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Resource Integration and CO₂ Conversion in Industrial Clusters

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Countries around the globe seek ambitious CO_2 emission reduction targets to avoid dangerous climate change effects. In this work, a tool was developed that produces a network of plants that can decrease emissions, maximize energy reuse and select products that maximize profit of an industrial cluster. The tool can integrate various plants and/or processes, such as industrial production plants, power plants etc., to enhance the potential of making financial profits. Recently, a focus has been put on integrating natural gas, energy, and CO_2 to reduce emissions or energy demand, which fall within end-of-pipe carbon capture utilization and storage (CCUS) solutions. This work designs an industrial cluster on the utilization of key materials including emissions. This approach introduces a new representation of resources management in a cluster that systematically integrates H₂O, N₂, O₂, CO₂ and energy (power and heat) converting them to value added products under a reduction target. The approach develops a Linear Program (LP), which can be easily applied to explore different combinations of plants. The method was applied on an illustrative example where several scenarios were investigated. The industrial cluster converts CO₂ by 76% and produces methanol, while making profit.

1. Introduction

CO₂ emissions have increased drastically from anthropogenic activity, mostly from stationary sources such as industrial activity. Individual Industrial process or plants have been optimized through energy and mass integration to increase profits by saving energy and at the same time, reduce emissions. However, integrating multiple industrial plants using an overall approach can achieve larger energy saving, bigger profits and larger emission reduction. This work falls under the umbrella of carbon capture utilization (CCU) where CO₂ was used as raw material to make value added products while only utilizing renewable energy in aim of creating a green CO₂ reducing cluster. Previous approaches have been developed to achieve footprint reduction in CO₂ emissions in industrial clusters. Manan et al. (2017) have summarized CO₂ emission reductions from an industrial cluster by energy reduction or using carbon capture utilization and sequestration (CCUS). Al-Mohanndi and Linke (2016) only looked into CO₂ conversion processes, while Hassiba et al (2017) expanded the representation to include waste heat exchange. Al-Mohannadi et al. (2017) studied managing resources in industrial processes focusing on natural gas and CO2 material exchange. Panu et al. (2019) expanding on the representation of Noureldin and El-Halwagi (2015) discussed a bi-objective CO₂ footprint reduction optimal design of Carbon-Hydrogen-Oxygen (CHO) symbiosis that integrate hydrocarbons streams between plants, while allowing the conversion of CO₂ to produce value added products. However, the approach allowed only the integration of hydrocarbon streams and did not consider the energy needed for the plants in the city. The approach presented in this work allows the integration of any possible resource is necessary for a holistic optimization approach. This method will allow the user to study multiple materials (H₂O, N₂, O₂, CO₂) and energy (heat and power) across plants to analyze the potential of meeting emission targets without offsetting other demands. The optimization approach will optimize several processes and/or plants coexisting in industrial parks. Moreover, renewable energy sources can be incorporated, which will further reduce CO₂ emissions. Several technologies exist that can convert CO₂ to value added products examples include the process presented by Van-Dal and Bouallou (2013) which produced methanol from CO₂, Pérez-Fortes et al. (2016), and more recently Alsayegh et al. (2019). This paper presents a systematic method that integrates several processes in a cluster

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to reduce CO₂. The next section will outline the approach, any assumptions taken to develop the model, and is followed by an example where several cases were studied.

2. Approach

In this paper, pre-existing plants in an industrial cluster are integrated to achieve maximum economic profit that can convert a given amount of CO₂. Figure 1 shows an industrial cluster that consists of a number of plants, where each plant has different materials that can be exchanged within the city. In addition to materials, energy can be exchanged either as heat or power through the illustrated power grid. The purpose of the study is to design the optimum integration network that results in the maximum profit, while maintaining a user specified environmental footprint e.g. consuming a given CO₂ flow within the city. A Linear Programming (LP) model is used to investigate the various route. User specified data are outlined below.





The formulation of the optimization problem takes the following steps:

- The identification of a capacity requirement for each plant 1.
- The identification of the maximum environmental footprint allowed as constraints, the minimum and 2. maximum flows of fresh feed and output of each flow to and from the industrial cluster.

(1)

3. The identification of an objective function, in which the profit of the industrial cluster is maximized

Max (profit of industrial cluster)

Subject to	
Equality constraints $h(x1, x2,, Xn) = 0$	(2
Inquality constraints $g(x1, x2,, Xn) \leq 0$	(3

Materials integrated within the cluster must meet specification of the recipient plant, which entails meeting inlet conditions such as temperature, pressure, and purity. Each material in any plant has energy demand, emission footprint, capital and operating cost parameters. The exchange of materials including heat carriers such as steam is carried through piping systems, where the cost of connection, in this case is neglected as industrial clusters are often built with an existing infrastructure. When it comes to energy management, each plant has an integrated utility system that provides all heating and cooling requirements for its processes. Any additional demands, either hot or cold utilities, are bought for a price and their emission is accounted for by a CO2 footprint parameter that scales with the flow. The LP was solved using "What'sBest!16.0" optimization tool in Microsoft Excel 2016 (Lindo Systems, 2019).

3. Case Study

In this study, an industrial city has been explored, which consists of the plants illustrated in Table 1. The table shows the materials involved in each plant, along with the main material the plant is designed to produce referred

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to as Resource R, and the maximum capacity associated with the plant. The purpose of the study is to maximize the profit under controlled CO_2 emissions. The capital cost for each is presented also in Table 1.

Plant	Products	Reference Resource	Max Capacity (t/y)	Capex (\$/t)
Air Separation	O ₂ , N ₂	O ₂	100,000	203
Water Splitting	O ₂ , H ₂	H ₂	15,000	7,108
Methanol Production	CH ₃ OH, H ₂ O, Power	CH₃OH	100,000	387
Ammonia Production	NH ₃ , Power	NH₃	100,000	153

Table 1: Industrial cluster plants and capacities

Figure 2 illustrates a schematic of the industrial cluster with the possible connections between the plants. Constraints specified for the fresh feed only allow air, water, CO_2 , and power to be imported, while the city allows ammonia, methanol, oxygen, and excess power to be sold. While waste streams include CO_2 emissions and N_2 waste stream. The cluster is required to convert imported 120,000 t CO_2/y to value added products. The industrial city imported energy from renewable sources with no CO_2 footprint. The main CO_2 emission sources are the unconverted CO_2 , and CO_2 emissions associated with water entering as fresh feed. The CO_2 emission parameters associated with the methanol plant and the fresh feed water plant are 0.383 t CO_2/t CH₃OH and 0.0329 t CO_2/t H₂O.



Figure 2: Schematic of the industrial cluster investigated

Parameters relating flows of resources and energy demand in each of the four plants are presented in Table 2 and Table 3. The parameters were obtained through performing mass and energy balances on collected data. A negative parameter represents an input requirement and positive parameters represents an output. A zero parameter indicates that the resource is not involved in the process of that plant. Costs of the resources entering and leaving the industrial city are presented in Table 4.

Resource	Air Separation	Water Splitting	Methanol Production	Ammonia Production
	(t R/t O ₂)	(t R/t H ₂)	(t R/t MeOH)	(t R/t NH₃)
Air	-4.330	0.000	0.000	0.000
O ₂	1.000	8.000	0.000	0.000
N ₂	3.270	0.000	0.000	-0.849
H ₂ O	0.000	-9.000	0.563	0.000
H ₂	0.000	1.000	-0.200	-0.182
CO ₂	0.000	0.000	-1.758	0.000
NH ₃	0.000	0.000	0.000	1.000
CH₃OH	0.000	0.000	1.000	0.000
CO ₂ Emissions	0.000	0.000	0.396	0.000
Dilute N ₂	0.000	0.000	0.000	0.031
Ar	0.060	0.000	0.000	0.000

Table 2: Parameters of flows in terms of reference products (R)

Table 3: Energy resources parameters in terms of reference products (R)

Resource	Unit	Air Separation	Water Splitting	Methanol Production	Ammonia Production
Chilled Water	GJ/t R	0	0	-0.885	0
Electricity	kWh/t R	-245	-5,370	0.111	458
Refrigeration	kWh/t R	0	0	0	-65

Data for the CO_2 conversion were obtained from (Demirel, 2015). Air separation energy consumption data were obtained (Alsultanny and Al-Shammari, 2014), and the H₂O splitting energy consumption data were obtained from (Gambhir et al., 2017). Also, the data for Ammonia production was obtained from (Canada, 2009).

Table 4: Prices of resources entering and leaving the industrial cluster

Resource	Price (\$)	Unit	
Air	0	\$/t	
H ₂ O	0.89	\$/t	
NH ₃	548	\$/t	
CH₃OH	380	\$/t	
O ₂	50	\$/t	
Electricity	0.06	\$/kWh	
Chilled water	4.5	\$/GJ	
Refrigeration	0.0033	\$/kWh	

The prices of methanol and ammonia were obtained from (Mevawala et al., 2019). The price of oxygen was obtained from (Ebrahimi et al. 2015) The refrigeration price was obtained from (Demirel, 2015). The chilled water price was obtained from (Towler & Sinnott, 2012). The price of electricity was obtained from (Kim et al., 2011). The cluster was assumed to have a lifetime of 15 years, with an interest rate of 8%. The model was used to design a network achieving a treatment of 120,000 tCO₂/y as fresh feed while maximizing the profit. Several options scenarios to deal with emissions were investigated namely, CO_2 can be imported to the cluster at no cost, the cluster can receive a monetary subsidy to convert CO_2 or the cluster can buy CO_2 feed at a cost. The breakdown of the two scenarios that were studied are shown in Table 5. Oxygen was sold as a byproduct while in Scenario 2 it was considered a waste product.

Table 5: Scenarios studied

Scenario	O ₂ Trade	Cases
1	On	Case 1: CO ₂ imported at \$0/t
		Case 2: CO ₂ bought at \$20/t
		Case 3: CO ₂ purchased by the city \$20/t
2	Off	CO ₂ imported at \$0/t

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All three cases emitted CO_2 28,934 t /y, resulting in a net conversion of 75.9 % of the inlet and had the same plants activated. Figure 3 illustrates the optimized network including the capacity of each plant and the total profit in each case.



Figure 3: Industrial city network and total profit for the three cases in scenario 1

The optimization resulted in minimizing the ammonia plant capacity to zero, due to its high operating cost. N₂ produced from the air separation did not have any use and leaves the cluster as a waste stream. Power was imported into the industrial cluster, while H₂ and H₂O were exchanged and consumed within the cluster. This indicates that if CO₂ was to be bought, sold, or obtained for free, profit can still be made from this industrial cluster. Results for the second scenario, where O₂ is not allowed to be sold, are shown in Figure 4. The cluster had a total capital cost of \$120 M, and generated a total profit of \$6.78 M /y. The plant capacities remained the same as those found in Figure 3.



Figure 4: Industrial cluster network without selling O2 and free of charge CO2

The air separation unit is excluded from the network, as its capacity was minimized to zero. In return, the power import requirement decreased, and the total profit of the industrial cluster decreased due to the O_2 limitation trade. This result shows that even if O_2 was not sold, the total CO_2 footprint can still decrease with a profitable outcome.

4. Conclusion

An integration network for an industrial cluster has been investigated through linear programming. An example was solved to illustrate the method. The cluster investigated converts CO_2 into value added products, producing methanol, ammonia and oxygen to be sold. Requirements of CO_2 treatment is 120,000 t/y of fed to the city. Three cases were studied with different CO_2 pricing scenarios, each resulting in different profits and costs. In the three cases the same net conversion of CO_2 (76%) was implemented, and the profits rendered ranged from

6.78 M/y to 15.79 M/y. Then, with the use of this tool, having CO₂ as a feedstock and converting it to profitable products can render an overall profit while meeting environmental constraints. Multiple options can be further investigated such as, the addition of more plants within the cluster, which allows for further interactions, and/or the addition of power inputs from non-renewable energy sources, while investigating the influence of the environmental impact constrain on the economic performance of the cluster.

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