this study is to design and simulate conceptual industrial scale processes for the carboxylation of PO to produce cyclic PC and PPC because of the considerable advancements achieved in the catalyst technology including shorter reaction time, solvent-free conditions, and an easy separation of catalyst system [18-25]. The inputs to the processes include the streams of CO₂ from an ethanol plant and propylene oxide from a petrochemical plant. In this process design and simulation, we have performed engineering and economic analyses with the sustainability metrics. Kinetics data and catalysts published in the literature [10,20,26] are used to determine the material and energy balances, the stream tables, list of the major equipment with operating

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conditions, the utilities necessary, and the sustainability indicators.

Material and Methods

An efficient catalyst is necessary to synthesize PC and PPC from the thermodynamically stable CO₂ molecule and a highly reactive substrate such as epoxide. Therefore, before presenting the simulation of production plants for PC and PPC, some recent research on possible catalysts and sustainability issue for such plants are discussed briefly in the following sections.

Advancements on catalyst

Current research activity has been the development of well-defined transition metal complexes as homogeneous catalysts for the synthesis of PC and PPC from CO₂ and epoxides [5,6,27-30]. Darensbourg et al. [25,26] presented an initial mechanistic study of the reaction between CO₂ and PO using chromium salen derivatives as catalyst. They reported kinetic study of these catalyst systems for producing copolymer versus cyclic carbonate as a function of the form of epoxide, such as for PO and cyclohexene oxide. Li et al. [11] also used the Cr salen complex, while Liu et al. [31] used cobalt salen complex, and North [32] used aluminium (salen) complexes for the synthesis reaction between CO₂ and PO. Chisholm et al. [12] studied zinc glutarate catalyst through adjusting the architecture of the ligands and optimizing reaction conditions, such as temperature, pressure, co-catalysts, and epoxide concentration. The catalysts could be immobilized on silica, allowing them to be used in a gas phase flow reactor as well as in batch reactors. The compatibility of the catalysts with CO₂ from power plant flue gas may enhance the commercial applicability of the catalysts [33].

The reaction between CO₂ and PO may be carried out in conventional organic solvents using catalysts such as dialkyltin methoxide, organoantimony halide, alkali metal salts, Mg-Al mixed metal oxide. However, the reactions using metallic catalysts have disadvantages, such as poor solubility of the catalyst, difficulties in catalyst recycling, air sensitivity, the need for co-solvent, or the requirement for high temperatures [27-29]. Ionic liquids (alkylphosphonium, *N*-alkylpyridinium, alkylammonium, and *N,N'*-alkylimidazolium), with low viscosity and no measurable vapor pressure, can be used as environmentally benign media for a range of industrially important chemical processes. Kim and Cheong [21] used the 1-alkyl-3-methylimidazolium cation because their synthesis is facile and neither oxygen nor water sensitive (but hygroscopic). With iodide as the counter anion, they can act as solvents as well as catalysts [16]. Hur et al. [20] used ionic liquids for synthesizing PC from CO₂ and PO. He et al. [27] also used ionic liquid catalysts including tetrabutylammonium bromide, functionalized and simple imidazolium ionic liquids, to a plethora of supported ionic liquid systems, and related systems for cycloaddition reactions of CO₂ with epoxides. Metal ions used in combination with ionic liquids, particularly ZnBr₂, can enhance conversions. Hydroxyl, carboxyl and other functional groups capable of hydrogen-bonding can be incorporated to improve catalysis [27]. Lim et al. [34] studied the direct carbonation mechanism of alcohols in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene, 1-butyl-3-methylimidazolium hexafluorophosphate, dibromomethane by O-labeling, and chiral alcohol experiments. Cyclic carbonates can also be synthesized from CO₂ and diols in ionic liquids via electrogenerated *N*-heterocyclic carbenes with good yields at mild reaction conditions of 40°C and 1 atm CO₂ [30].

Cellulose/KI is also active, selective, stable, and recyclable catalyst for the cycloaddition reactions of CO₂ and epoxides due to the

synergetic effect of cellulose and KI [5]. A continuous process for cyclic carbonate production is obtained in good to excellent yield (51-92%) with residence time of 30 minutes. A series of kinetics experiments show a reaction mechanism involving epoxide activation by electrophilic bromine and CO₂ activation by an amide [28]. Using the polymer-supported quaternary onium salts and aqueous solution of metal salts, the reaction of CO₂ with selected epoxides can be conducted with high product yield (71-91%) and selectivity (97-99%) under mild reaction conditions (110°C and initial CO₂ pressure of 0.9 MPa). The best yield for PC is around 91%. In addition, the advantages of this method include a short reaction time, solvent-free conditions, and an easy separation of catalyst system [29].

Cycloaddition of CO₂ with PO to produce PC may be catalyzed by potassium halides (KCl, KBr, and KI) in the presence of cucurbit [6] uril effectively at various conditions. The decrease of the activity and selectivity of KI/CB [6] is negligible after the catalytic system is reused five times. The KI/CB [6] catalytic system is also active and selective for the cycloaddition of CO₂ with other epoxides, such as glycidyl phenyl ether, epichlorohydrin, and styrene oxide [35]. Niobium stands out among neighboring transition metals for its catalytic performance in the synthesis of cyclic carbonates. Readily available NbCl₅ is an efficient catalyst for the preparation of industrially relevant carbonates at ambient temperature, low CO₂ pressure, and low concentrations [22].

The addition of CO₂ to PO may be used to examine the effect of catalytic systems formed from Lewis bases, mainly *N,N*-dimethylformamide and tributylamine, and preferentially halides of transition metals of the iron triad (CoCl₂, FeCl₃ and NiCl₂) and some Group 2 metal halides (CaCl₂, MgBr₂, ZnCl₂, CaI₂, and SnCl₄) on the conversion of the addition and its selectivity to PC formation [23]. As seen, beside salen metal complexes and ionic liquids there are various catalysts emerging for the reaction between PO and CO₂. Expensive and inefficient catalysts may impede the commercialization of the routes for producing PC and PPC at industrial scale. Advancements in the catalyst technology summarized above could lead to improved operating conditions for the synthesis of PC and PPC from CO₂ with PO and hence to continuous industrial scale processes for the production of carbonates [36].

Sustainability in chemical process industries

'Sustainability' is maintaining or improving the material and social conditions for human health and the environment over time without exceeding the ecological capabilities that support them [37]. The dimensions of sustainability are economic, environmental, and societal as seen in

1. One- and two-dimensional metrics, while useful, cannot alone certify progress towards sustainability. Progress towards sustainability occurs only when all three aspects are improved [38,39]. Economic and societal indicators may also be constrained with the environment, as seen in Figure 1. Suitable assessment tools are needed for the development of sustainable chemical products and processes [38]. The collective environmental regulations and technical advances, such as pollution control, waste minimization, and pollution prevention has greatly diminished adverse environmental impacts of chemical process industries [39,40]. Furthermore, several companies have integrated the use of sustainability tools including sustainability decision checklists, life cycle assessment, total cost assessment, and others. These tools, however, are not yet widely used [38]. The Center for Waste Reduction Technologies (CWRT) of the American Institute of Chemical Engineers (AIChE) [41,42] and the Institution of Chemical Engineers (IChemE)

[43] proposed a set of sustainability metrics that are applicable to a specific chemical process:

Material intensity (nonrenewable resources of raw materials, solvents/unit mass of products)

Energy intensity (nonrenewable energy/unit mass of products)

Potential environmental impact (pollutants and emissions/unit mass of products)

Potential chemical risk (toxic emissions/unit mass of products)

This study estimates the sustainability metrics of 'material intensity,' 'energy intensity,' and 'potential environmental impacts.' The 'Carbon Tracking' and 'Global Warming Potential' features of the Aspen Plus simulation package [44] has been used to estimate the CO₂ emission during the production of PC and PPC. The results provide guidance on the relative impacts of different types of products or industries with respect to resource use and emissions throughout the production line. Carbon tracking capability of the Aspen Plus simulator [44] allows the calculation of equivalent CO_{2e} emissions after specifying 'CO₂ emission factor data source' and 'ultimate fuel source.' The CO₂ emission factor data source can be from European Commission decision of '2007/589/EC' [45] or United States Environmental Protection Agency Rule of E9-5711 [46]. This study employs the CO₂ emission factor data source of US-EPA-Rule-E9-5711 and the fuel source of natural gas as seen in Table 1. The carbon equivalents of streams are based on data from three popular standards: (1) the IPCC's 2nd (SAR), (2) 4th (AR4) Assessment Reports, and (3) the U.S. EPA's (CO2E-US) proposed rules from 2009 (Table 2) [44]. This study uses US-EPA with a predetermined cost for CO₂ fee/tax.

Process simulation results and discussions

Production of propylene carbonate: Figure 2 shows a possible conceptual process flow diagram for the production of PC from PO and carbon dioxide. The process based on the chemical reaction $C_3H_6O (PO) + CO_2 \rightarrow C_4H_6O_3 (PC)$ utilizes the rate constant k in the form of the Arrhenius equation [20].

$$k = k_0 \exp(-E / RT) = 17452614 \exp(-67600.00 / RT) \quad (1)$$

where k_0 is the pre-exponential factor, E is the activation energy in kJ/mol K, and R is the gas constant in 8.314 kJ/kmol K. The catalyst ionic liquid-1-n-ethyl-3-methylimidazolium chloride (EMImCl) is used in a stirred tank reactor at 212°F and 114.7 psi. The initial amount of the catalyst introduced into the process is around 660 lb to produce around 23174 lb PC/hr (200,227,000 lb years) by using 9990 lb CO₂/

Fuel Source	US-EPA-Rule-E9-5711 lb/MMbtu	EU-2007/589/EC lb/MMbtu
Natural gas	130.00	130.49
Coal bituminous	229.02	219.81
Coal anthracite	253.88	228.41
Crude oil	182.66	170.49
Bio gas	127.67	0

Table 1: Emission rates for various CO₂ emission factor data sources and fuel sources.

Standards for reporting CO ₂ emissions	Prop-Set properties corresponding to each standard
IPCC AR4 (2007)	CO2E-AR4
USEPA (2009)	CO2E-US

Table 2: Standards used in global warming potential for reporting CO₂ emissions.

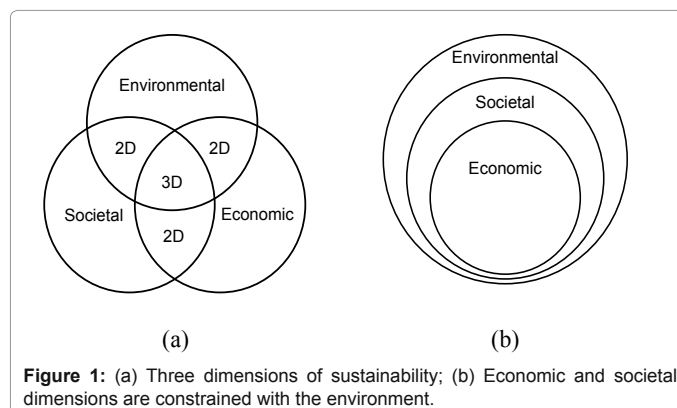


Figure 1: (a) Three dimensions of sustainability; (b) Economic and societal dimensions are constrained with the environment.

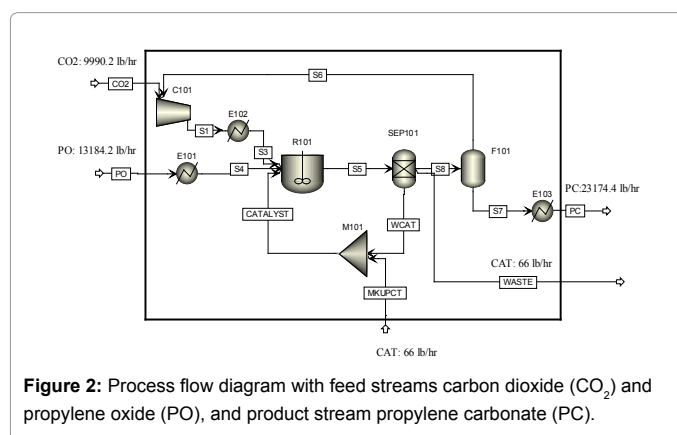


Figure 2: Process flow diagram with feed streams carbon dioxide (CO₂) and propylene oxide (PO), and product stream propylene carbonate (PC).

hr and 13184 lb PO/hr. It is assumed that 90% of the initial catalyst is recoverable and recyclable, while 10% of the initial amount of the catalyst (66 lb/hr) was considered waste catalyst. The makeup stream (MKUPCT) is used to replenish the catalyst. The stream of CO₂ is compressed to 114.7 psi in compressor C101 and its temperature is adjusted to the reaction temperature (212°F) in heat exchanger E102 before it is fed into the reactor R101. The temperature of PO is adjusted to 212°F in E101 and pumped into the reactor. The catalyst is dispersed in the PO within the reactor. Stream 5, the reactor output, is sent to the separator SEP101 to separate and recover the catalyst. Stream S8, containing the unused CO₂, PO, and produced PC, is flashed at around 5 psi in the F101 and unused CO₂ and PO are recycled to compressor C101, and eventually to reactor R101. Stream S7 containing almost pure PC is cooled and stored at 68°F. The results are obtained by using the Soave-Redlich-Kwong (SRK) equation.

Production of polypropylene carbonate: Figure 3 shows a possible conceptual process flow diagram. The process uses (salen) CrIII Cl complex as catalyst. The kinetics data published by Darenbourg et al. [26] is used

$$k = k_0 \exp(-E / RT) = 17452614 \exp(-67600.00 / RT) \quad (2)$$

Where k_0 is the pre-exponential factor, E is the activation energy in kJ/mol K. The reaction takes place at 850 psi and 86°F and produces a small amount of a cyclic PC. The reaction initially forms segments from CO₂ and PO and then proceeds in the copolymerization of these segments as the repeating units to form the polymer:

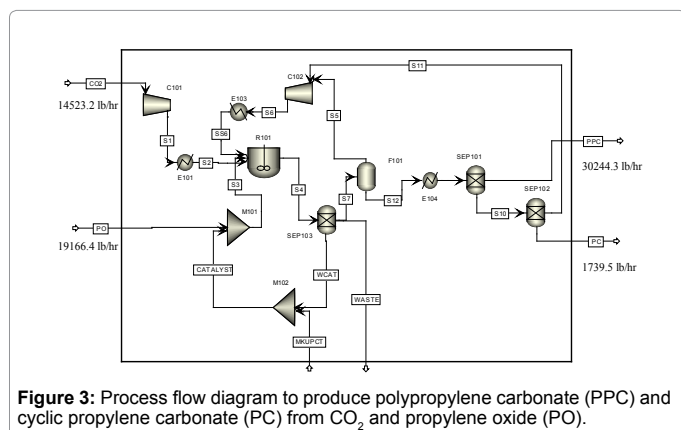
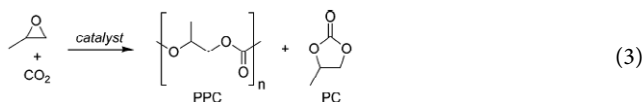


Figure 3: Process flow diagram to produce polypropylene carbonate (PPC) and cyclic propylene carbonate (PC) from CO₂ and propylene oxide (PO).



When the reaction is performed at elevated temperatures, cyclic propylene carbonate is the dominant product as a result of a unimolecular depolymerization reaction of the polymer-catalyst complex, i.e., a backbiting mechanism [25,26]. The initial mass of the catalyst within the reactor is around 80 lb. The process produces around 30224.3 lb/hr of PPC (261 million lb year) and 1739.5 lb/hr PC by using 14523.2 lb/hr CO₂ and 19166.4 lb/hr PO.

The stream of CO₂ is compressed to 850 psi in compressor C101 and its temperature is adjusted to reaction temperature (86°F) in heat exchanger E101 before it is fed into the reactor R101. The temperature of propylene oxide is adjusted to 86°F in E104 and pumped into the reactor. The catalyst is dispersed in the propylene oxide within the mixer M101 and sent to reactor. The reactor output, stream S4, is sent to the separator SEP101 to separate and recover the catalyst. It is assumed that 90% of the catalyst is recovered and recycled back to the reactor, while 10% of the catalyst, stream WASTE, is to be treated before it is recycled into the reactor within the makeup stream, MKUPCT. The process is capable of supplying a fresh makeup catalyst if necessary through stream MKUPCT. Stream S7, containing the unused CO₂, propylene oxide, and produced propylene carbonate and poly(propylene carbonate), is flashed at around 5 psi in the F101 and most of the unused CO₂ and PO are recycled to compressor C102, and eventually to reactor R101 after cooling down in E102. Stream S12, containing the mixture of PC, PPC, and little of CO₂, and PO, is cooled to 68°F and 14.7 psi, and sent to SEP102 to separate and store the PPC. Stream S10 is separated in SEP103 and the remaining unused CO₂ and PO are recycled back to compressor C102, while PC is stored. The results are obtained by using the RK-SOAVE model.

Sustainability

The following sustainability metrics are considered for propylene carbonate and polypropylene carbonate production processes:

Material intensity (nonrenewable material/unit mass of products)

Energy intensity (nonrenewable energy/unit mass of products)

Potential environmental impact (pollutants and emissions/unit mass of products)

Here, it is assumed that there is no toxic material emission in both the processes. These approximate sustainability analyses do not include

the energy cost and emission during the carbon capture, propylene oxide production, storage, and transportations. Table 3 displays the sustainability metrics for both the productions of PC and PPC.

Sustainability in propylene carbonate production process: As Table 3 shows, the material intensity metric that is the net propylene oxide, as nonrenewable material, consumption per unit mass of propylene carbonate is 0.569. The lower values of these metrics are preferable. The approximate net duty and the net cost required are -1.314×10^7 Btu/hr and \$44.5/hr, respectively where the minus sign indicates reduction in a quantity. The net duty per unit mass of PC is -567.0 Btu/lb. The net cost of utility per unit mass of PC is 1.920×10^{-3} /lb PC. These costs are estimated by the unit cost of utilities listed in Table 4. The net amount of CO₂ fixed, after taking into account the emitted CO₂ by the utility production, is -7389.0 lb/hr or 63.84×10^6 lb/year, with 8640 hr working hours per year. The total CO₂ fixed per unit mass of PC is -0.318 , as seen in Table 3. Higher absolute values of this indicator are favorable for environmental impact of the operation. The plant fixes considerable amount of CO₂ and saves carbon fee/tax of \$57888/year due to use CO₂ as feedstock after accounting the emissions for the utilities.

Sustainability in polypropylene carbonate production process: In Table 3, the material intensity metric shows that the net propylene oxide consumption per unit mass of polypropylene carbonate is 0.634. This ratio becomes 0.599 when the byproduct propylene carbonate is also accounted (PPC+PC). The approximate net duty and the net cost required are 1.257×10^7 Btu/hr and \$241.0/hr, respectively, where the minus sign shows the reduction. The net duty per unit mass of PPC is -410 Btu/lb. The net cost of utility per unit mass of PPC is 7.978×10^{-3} /lb PPC. The net amount of CO₂ fixed, after taking into account the emitted CO₂ by the utility production, is -10350.6 lb/hr or 89.42×10^6 lb/year, with 8640 hr working hours per year. The cost data of the utilities are shown in Table 4. The total CO₂ fixed per unit mass of PPC

	Propylene carbonate (PC)	Polypropylene carbonate (PPC)
Material intensity		
Net stream of propylene oxide (PO), lb/hr	13184.2	19166.4
Mass of product, lb/hr	23143.3	30224.2
Net PO/Unit mass of product	0.569	0.634
Net PO/Unit mass of (PPC+PC)		0.599
Energy intensity		
Total heating duty, Btu/hr	$+2.678 \times 10^6$	$+2.927 \times 10^7$
Total cooling duty, Btu/hr	$+1.582 \times 10^7$	$+4.202 \times 10^7$
Net duty (heating- cooling), Btu/hr	-1.314×10^7	-1.257×10^7
Net duty/Unit mass of product, Btu/lb	-567	-410
Net duty/Unit mass of (PPC+PC), Btu/lb		-390
Cost		
Total heating cost, \$/hr	40.9	231.7
Total cooling cost, \$/hr	3.5	9.4
Net cost (heating + cooling), \$/hr	44.5	241.1
Net cost/Unit mass of product, \$/lb	1.920×10^{-3}	7.978×10^{-3}
Net cost/Unit mass of (PPC+PC), \$/lb		7.542×10^{-3}
Environmental impact		
Feed stream CO ₂ , lb/hr	-9976.8	-14523.2
Utility CO _{2e} , lb/hr	+2587.8	+4172.6
Net stream CO ₂ , lb/hr	-7389.0	-10350.6
Net stream CO ₂ /Unit mass of product	-0.318	-0.342
Net stream CO ₂ /Unit mass of PPC+PC		-0.323

Table 3: Sustainability metrics for propylene carbonate (PC) and polypropylene carbonate (PPC) production processes.

is -0.342, as seen in Table 3. The absolute value of this indicator should be higher for a sustainable environmental impact of the operation. The plant saves carbon fee/tax of \$81216/year. Table 5 shows the reductions in net carbon fee and hence the positive impact of the production plant in Global Warming Potentials because of using CO₂ as feedstock. The emission indicators for CO₂ based on the standard USEPA (2009). As Table 5 shows, the fixation of CO₂ in carbonates helps moderately reduce the CO₂ emission.

Economic analysis

For both the processes, the competitive operational life is ten years. The fixed capital investments as bare module costs are estimated by using the CAPCOST program [46]. The interest rate is 4.5% while the tax 30%. The deterministic discounted cash flow diagrams have been prepared using the depreciation method of 'Maximum Accelerated Cost Recovery System' with a 7-year recovery period. Using the cash flow diagrams, the feasibility criteria of 'Net Present Value' (NPV), 'Payback Period' (PBP), and 'Rate of Return' (ROR) have been estimated. At least two out of three criteria should be favorable for a feasible operation: NPV ≥ 0, PBP ≤ useful life of operation, and ROR ≥ interest rate. Chemical Engineering Plant Cost Index (CEPCI-2014) (= 576.1) [47] is used to update the cost of equipment to the present date:

$$Cost_{New} = Cost_{New} \frac{CEPCI_{New}}{CEPCI_{Old}} \left(\frac{Capacity_{New}}{Capacity_{Old}} \right)^x \quad (5)$$

where x is the factor, which is usually assumed to be 0.6. The analysis, therefore, is based on the recovery of 90% of the catalyst and recovery and treatment/reactivation of the remaining 10% and no net catalyst loss is allowed during the process.

Propylene carbonate production plant

The approximate fixed capital investment is approximately \$18.2×10⁶. For a capacity of 200, 226, 816 lb PC estimated cost of manufacturing and revenue are \$154.7×10⁶ and \$158.7×10⁶, respectively. The economic analysis shows that the approximate values of NPV, PBP, and ROR are \$13.0×10⁶, 3.5 years, and 24 %, respectively when the selling price of PC ≥ \$0.72/lb. Figure 4 shows how the values of NPV, PBP, and ROR change with the selling price of PC [48].

Conclusion

Economic analyses show that the processes for producing propylene carbonate and polypropylene carbonate from propylene oxide and CO₂ may be economically feasible depending on the selling prices of the products with the projected advancements in the catalyst

Utilities	Energy Price, \$/MJ	T _{in} °C	T _{out} °C	Factor*	U** kW/m ² K
Electricity	\$0.0775/kWhr			0.58	
Cooling Water	2.17×10 ⁻⁴	20	25	1	3.75
Medium Pressure Steam	2.2×10 ⁻³	175	174	0.85	6.00
High Pressure Steam	2.5×10 ⁻³	250	249	0.85	6.00

*CO₂ energy source efficiency factor; ** Utility side film coefficient for energy analysis.

Table 4: Unit energy cost for various utilities with energy source of natural gas for 2014 [44].

	CO ₂	PC
CO ₂ E-US lb/hr (PPC)	14523.2	0.025
CO ₂ E-US lb/hr (PC)	9990.2	13.4
	Propylene Carbonate (PC)	Poly(propylene) Carbonate (PPC)
Net carbon fee/tax, \$/hr	- 6.7	-9.4
Net carbon fee/Unit mass of product, \$/lb	- 2.891×10 ⁻⁴	- 3.110×10 ⁻⁴
Net carbon fee/Unit mass of PPC+PC, \$/lb		- 2.940×10 ⁻⁴

Standard: US-EPA-Rule-E9-5711; Fuel source: natural gas; Carbon fee: \$2/tonne; These indicators do not include the energy cost and CO₂ emission during the CO₂ and PO productions, storages, and transportations.

Table 5: Global warming potential indicators [44].

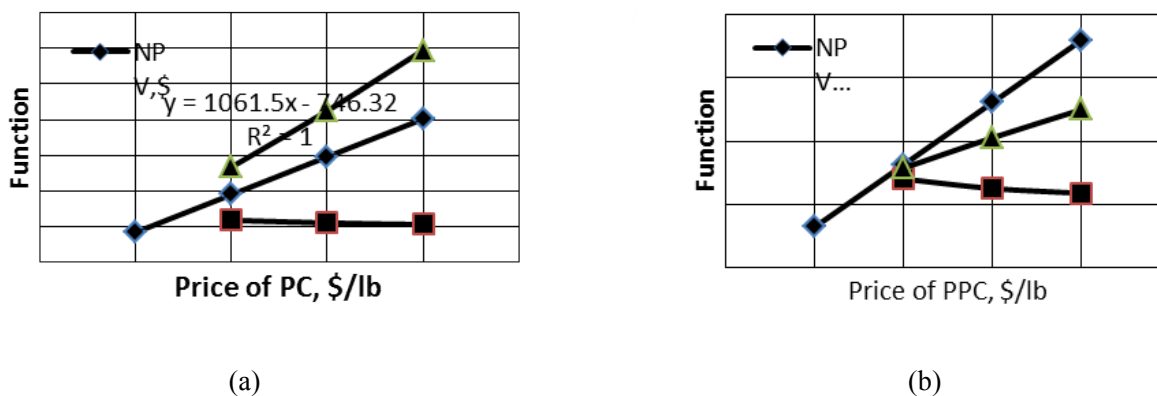


Figure 4: The values of net present value (NPV), payback period (PBP), and rate of return (ROR) with the selling prices of products: (a) NPV ≥ 0 for manufacturing PC with an approximate selling price ≥ \$0.72/lb PC; (b) NPV ≥ 0 for manufacturing PPC with an approximate selling price ≥ \$0.97/lb PPC.

technology under the current economic data, available technology, and catalyst utilized. The approximate sustainability analyses indicate that these processes may have positive effects on fixing the carbon in high value chemicals and may be sustainable. As the assumptions made in this investigation had a significant effect on the outcome of the study, a closer look at these assumptions, in particular the use of catalyst, reactor configuration, and use of propylene oxide as the starting material are essential. Beside the economics, the feasibility evaluation should take sustainability into account for chemical process technologies which have ecological, economic and societal components.

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