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A Planning Tool for Long-term Enterprise-scale Decarbonisation with Carbon Dioxide Removal Technologies

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To combat severe climate change, several governments around the world have set ambitious targets to reach net-zero emissions in the coming decades. To this end, policymakers will need decarbonisation planning tools, such that a decarbonisation pathway optimised to local constraints is selected and implemented. There are several policymaking planning tools available for macro-scale planning and operations at region-wide level, however tools and research on smaller, enterprise-level scale remain limited, despite commitments being made by several large companies to become net-zero carbon emitters. This work presents an optimisation-based decarbonisation planning tool for use by industrial companies to plan for carbon emission reduction by implementing a variety of different technologies. The model can consider feedstock changes and alternative energy sources and, given a set of demands and constraints, can suggest the optimal technology selection of carbon, capture and storage (CCS), low emission energy and feedstocks, and negative emissions technologies to achieve emissions targets. Unlike previous models, the model accounts for price changes across decades and provides a plan on how companies can invest in the right technologies, either constrained by a budget or given an emissions target, while still delivering products to satisfy demands. The model is demonstrated on a case study based on ExxonMobil's Baytown refinery complex which consists of an oil refinery, a plastics plant, an olefins plant and a chemical plant, where a net-zero emission limit is set within six 5-year periods. The pathway created by the model is able to suggest a full reduction of emissions in the chemical, plastics and olefins plant respectively within a 10-year implementation of biogas and negative emissions technologies and is able to reduce the oil refinery from 44 Mt/y of CO_2 emissions to 4.5 Mt/y after 25 years by phasing out oil in favour of renewable biogas refining.

1. Introduction

Due to human activities such as over-farming, deforestation and extensive overuse of fossil fuels, the concentration of greenhouse gases in the atmosphere has increased, causing an increase in the Earth's mean temperature. The effects of this have already been clear to see with increases in flooding, droughts and other extreme weather events caused by such climate change and will likely continue to worsen unless humans curb their practices. Governments around the world have attempted to minimise and, in some cases, reverse the effects of global warming, by entering The Paris Agreement. Signed in December 2015 by 196 parties, the goal of this legally binding treaty is to ensure that global warming is limited to far below 2°C, with a total of 24 countries having reduced their greenhouse gas emissions for at least 10 years (Skea et al., 2022). More than 70 countries have formed a coalition pledging to reduce their carbon emissions to net zero, including China, the United States, the UK, and the European Union (United Nations, 2022). This ambitious target includes reducing fossil fuels in a number of sectors, where energy and transport have been highlighted as the key sectors for change (Skea et al., 2022). While on a macro scale there is some understanding of how to reach this target, policies alone will not be enough to reach this goal. Despite the pledges made, current commitments are falling short of

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what is required and until effective measures are implemented, the usage of fossil fuels will still be required at an unsustainable rate (United Nations, 2022). Many sectors of the world economies rely on fossil fuels, and the production and refining of these fuels can be as damaging to the environment as their usage. Oil refining is the industrial process of transforming and refining crude oil into a number of useful products. These products include petroleum, naphtha, gasoline, diesel fuel and other heavier hydrocarbons which are used in a variety of industries. The most recent data from 2020 suggests world oil refineries refine over 76 million barrels of oil per day, with the US containing the largest oil refinery capacity at 18.14 million barrels per day (Statista, 2021). It is believed that between 2020 and 2030, the emissions released by refining this quantity of oil may be as large as 16.5 Gt of CO_2 (Lei et al., 2021). Reducing these high levels of carbon emissions will not only help reduce the effects of climate change but may also save companies money as several major economies explore the possibility of introducing a carbon tax on those who do not comply with decarbonisation (Morton, 2021). The difficulties with fulfilling government targets often lie in implementation, as while pledges are made, there is not always enough impetus on how the target can be successfully and cost effectively reached. The use of technology will prove vital in the decarbonisation of industrial sectors, with carbon capture and storage (CCS) and negative emissions technologies (NETs) at the forefront of possible options for policymakers, as well as low-carbon fuels (Haszeldine et al., 2018). There are several policymaking planning tools currently available for macro-scale planning and operations, on either a country or regional level, such as OSeMOSYS, TIMES and SimCCS. These tools are effective in providing cost-based optimisation for policymakers relating to regional energy problems. Tools and research on smaller, company-level scale remains limited, and there are no current models that consider production-based processes. To address this research gap, we develop a novel optimisation model that informs local policymakers how to decarbonise while fulfilling production targets. Unlike previous work, this model provides a tool for industrial processes to plot decarbonisation pathways while fulfilling current demands, either based on a budget or emission limit. This paper first discusses the problem statement before displaying the mathematical formulations that the model is based on. The paper then demonstrates the model on a prospective case study of the ExxonMobil Baytown facility, showcasing a potential pathway of how the complex can decarbonise over a 30-year period.

2. Problem Statement

Given a set of plants and their production and carbon intensity data, find the optimal pathway of reducing emissions while meeting product demands over several time periods. Given a set of plants $z \in Z$ and their production demand D, this model chooses from a variety of different technologies, including CCS, NETs and renewable fuels, and returns output values of emissions, suggested technologies and total cost of production in each period $k \in K$.

3. Methodology

This section presents the constraints of the mathematical model created for the planning tool. For a period k, the sum of the total production from the various types of production plants should be equivalent to the total demand:

$$\sum_{k=1}^{K}(\sum_{z=1}^{Z} FS_{z,k}) = \sum_{k=1}^{K} D_k \qquad \forall k \tag{1}$$

where $FS_{z,k}$ is the production output of production plant $z \in Z$ in Mt/y. This is due to the fact an industrial process can either be made up of a single plant with a single product, or multiple plants making products in a complex. As many or as few plants can be added/ taken away from this equation depending on the type of case study being investigated. Parameter D_k is the total production demand D in period $k \in K$ in Mt/y. Although in reality there is a possibility that a company will not be able to fulfil demand due to a delay in supply chain, in this model it has been assumed that such delays are insignificant on average over the length of the time period considered, hence demand would overall be met. The next equation is that of the carbon intensity of the various plants when carbon, capture and storage (CCS) technology n is implemented. The equations are adapted from Nair, Tan and Foo (2021), where the carbon intensity of plant z etc in period k are as follows:

$$CR_{z,n} = \frac{CS_z \times (1 - RR_n)}{1 - X_n} \qquad \forall z \; \forall n \tag{2}$$

Here $CR_{z,n}$ are the carbon intensities of the plants in Mt CO_2/Mt, RR_n is the removal ratio of the CCS technology and X_n is the parasitic power loss associated with CCS implementation.

The net production output of the production plants with the CCS technology n in a period k can be calculated with the following equation:

$$FR_{z,k,n} \times (1 - X_n) = FNR_{z,k,n} \qquad \forall z\, \forall k\, \forall n \tag{3}$$

where $FR_{z,k,n}$ is the extent of CCS retrofit of plant z with CCS technology n in period k, given as the amount of CO2 the retrofit would have to capture in Mt/y, and $FNR_{z,k,n}$ is the net production output by plant z with CCS technology n in period k in Mt/y. This term $FNR_{z,k,n}$ should also not exceed its upper bound of production output in period k:

$$FNR_{z,k,n} \leq F_{z,UB} \times B_{z,k,n} \qquad \forall z\, \forall k\, \forall n \tag{4}$$

In this equation, $F_{z,UB}$ represents the upper bound of production output by power plant z and $B_{z,k,n}$ the binary variable for selection of plant z with CCS technology n in period k. Eq(5) shows a summation of the extent of CCS retrofitting applied to production plant z with all the CCS technologies applied in period k, and Eq(6) is a constraint to ensure that the total extent of retrofitting does need exceed the production output within period k:

$$\sum_{z=1}^{Z} FR_{z,k,n} = FR_{z,k} \times B_{z,k,n} \qquad \forall z\, \forall k \tag{5}$$

$$FR_{z,k} \leq FS_{z,k} \qquad \forall z\, \forall k \tag{6}$$

Here, the term $FR_{z,k}$ represents the extent of the CCS retrofit with all technologies to plant z. Additional equations have also been added to signify the summation of net production output if the production plants do not have CCS technology retrofitted to them ($FNS_{z,k}$) alongside the possibility of retrofitting ($FR_{z,k,n}$) and ensuring that they equate to the production output, shown in Eq(7). This possibility has been explored only for mixed or liquid fuel plants, while Eq(8) and Eq(9) incorporate the possibilities of alternative low CO2 intensity solid or gas-based fuels respectively.

$$FNS_{z,k} + \sum_{z=1}^{Z} FR_{z,k,n} = FS_{z,k} \qquad \forall k;\ when\ z\ is\ a\ mixed\ or\ liquid\ fuel\ plant \tag{7}$$

$$FNS_{z,k} + \sum_{z=1}^{Z} FR_{z,k,n} + \sum_{w} FAS_{z,k,w} = FS_{z,k} \qquad \forall k;\ when\ z\ is\ a\ solid\ fuel\ plant \tag{8}$$

$$FNS_{z,k} + \sum_{z=1}^{Z} FR_{z,k,n} + \sum_{v} FAS_{z,k,v} = FS_{z,k} \qquad \forall k;\ when\ z\ is\ a\ gas\ fuel\ plant \tag{9}$$

Here, w and v represent alternative fuel types for the production plants to run on. Eq(10) demonstrates the requirement for all production outputs from production plants, including compensatory production to make up for losses due to CCS and negative emission technologies equating the total demand for the period k.

$$\begin{aligned}\sum_{z=1}^{Z}\sum_{n}(FNS_{z,k} + FNR_{z,k,n}) + \sum_{z}^{Solid\ fuel}\sum_{w} FAS_{z,k,w} + \sum_{z}^{Gas\ fuel}\sum_{v} FAG_{z,k,v} + \sum_{r} FC_{k,r} + \sum_{p} FEP_{k,p} \\ = \sum_{q} FEC_{k,q} + \sum_{k=1}^{K} D_k \qquad \forall k\end{aligned} \tag{10}$$

In this equation, $FC_{k,r}$ represents the compensatory production in Mt/y, $FEP_{k,p}$ the production producing negative emission technologies (NETs) in Mt/y and $FEC_{k,q}$ the production consuming NETs in Mt/y. Constraints have also been added to ensure that the total emissions equal emission limits and total costs do not exceed budgetary constraints respectively, where L_k from Eq(11) represents the total emission limit in Mt/y and BD_k from Eq(12) represents the maximum budget in US$.

$$TE_k = L_k \quad \forall k \tag{11}$$

$$TC_k \leq BD_k \quad \forall k \tag{12}$$

Eq(13) shows total CO2 load from production equating total CO2 emissions at end of production period k.

$$\begin{aligned}&\sum_{z=1}^{Z}\sum_{n}(FNS_{z,k}CS_z + FNR_{z,k,n}CR_{z,n}) \\ &+ \sum_{z}^{Solid\ fuel}\sum_{w} FAS_{z,k,w}CIAS_{z,k,w} + \sum_{z}^{Gas\ fuel}\sum_{v} FAG_{z,k,v}CIAG_{z,k,v} + \sum_{r} FC_{k,r}CIC_{k,r} \\ &+ \sum_{p} FEP_{k,p}CIEP_{k,p} + \sum_{q} FEC_{k,q}CIEC_{k,q} = TE_k \qquad \forall k\end{aligned} \tag{13}$$

In Eq(13), CS_i, $CR_{z,n}$, $CIAS_{z,k,w}$, $CIAG_{z,k,v}$, $CIC_{k,r}$, $CIEP_{k,p}$ and $CIEC_{k,q}$ represent the carbon intensities of each term respectively in Mt CO2/Mt. The final term TE_k represents the total CO2 emissions at the end of production planning in period k. Eq(14) calculates the total cost of production in period k, represented by term TC_k which is in US$. Terms $CT_{z,k}$, $CTR_{z,k,n}$, $CTAS_{z,k,w}$, $CTAG_{z,k,v}$, $CTC_{k,r}$, $CTEP_{k,p}$ and $CTEC_{k,q}$ represent the costs of each respective technology.

$$\sum_{z=1}^{Z}\sum_{n}(FNS_{z,k}CT_{z,k} + FNR_{z,k,n}CTR_{z,k,n}) \\ + \sum_{z}^{Solid\,fuel}\sum_{w} FAS_{z,k,w}CTAS_{z,k,w} + \sum_{z}^{Gas\,fuel}\sum_{v} FAG_{z,k,v}\,CTAG_{z,k,v} + \sum_{r} FC_{k,r}CTC_{k,r} \\ + \sum_{p} FEP_{k,p}CTEP_{k,p} + \sum_{q} FEC_{k,q}CTEC_{k,q} = TC_k \quad \forall k \tag{14}$$

Further constraints have been made to ensure that any potential CCS retrofit carried out on a production plant is not reversed in a previous period, as shown in Eq(15):

$$(FR_z)_{k,n} \;\geq\; (FR_z)_k \qquad k = 1,2,\ldots,K-1 \tag{15}$$

The objective function for optimisation is a choice made by the user. They can either choose to minimise emissions in Mt/y based on some budget constraints, or to minimise costs in millions US$ to meet some emissions targets. These are shown below, with Eq(16) referring to budget and Eq(17) the objective function for emissions.

$$minTC_k \qquad \forall k \tag{16}$$

$$minTE_k \qquad \forall k \tag{17}$$

The mathematical model is a mixed-integer linear programming (MILP) model which was implemented in Pyomo, with a spreadsheet user interface for ease of data input. The values inputted for each period were the prospective productions in Mt/y and the initial carbon intensity values shown in Table 2. The increase in production from period to period were implemented to reflect the increasing demand of the respective products in reality, and the different increases depending on production plant were chosen to test the model as rigorously as possible with regards to the case study. As implemented, the time periods in this model represent five year periods. While it is accepted that there will be a discount rate for the cash flow between periods, the model will not be able to account for the unpredictable future pricing of technologies, or their readiness level in each future time period. The model has therefore adopted a uniform reduction in cost of technology between each time period, which can be changed by the user unique to each particular case. The model also does not account for every possible renewable technology available – instead it provides two or three options per technology which have different costs and levels of effectiveness.

4. Case Study

The model is demonstrated using a semi-hypothetical case study, with data taken from literature. As highlighted in previous literature, compiling accurate and recent data is a difficult task and is a common weakness shared in many policymaking planning projects (Musonye et al., 2021). In order to combat this, a hybrid case study was created, sourcing real life data from a range of sources. As many companies operating stationary sources have no sufficient data available for use, ExxonMobil's Baytown refinery complex was chosen as the ideal base for the hybrid case study due to its published production data, and the fact it had a range of different product plants on-site, making it ideal to test how the model would handle multiple data sources (ExxonMobil, 2021). The ExxonMobil Baytown refinery complex based in Texas, USA, is one of the biggest facilities of its kind in the US. Originally solely a refinery that began operations in 1920, the complex now boasts an additional three plants: a chemical plant, that activated in 1940, an olefins plant, activated in 1979 and a plastics plant, activated in 1982 (NS Energy, 2021). The exact product of each plant is unknown, and as a result, for the purposes of implementation they have been simplified to just 'products' (e.g., the products of Baytown refinery become 'Refinery products' instead of each individual element). To adapt equations 1 to 13 to the case study, general term z has been changed to reflect each plant, such that Baytown refinery is production plant i, Baytown Chemical plant is production plant j, Baytown Olefins plant is production plant l and Baytown Plastics plant is production plant m. The production data for the Baytown refinery was compiled from the ExxonMobil's website. The carbon intensity data was compiled from a variety of sources based on the processes required to produce the primary product. Many of the sources gave a range of data values for each process as it can differ from plant to plant and operation to operation, and so to simplify, a value was chosen from within the ranges, as shown in Table 1.

Table 1: Production of each plant in the Baytown refinery complex 2020 and approximate carbon intensities of Baytown complex plants with references of data

Plant name	Production in 2020 (Mt/y)	Process	Carbon Intensity (Mt CO_2/Mt)	Reference
Baytown Refinery	20	Refining	2.2	Jing et al., 2020
Baytown Chemical	1.6	Polymerisation	1.0	Pilz et al., 2010
Baytown Olefins	4.0	Cracking	0.8	Benchaita, 2013
Baytown Plastics	2.2	Polymerisation	0.6	Pilz et al., 2010

5. Results

With all the data compiled, the production, carbon intensities and emissions limits (reducing the emissions gradually to 0 Mt/y) were inputted into the model. The results are shown in Table 2 and Table 3 below:

Table 2: Results of Baytown Refinery and Chemical plant

	Baytown Refinery				Baytown Chemical			
	Production (Mt/y)	Technologies	Emissions (Mt/y)	Cost (Millions US$)	Production (Mt/y)	Technologies	Emissions (Mt/y)	Cost (Millions US$)
P1	20	None	44	980	1.3	None	1.3	139
P2	22	Renewable Biogas	45	1077	1.6	Renewable Biogas	0.37	158
P3	24	Renewable Biogas	40	1179	1.9	Renewable Biogas and NET	0	483
P4	26	Renewable Biogas	35	1272	2.2	Renewable Biogas and NET	0	451
P5	28	Renewable Biogas	30	1356	2.5	Renewable Biogas and NET	0	434
P6	30	Renewable Biogas	4.5	1430	2.8	Renewable Biogas and NET	0	421

Table 3: Results of Baytown Olefins plant and Plastics plant

	Baytown Olefins				Baytown Plastics			
	Production (Mt/y)	Technologies	Emissions (Mt/y)	Cost (Millions US$)	Production (Mt/y)	Technologies	Emissions (Mt/y)	Cost (Millions US$)
P1	4	None	3.2	260	2.2	None	1.32	179
P2	4.5	Renewable Biogas	1.03	301	2.4	Renewable Biogas	0.55	198
P3	5	Renewable Biogas and NET	0	749	2.6	Renewable Biogas and NET	0	541
P4	5.5	Renewable Biogas and NET	0	678	2.8	Renewable Biogas and NET	0	493
P5	6	Renewable Biogas and NET	0	655	3	Renewable Biogas and NET	0	467
P6	6.5	Renewable Biogas and NET	0	636	3.2	Renewable Biogas and NET	0	454

The suggested technologies from the model highlight the costs associated of attempting carbon neutrality when demand for resources is ever-expanding. The Baytown refinery would require a radical change in operation, as the model suggests replacing traditional natural gas with renewable biogas instead. This option would be difficult to implement in reality due to the abundant nature of traditional natural gas, however, it is predicted that methods of refining the renewable biogas options would be financially competitive by 2050 if carbon tax is introduced (Van der Zwaan et al., 2022). All three of the other plants in the complex were able to reduce emissions to zero by the third period by implementing a mix of renewable biogas fuels and NETs, with costs of production eventually decreasing as technologies become more affordable.

6. Conclusion

This study presents a new planning tool for decarbonisation in industrial enterprises over multiple time periods. Unlike previous tools, the model allows for planning decarbonisation pathways on a micro-scale, accounting for meeting production demand targets and energy demands, and the first to cover both. The model is formulated as an MILP, which can quickly provide optimised decarbonisation pathways from user inputs of production targets, carbon intensity data, to minimise emissions or budget. The model selects from a range of renewable technologies, namely CCS, NETs and renewable fuels. When used on the ExxonMobil Baytown Complex case study, the model suggests NETs and renewable biogas fuels as the most attractive options in helping the chemical, plastic and olefins plants to achieve zero emissions by the third period. Renewable biogas is also suggested to help reduce the oil refinery emissions from 44 Mt/y to 4.5 Mt/y over the course of six time periods. In future work, the model will be tested on an industrial case study, making use of real production data. Additional constraints will be added, accounting for the feasibility of introducing different technologies based on maturity relative to the host country, ensuring that the pathway provided by the model can be realistically achieved. Other constraints to be included would be the possibility that demand is not met immediately due to supply chain issues, and the inclusion of discount rates and technology learning curves to simulate cost decreases associated with technology readiness.

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