Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale, Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Pareto optimal solutions for decarbonization of oil refineries under different electricity grid decarbonization scenarios

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ABSTRACT

In response to global efforts to reduce carbon emissions, the oil refining sector, a major source of industrial emissions, has set ambitious decarbonization targets. This study analyzes trade-offs between minimizing CO_2 emissions and costs through the use of Pareto optimal solutions. A superstructure optimization framework evaluates various technological pathways and timelines, employing a bi-criterion optimization approach using the ϵ-constraint method. Results show that cost-effective, higher-emission solutions often involve natural gas-based technologies with carbon capture, while expensive, low-emission solutions favor electric power-based technologies. The analysis incorporates detailed assumptions about grid carbon intensity of varying degrees and accounts for varying national policies. Comparative case studies across locations highlight how grid carbon profiles influence optimal strategies, providing insights to inform local policies and incentivize technologies.

Keywords: Process Design, Optimization, Renewable and Sustainable Energy, Energy Policy, Carbon Capture, Decarbonization, Electrification

INTRODUCTION

With each successive UN Climate Change Conference, the need for decisive climate action becomes increasingly evident. This year, for the first time, Earth is projected to exceed the 1.5°C of warming above pre-industrial levels, emphasizing the need for immediate action [1]. In response, nations worldwide have implemented stricter carbon pricing mechanisms, and set more ambitious net-zero targets to mitigate the accelerating climate crisis. The industrial sector is a major contributor to these global GHG emissions, with the key contributors in the US being oil refining (15%), cement production (7-8%), steel manufacturing (7-9%), and chemical production (4-6%) [2]. In particular, the oil refining sector faces increasing pressure to align with these climate objectives, while maintaining economic viability.

A conventional refinery processes various types of crude oil with variable compositions to produce various products, including liquified petroleum gas, gasoline, jet fuel, diesel, and paraffin through distillation and conversion units like hydrotreaters, crackers, and reformers. Burning of fossil fuels for heat, the Fluid Catalytic Cracker (FCC), and the Steam Methane Reformer (SMR), are identified as the main primary sources of scope 1 emissions accounting for 94% of total CO_2 emissions [4]. Recent studies have explored future refinery configurations and potential decarbonization pathways. Griffith et al. [3] highlight the dual role of refineries as both major contributors to greenhouse gas emissions, and critical actors in transitioning to sustainable energy systems in their critical review of socio-technical systems. They emphasize the importance of tailored strategies, including carbon pricing, stricter emissions controls, renewable technology investments, and subsidies. Bryum et al. [4] advocate for low-carbon hydrogen fuels, electrification, and Carbon Capture and Storage (CCS) as key measures, proposing two conceptual designs for low-emission refineries. However, both studies offer qualitative insights without quantitative optimization strategies. Complementary analyses, such as those by Nixon et al. [5] evaluate the feasibility of CCS for oil refineries, and emphasize the need for combined approaches involving fuel substitution and emission offsets, while Li et al. [6] assess cost-effective CO_2 abatement technologies in China's refineries. These studies perform techno-economic assessments for different decarbonized technologies. Yáñez et al. [7] analyze CO_2 mitigation pathways for a Colombian oil refinery, while Sachs et al. [8] emphasize diverse technology mixes to meet climate targets, although their methodologies may not yield optimal solutions. Optimization-based approaches provide a more systematic perspective on refinery decarbonization. De Maigret et al. [9] employ a multiobjective optimization framework to minimize CO_2 emissions and costs for an Italian refinery, though their model focuses on short-term cost minimization without a transition timeline. Similarly, a paper by Zhang et al. [10] develops a multiperiod optimization model to obtain biomass-based retrofits, but omits options for scope-1 and scope-2 emission reductions. Beyond the refining sector, Sotiriou et al. [11] have developed a multi-objective optimization framework tailored to the dynamic policy context of EU member states, exploring trade-offs between stronger decarbonization ambitions and associated costs. This study has demonstrated the use of multi-objective optimization in planning problems involving longer time horizons.

Although techno-economic analyses are available for individual decarbonization initiatives, Chattopadhyay et al. [12][13] have highlighted the need for a specialized tool that can find decarbonization pathways for individual refineries based on specific factors such as production capacity, plant structure, and the cost of renewable energy sources. They have developed an optimization tool to address this problem. However, scope 2 emissions (stemming from the indirect consumption of purchased electricity) were not accounted for in their paper. The reality presents a complex landscape where scope 2 emissions significantly influence the economic viability, especially for electrification-based alternatives. This is relevant for multinational corporations whose refineries operate across different regions, each with unique regulatory frameworks and economic conditions. Our study addresses these limits and proposes a multi-objective optimization (MOO)-based framework for analysis. The rest of the paper is organized as follows; the various decarbonization pathways considered in the superstructure are presented, followed by the problem statement considered. A MOO problem modeling the superstructure by minimizing CO_2 emissions, and the present value of cost, are presented in the methodology section. Finally, in the results section, we compare the results obtained for Canada and the United States, subject to respective natural gas and electricity prices and carbon emission reduction policies.

The superstructure (Fig.1) consists of several decarbonized and current pathways for hydrogen production and steam generation. Alternatives for hydrogen production include traditional fossil-based processes, blue hydrogen production (involving steam methane reforming (SMR) augmented with post combustion or precombustion-based capture), and green hydrogen production via electrolysis, supported by technologies like proton exchange membrane electrolyzer (PEME) and alkaline electrolyzers (AE). Precombustion carbon capture requires less energy and is more cost-effective in terms of both capital and operational expenses. However, it is compatible only with gasification units that generate flue gas containing higher CO_2 concentrations. In contrast, post-combustion CO_2 capture, while demanding more energy, is capable of managing flue gas with lower CO_2 concentrations. Alkaline electrolyzers (AEs) are less energy efficient and have the drawback related to their shutdown current as they cannot operate at low current densities, but are cheaper than PEMEs. Process heating is achieved using high pressure steam (HPS), which is produced by natural gas boilers with or without carbon capture, or electric boilers. The superstructure also includes a pathway to capture CO_2 from flue gas emissions from other units such as FCC or furnaces, using post-combustion carbon capture. The problem involves strategic selection and timely implementation of the best set of initiatives for retrofitting the supply of HPS and hydrogen to the given refinery considering the operating data for a typical crude-based refinery, with a distillation capacity of 220 kbbl crude oil per day to minimize emissions and present value of cost.

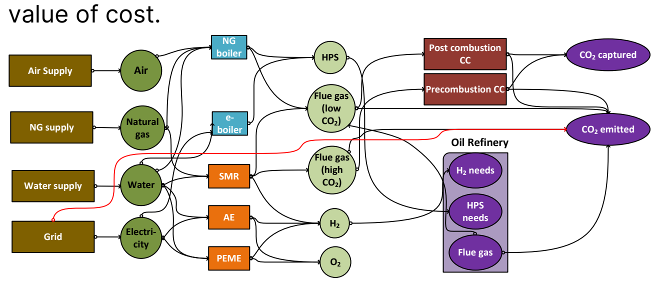

Figure 1. Superstructure showing options considered for decarbonization

METHODOLOGY

The variables used in the model are, $F_{k,j,yr}$, a positive continuous variable representing the amount of component k present in a stream flowing to or from a unit j in year yr. $y_{j,yr}$ is a binary variable indicating whether the installation of a specific unit of technology j (e.g. PEME, AE) takes place in the year yr. $Q_{j,yr}$; $(QE_{j,yr}/QD_{j,yr})$), a continuous variable indicating the total (expansion in/decommissioned) capacity of a technology j in a given year yr. These constraints apply to all years in the entire time horizon i.e. 2022-2040 unless specified otherwise.

Mass balance constraints

The proposed formulation requires specifying balances across the task nodes (or the technology units) and the resource nodes (or the components). The task balance involves Eqs. (1) and (2) relating the amount of components present in the inlet and outlet streams to a certain key component through simplified yield-based models. Eq. (1) represents a yield-based model where $\mu_{k,j}$ is the yield coefficient relating the flowrate of reactant k to produce a certain flowrate of key component k'_j in unit j. Similarly, in Eq. (2), $-\mu_{k,j}$ denotes the amount of by-product (e.g. CO_2) k in the outlet stream of unit j, given a certain amount of key component k'_j in the outlet stream. The total hydrogen and HPS produced across all pathways must match the refinery's overall hydrogen and HPS requirements. The CO_2 captured and emitted after passing through carbon capture units are proportional, determined by the efficiency of the respective CC equipment. Likewise, the steam generation and losses via the purge stream (blowdown) from boilers are proportional, governed by a constant factor.

$$F_{k,j,yr} = \mu_{k,j} F_{k_{j}',j,yr} \; if \; k \in \{In(j)\}, \mu_{k,j} \geq 0, \forall yr,$$

$$\forall j \in \{\text{AE, PEME, e-boiler, CC units, NG boiler, SMR}\} \; (1)$$

$$F_{k,j,yr} = -\mu_{k,j} F_{k_{j}',j,yr} \; if \; k \in \{Out(j)\}, \mu_{k,j} \leq 0, \forall yr,$$

$$\forall j \in \{\text{AE, PEME, e-boiler, CC units, NG boiler, SMR}\} \; (2)$$

Here, the notations $In(j)$ and $Out(j)$ represent the set of resource nodes connected at the inlet and outlet of node j respectively. Additionally, mass balances are imposed across the resource nodes as shown in Eq. (3). Here k denotes a particular component node and $In(k)$ and $Out(k)$ denote the set of task nodes connected at the inlet and outlet of resource node k. K denotes the set of all component nodes.

$$\sum_{l \varepsilon\, In(k)} F_{k,l,yr} = \sum_{j \varepsilon\, Out(k)} F_{k,j,yr} \quad \forall k \in \text{K}, \forall yr \; (3)$$

Energy balance and CO_2 intensity constraints

Energy balances for e-boilers, and electrolyzers are given by Eqs. (4) and (5) respectively where $P_{j,yr}$ denotes the power drawn from equipment j in a given year yr.

$$P_{\text{e-boiler},\, yr} \eta_{\text{e-boiler}} = \Delta H_{vap} F_{H_2O,\text{e-boiler},\, yr} \; \forall yr \; (4)$$

$$F_{Hydrogen,j,yr} \Delta H_{electrolysis} = P_{j,yr}\, \eta_j, j \in \{PEME, AE\}, \forall yr \; (5)$$

where η_j denotes the energy efficiency of equipment j. The emissions from the grid are calculated using the Eq. (6) Here CI_{yr} denotes the CO_2 intensity of the grid.

$$CI_{yr} \sum_{j \varepsilon\, Out(Grid)} P_{j,yr} = \text{F}_{\text{grid},\text{CO}_2,yr} \; (6)$$

Capacity expansion constraints

Eqs. (7) and (8) impose logical constraints on the capacity expansion/decommissioning capacity reduction in any year.

$$LB_j y_{j,yr} \leq QE_{yr} \leq UB_j y_{j,yr}$$

$$\forall \text{ j} \in \{\text{AE, PEME, e- boiler, CC units}\} \; (7)$$

$$LB_j y_{j,yr} \leq QD_{yr} \leq UB_j y_{j,yr} \; \forall \text{ j} \in \{\text{SMR, NG-boiler}\} \; (8)$$

Eqs. (9) and (10) evaluate the total capacity at the end of any year yr. [23, 19].

$$QE_{j,yr} + Q_{j,yr-1} = Q_{j,yr}$$

$$\forall \text{ j} \in \{\text{AE, PEME, e-boiler, CC units}\} \; (9)$$

$$-QD_{j,yr} + Q_{j,yr-1} = Q_{j,yr} \; \forall \text{ j} \in \{\text{SMR, NG boiler}\} \; (10)$$

Eqs. (11) and (12) state that the operating flow rate or power is less than the installed capacity and greater than a certain fraction (the minimum possible turn down χ_j) of the installed capacities.

$$\chi_j Q_{j,yr} \leq P_{j,yr} \leq Q_{j,yr} \;\; \text{j} \in \{\text{e-boiler, PEME, AE}\} (11)$$

$$\chi_j Q_{j,yr} \leq F_{k'j,yr} \leq Q_{j,yr} \; \text{j} \in \{\text{NG boiler, SMR, CC}\} (12)$$

We assume that the capacity expansion for e-boilers and CC facilities can vary continuously, while the expansion of electrolyzer capacity is restricted to discrete increments corresponding to standard sizes. To handle this, we introduce non-negative integer variables $w_{j,s,yr}$ which denote how many electrolyzers, in year yr, of type $j \in \{\text{PEME, AE}\}$ are of size s, where $s \in [1, \text{Num. of available discrete sizes}]$, with $d_{j,s}$ denoting the available sizes for each type of electrolyzer. Eq. (13) adds the size of all installed electrolyzers to calculate the total capacity expansion in any given year [10].

$$\sum_s w_{j,s,yr} d_{j,s} = QE_{j,yr} \;\; \text{j} \in \{\text{PEME, AE}\} \; (13)$$

Cost constraints and objective function

Eq. (14) expresses the total CAPEX for an expansion as $\alpha + \beta QE$, where α represents the fixed cost and βQE represents the variable cost, $dur(j)$ represents the time taken to build a unit of tech. j. Eq. (15) enforces an upper limit on the annual capital expenditure (CAPEX) that can be allocated to these decarbonization initiatives.

$$CAPEX_{yr} =$$

$$\sum_j \sum_{h=0}^{dur(j)-1} \frac{\alpha_{j,yr+h} y_{yr+h}}{dur(j)} + \sum_{h=0}^{dur(j)-1} \frac{\beta_{j,yr+h} \; QE_{j,yr+h}}{dur(j)} \; (14)$$

$$CAPEX_{yr} \leq CAPEX\; CAP \; (15)$$

The annual OPEX associated with decarbonization efforts, shown in Eq. (16), includes two key components: one arising from the use of natural gas and electricity, and the other, associated with the energy related to capture in CC units. The capture cost is directly proportional to the amount of emissions reduced via carbon capture.

$$OPEX_{yr} = \Bigg(\sum_{j \epsilon Out(NG)} \$_{\frac{NG}{unit\, mass}} F_{NG,j,yr} + \sum_{j \epsilon Out(Power)} \$_{\frac{electricity}{unit\, energy}} P_{j,yr} + \sum_{j \epsilon CCS\; Units} OPEX_j \, F_{Captured\; CO_2,j,yr} \Bigg) time \;\; (16)$$

Finally, we formulate the objective functions as the present value of the cost of the decarbonization project (17), and the total emissions over the transition period

(18). The amount of CO_2 and other gases present in the flue-gas released from the rest of the operations in the refinery are specified additionally.

$$Minimize\ \sum_{yr=1}^{19}(CAPEX_{yr} + OPEX_{yr})/(1+i)^{yr} \quad (17)$$

$$Minimize\ \sum_{yr=1}^{19}\sum_{j\,\epsilon In(CO_2\,emission)} F_{CO_2 emission,\,j,yr} \quad (18)$$

The ϵ-constraint method [14] is used to convert the second objective Eq. (18) into a constraint and the Pareto front is generated by plotting the ordered pair of objective values for the non-dominated solutions.

RESULTS

The retrofit MILP model was implemented in Pyomo 6.6.1 with the Gurobi 10.0.1 solver [15] for a 19-year horizon, involving 1,160 variables (133 discrete, 1,027 continuous) and 1,197 constraints. Results are presented for two case studies, based on energy prices, policies, and grid carbon intensities for Canada and the USA. The Pareto fronts from the bi-criterion optimization highlight the effects of carbon mitigation policies, such as carbon taxes and tax credits, on the cost-emissions trade-off. The analysis also examines the role of scope-2 emissions on the non-dominated solutions. The CAPEX for carbon capture technologies was modeled as a linear function of the processed CO_2, with an intercept. Similarly, CAPEX for electrolyzers and e-boilers vary linearly with an intercept installed capacity, reflecting economies of scale. OPEX for carbon capture was tied to the amount of CO_2 captured.

Canada

Electricity and natural gas prices for Canada, sourced from [16] [17] and shown in Figure 2 (a) and (b), were used to estimate the operational costs. While Canada aims for a net-zero electricity grid by 2035 [18], our scenarios project a 100% emissions reduction by 2040 (optimistic), 2043 (baseline), and 2045 (pessimistic), based on predicted greenhouse gas emissions from Annesley et al. [19] and grid mix forecasts from Canada's Energy Future 2021 [20] (shown in Fig. 2 (c)).

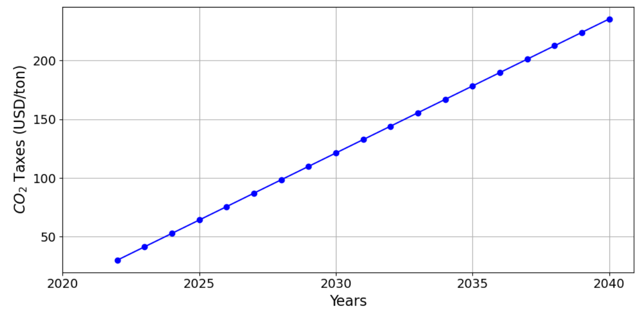

Figure 3. CO_2 taxes implemented as per Canadian rates

When CO_2 taxes are implemented as per the rates shown in Figure 3, we see that the Pareto front compresses towards low emission solutions as compared to the baseline solution (shown in Figure 4). Beyond a certain point, increasing the ε value does not reduce CO_2 emissions further, as the ε-constraint becomes inactive. Remaining within the ε limit is financially advantageous due to the penalties for exceeding it. Non-dominated solutions incur higher costs than the baseline due to the imposed penalties. Figure 5 shows that low-cost, non-dominated solutions obtained when CO_2 taxes are

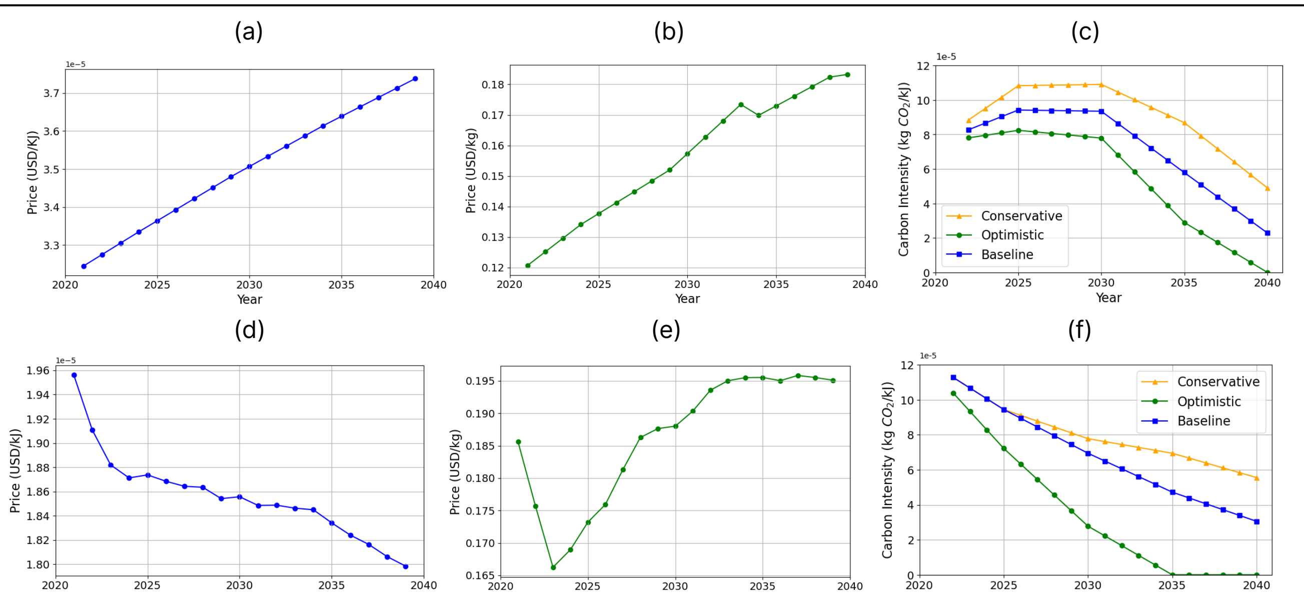

Figure 2 (a) Canadian electricity price forecasts (b) Canadian natural gas price forecasts (c) Carbon intensity scenario forecasts for Canadian grid (d) US electricity price forecasts (e) US natural gas price forecasts (f) Carbon Intensity Scenarios for US grid

implemented. These favor carbon capture options. For higher cost and lower emission non-dominated solutions earlier, and higher adoption of both pre- and post-combustion carbon capture takes place. Since no cases include e-based options, variations in grid intensity profiles have no significant impact on the Pareto front.

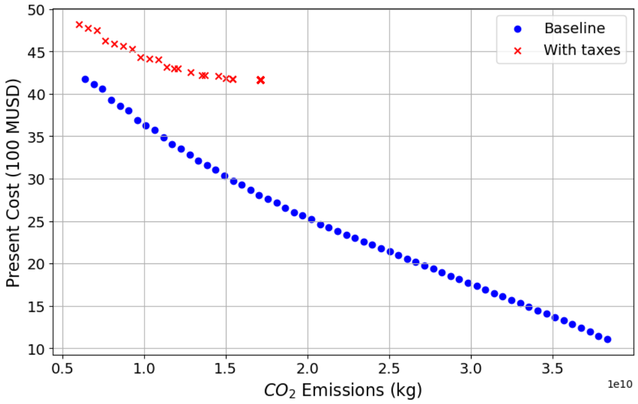

Figure 4. Pareto front with CO_2 taxes implemented

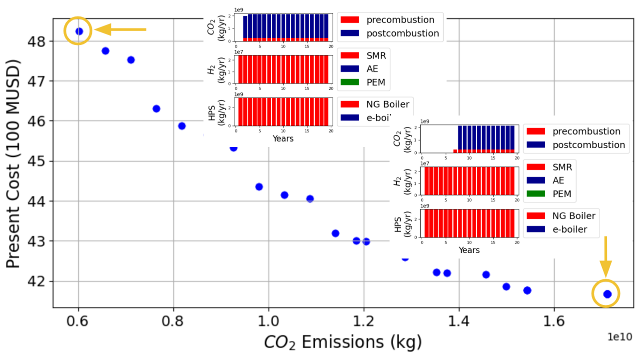

Figure 5. Canada with CO_2 taxes: Pareto front with the solutions shown for a few points.

United States

The electricity and natural gas price projections, based on EIA data (Figure 2 (d) and 2 (e)), were used to estimate the operational cost estimates. Carbon intensity scenarios for the electricity grid included 3 cases with the optimistic case, predicting a 100% reduction in emissions by 2035, baseline 95% by 2050, and the pessimistic case 65% by 2050, informed by Leard et al [21]. Evaluating the effect of scope-2 emissions for different carbon intensity profiles of the grid (as shown in Figure 2 (f)) on the non-dominated solutions, we see in Figure 6 that with higher grid CO_2 intensities, carbon capture (CC)-based solutions were favored over e-based alternatives. The point on the Pareto-front with the lowest CO_2 emissions involve e-based solutions but was feasibly obtained only with the optimistic grid intensity predictions as shown in Figure 6. As per the 45Q tax credit rates under the Inflation Reduction Act USD [22], $ 85 are provided per metric ton of CO_2 captured and stored securely underground. It is assumed that the 45 Q credits increase at the same rate as the carbon taxes. Additionally, according to the 45 V tax credits, at least 0.6 USD tax credits are provided per kg of green H_2 produced. With the imposition of these incentives, as shown in Figure 7, the Pareto front shifts towards low-emission solutions, though the NPV values are lower than the base case due to the received credits. As shown in Figure 8, the non-dominated solutions resemble those in Figure 3, but the highest-cost, lowest-emission solution includes partial adoption of e-boilers.

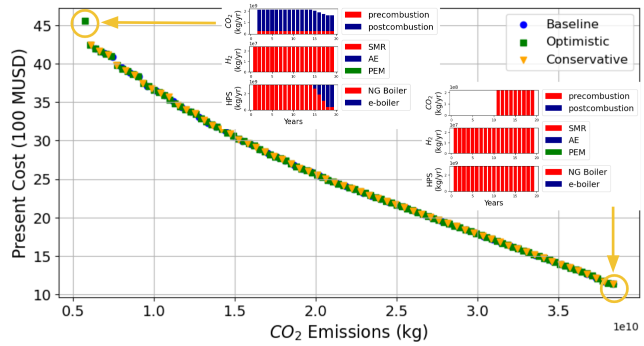

Figure 6. US : Pareto front under changing grid intensity profiles.

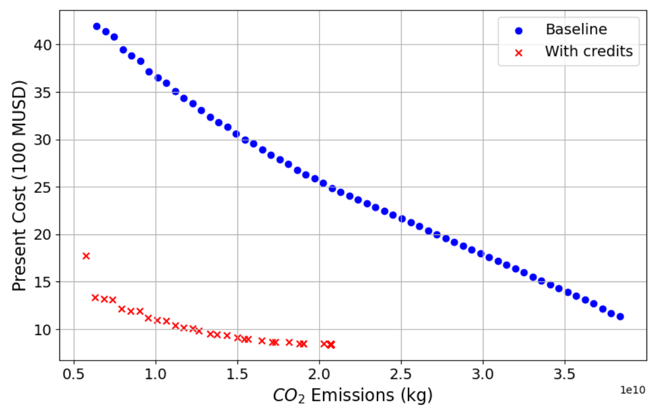

Figure 7. Pareto front with CO_2 credits implemented

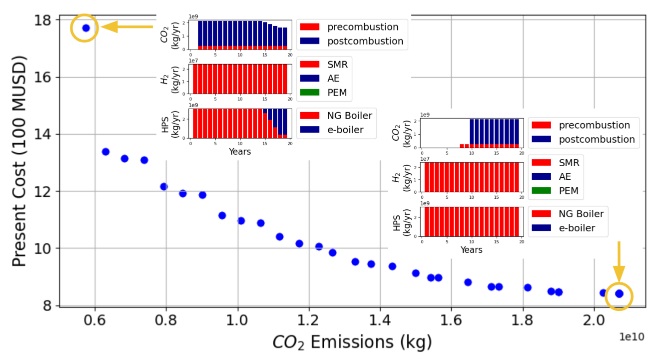

Figure 8. US with carbon credits: Pareto front with the solutions shown for a few points

CONCLUSIONS

The multi-objective optimization framework developed in this paper, minimizes retrofit decarbonization costs and CO_2 emissions, providing insights into the trade-offs between cost and emissions under various scenarios. Solutions incorporating carbon capture (CC) equipment were unaffected by changes in grid intensity, with several non-dominated solutions favoring earlier adoption of CC. E-based technologies are chosen exclusively when CO_2 emissions reach their minimum on the Pareto front, assuming the grid's CO_2 intensity decreases in line with optimistic projections. Carbon mitigation policies, such as carbon taxes and 45Q/V tax credits. compress the Pareto frontier toward low-emission, high-cost solutions, demonstrating their effectiveness in incentivizing aggressive emission reductions.

ACKNOWLEDGMENTS

This work was financed [in part] by a grant from the Commonwealth of Pennsylvania, Department of Community and Economic Development. We acknowledge the support and funding from Shell Global and Shell Polymers Monaca.

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