

Economic Optimization and Impact of Utility Costs on the Optimal Design of Piperazine-Based Carbon Capture

Ilayda Akkor^{a*}, Shachit S. Iyer^b, John Dowdle^b, Le Wang^b, and Chrysanthos Gounaris^a

^a Carnegie Mellon University, Department of Chemical Engineering, Pittsburgh, PA, USA

^b The Dow Chemical Company, Lake Jackson, Texas, USA

* Corresponding Author: iakkor@andrew.cmu.edu.

ABSTRACT

Recent advances in process design for solvent-based, post-combustion capture (PCC) processes, such as the Piperazine/Advanced Flash Stripper (PZ/AFS) process, have led to a reduction in the energy required for capture. Even though PCC processes are progressively improving in Technology Readiness Levels (TRL), with a few commercial installations, incorporating carbon capture adds cost to any operation. Hence, cost reduction will be instrumental for proliferation. The aim of this work is to improve process economics through optimization and to identify the parameters in our economic model that have the greatest impact on total cost to build and operate these systems. To that end, we investigated changes to the optimal solution and the corresponding cost of capture considering changes in the price of utilities and solvent. We found that changes in solvent price had the most effect on the cost of capture. However, re-optimizing the designs in the event of price changes did not lead to significant improvements in the case of piperazine, cooling water and electricity, whereas re-optimizing for changes in steam prices lead to yearly saving of 3.8%. These findings show that the design choices obtained at the nominal optimal solution are insensitive to utility price changes except for the case of steam and that there is a need for altered designs for locations where the steam prices are different.

Keywords: post-combustion carbon capture, rate-based model, optimization, nonlinear programming, sensitivity analysis.

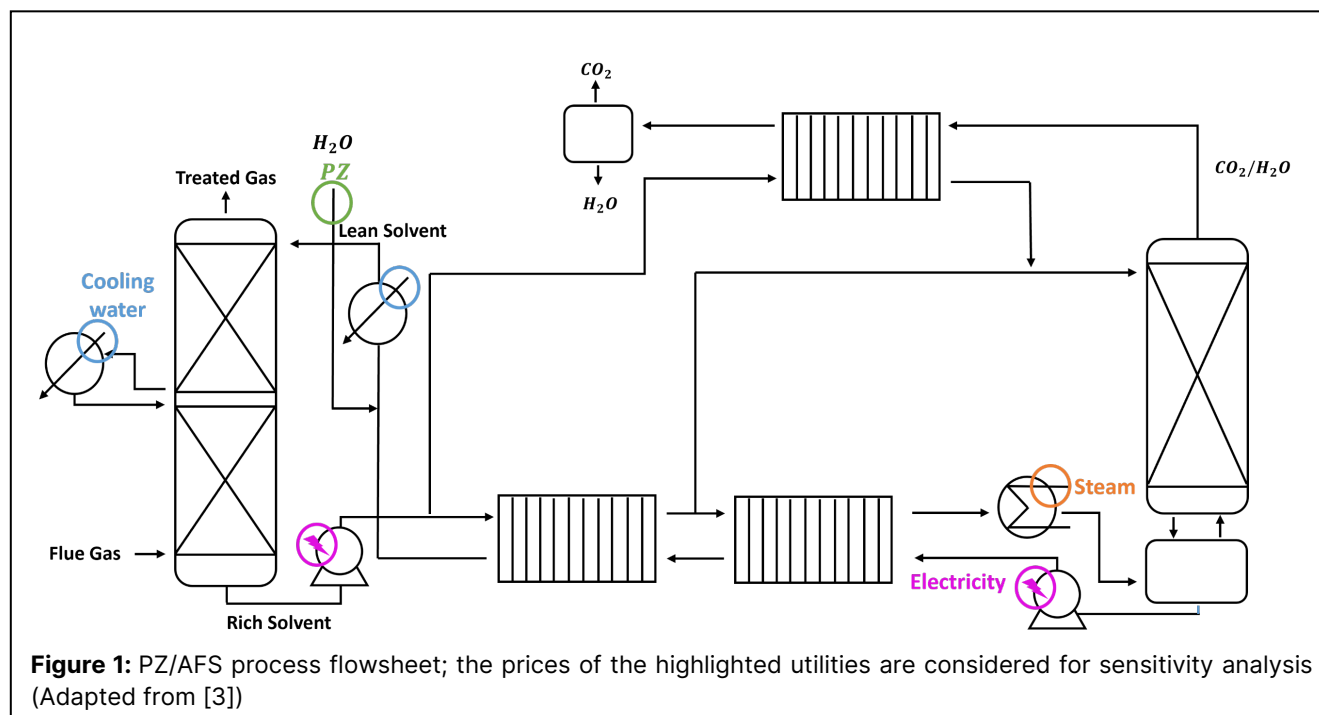
INTRODUCTION

Solvent-Based Carbon Capture Process Modeling

Solvent-based post-combustion carbon capture (PCC) processes are the most promising way to mitigate the increasing CO₂ emissions. There has been significant focus on trying to reduce the energy and cost required for capture, one prominent example being the Piperazine/Advanced Flash Stripper (PZ/AFS) process [1], shown in Fig 1. This novel process uses PZ as the solvent and the AFS process design, as shown. Flue gas containing CO₂ is contacted with the CO₂-lean solvent in a packed absorber column. An intercooler in the middle of the column, as well as a cooler at the top, are used to drive down the solvent temperature to improve absorption. After leaving the absorber, the CO₂-rich solvent passes through a heat exchanger network that has two

split streams; one of which is pumped directly to the top of a stripper column, while the other is pumped to a steam heater as shown in Fig 1. After the solvent is further heated in a steam heater, it gets flashed inside of a flash tank where the resulting vapor then enters the stripper column. After stripping, a vapor phase containing a CO₂ - water mixture exits the column from the top. It is then cooled down in a heat exchanger and finally separated out in a condenser drum. The lean solvent recovered in the flash tank is pumped back to the absorber column with the addition of make-up PZ and water.

The economics of PCC processes can be improved by optimization, which requires a mathematical model of the process. Hence, a detailed model of the PZ/AFS process was built using an equation-oriented approach in the IDAES framework, an open source, Python-based modeling medium [2]. In addition to the absorber and stripper columns, our model also includes the flash tank, all heat exchangers, and a recycle stream with solvent



make-up. For the columns, a rate-based modeling approach was used (as opposed to equilibrium-based), and a finite-difference scheme was used for discretization of the system of differential algebraic equations (DAE). This led to a highly nonlinear programming (NLP) model with over 8600 variables and constraints. The solution strategy includes a tailored, multi-level initialization cascade for reliable model convergence [3]. Once the model results were validated with pilot plant data [4], economic optimization was performed, which resulted in identifying the design and operating conditions that led to a considerable reduction in the capital and operational costs compared to the baseline, at the pilot scale [3]. To test the robustness of the model and to aid the commercialization of this process, optimization was performed for varying plant capacities (processing up to 1500 times more flue gas than the pilot scale) and for feed gases with different CO_2 concentrations to represent different flue gas sources that may arise in practice [3].

Parameter Uncertainty and Variability

In chemical process models, there are many parameters that are uncertain or subject to variability which, if disregarded by the model, lead to solutions that may not be truly optimal or even feasible in real life. Hence, it is crucial to account for these during the design phase. Uncertainty in a parameter stems from a lack of knowledge of its exact value, whereas variability is concerned with a parameter that may take on a different value, for example at a different point in time or at another location [5]. In the context of process models, these parameters can be categorized into three groups: (1) *epistemic parameters*, which are inherent in any process model, and which stem

from the approximating nature of correlations used to evaluate properties (kinetic, thermodynamic, transport) and the overall assumptions made therein; (2) *operational parameters*, which pertain to the upstream conditions and may be subject to temporal variations, e.g., composition, flowrate and/or temperature of the flue gas; and (3) *economic parameters*, such as the applicable prices for utilities and the solvent.

To identify which of the above are most impactful and to quantify the extra costs necessary for designs to insure against them, a series of sensitivity analyses were conducted. More specifically, the aim of this work was to leverage the equation-oriented model that we had previously built to gather insight on the impact of the economic parameters on the optimal process designs. In our previous study it was seen that, at the commercial scale, along with the purchase cost of the absorber column, the operating expenses for cooling water, steam, electricity, and solvent renewal were the dominating costs [3]. Therefore, this study further investigated the sensitivity of the plant design and its total cost to the prices of said utilities and to the piperazine solvent.

METHODOLOGY

For this study, we chose to perform sensitivity analyses on the commercial scale, natural gas combined cycle (NGCC) flue gas processing plant. The feed gas flowrate was 30,000 mol/s, and the parallel train configuration was used as it was done in the Mustang Station plant, presented in the work of Clossmann et al. [6]. The optimization problem was structured to minimize the total annualized cost (TAC), subject to some performance

constraints, such as a 96% capture target and flooding constraints for the columns [3]. Thirteen degrees of freedom were the packed length and the inner diameter of the absorber and stripper columns, the areas of the three heat exchangers, the two coolers and the steam heater, two bypass ratios, and solvent circulation rate. The first ten were the decision variables related to design, which must be committed before building the plant, whereas the bypass ratios and the solvent amount were operational decisions that can be adjusted.

The parameters that we focused on were the prices of the utilities (e.g., steam, cooling water and electricity) and piperazine, which were nominally assumed to be at the values given in Table 1. Cooling water was used for the two coolers, as shown in Fig 1. It must be noted that the optimal solution for the nominal case for the commercial-scale natural gas combined cycle (NGCC) flue gas processing plant does not use the intercooler. Hence, in the nominal solution, cooling water is only needed for the lean cooler at the top of the absorber column. However, the optimal solution for the cases that consider price variation, the inclusion of intercooler is allowed as a degree of freedom. Steam is used to heat up the rich solvent in a heater before it enters the flash tank. Electricity is needed for pumping the lean and rich solvents between columns. Our economic model considers operational expenses for these utilities as a fixed per unit price. To compensate for any losses, make-up of water and piperazine is needed to close the recycle loop. However, in a real-world plant operation, the lost piperazine is mostly

recovered in a water wash section above the absorber column. Therefore, cost of make-up is not additionally considered in our economic model. Instead, the cost of the solvent initially used in loading up the system is included in the capital costs at the design stage. Thereafter, it is assumed that the entirety of the solvent will be renewed every three years to make up for losses and degradation. This cost is included in the operational costs.

Table 1: Fixed prices assumed for utilities and piperazine.

Utility	Price
Piperazine	3750 \$/ton
Steam	14.5 \$/ton
Cooling water	0.0329 \$/ton
Electricity	0.06 \$/kWh

Optimal designs and corresponding operating conditions are obtained for cases for which the prices of selected parameters are changed stepwise up to a range of ± 50 . CONOPT was used as the solver for solving this nonlinear optimization problem [7]. By reoptimizing the system for each case with respect to all degrees of freedom (both design and operational), we can see how designs change and how the overall cost changes with the utility prices. The insights gained from this study are particularly useful when designing plants for geographies or markets with different applicable utility prices. Additionally, the parameter that has the greatest impact on total

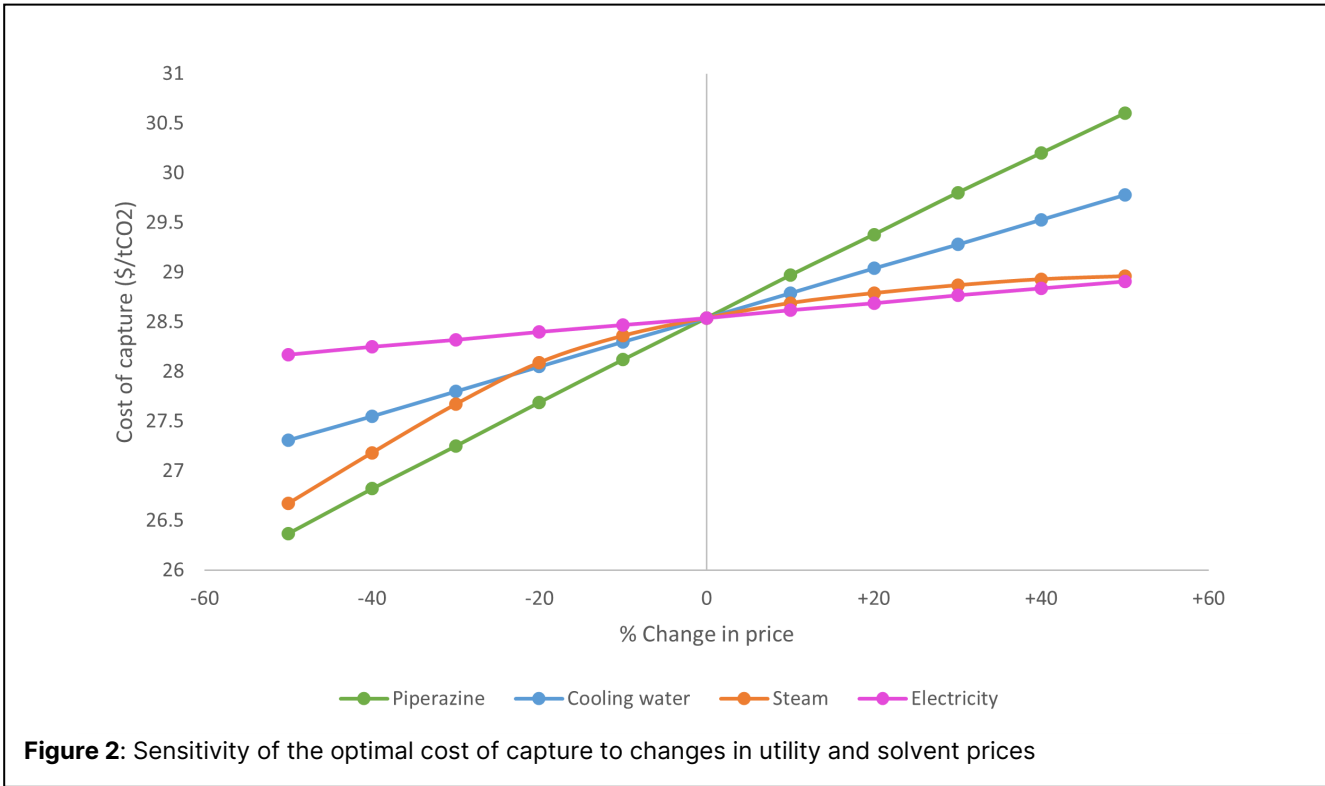


Figure 2: Sensitivity of the optimal cost of capture to changes in utility and solvent prices

cost can be identified along with design optimizations that can mitigate the impact of its price change.

SENSITIVITY OF OPTIMAL DESIGN TO ECONOMIC PARAMETERS

The corresponding changes in the optimal cost of capture with changing utility and solvent prices is shown in Fig 2. It is observed that the change in the price of piperazine has the most significant effect on the cost. This is due to the way solvent renewal is accounted for in our economic model, where it is a part of both capital and operational expenditures. Moreover, while there is flexibility in the usage amounts of utilities, a certain base amount of solvent needs to be used to achieve a given capture target no matter what. It is observed that electricity has the least impact on the cost of capture. This could be because our model does not consider a compressor train, so electricity is only used for running the pumps. The column pressures are not allowed to vary, therefore the only decision variable that would affect the electricity consumption is the amount of solvent circulated. While all cost curves are mostly linear, the curve representing steam becomes non-linear at lower prices, with the cost of capture becoming more sensitive to steam for price decreases beyond 20%.

To further investigate the sensitivities to price changes, the optimal solutions were compared to results from the baseline case, where price changes were implemented on the nominal solutions but without any optimization. For steam, reoptimizing the process design for price changes can lead to savings up to 3.8% (around \$1.6M yearly) compared to the baseline solution. The most significant difference is observed in the case of steam as compared to other parameters. Reoptimizing for different prices of piperazine leads to savings up to 0.2% (around \$100k yearly). However, for cooling water and electricity, reoptimizing did not lead to significant changes. The new solutions did not deviate from the original solution significantly. The nominal optimal solution is therefore robust for the changes in the price of electricity and cooling water. However, it must be noted that these are local optimal solutions, which can be dependent on initialization. Since each problem is initialized from the nominal solution, a better solution further away from the nominal case can not be ruled out.

Sensitivity to Steam

The effect of changes in steam price on the optimal solution along with the percent reduction in the optimal Total Annualized Cost (TAC) were further investigated. Fig 3 shows the change in the steam consumption with price changes. When the price is increased by 50%, very little steam is used, with a steam heater area that is almost $1/6^{\text{th}}$ of its original size. When the price is decreased

by 50%, the change in steam consumption is much more pronounced. This also reflects in the reduction of TAC as seen in Fig 3. For price changes between -50% and -30%, we can see a significant reduction in TAC. The steam consumption also changes sharply after the -30% price change point. This is also evident in Fig 2, where the curve representing steam shows nonlinear behavior.

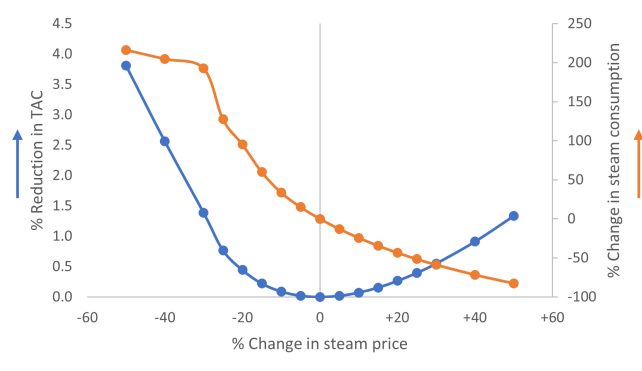
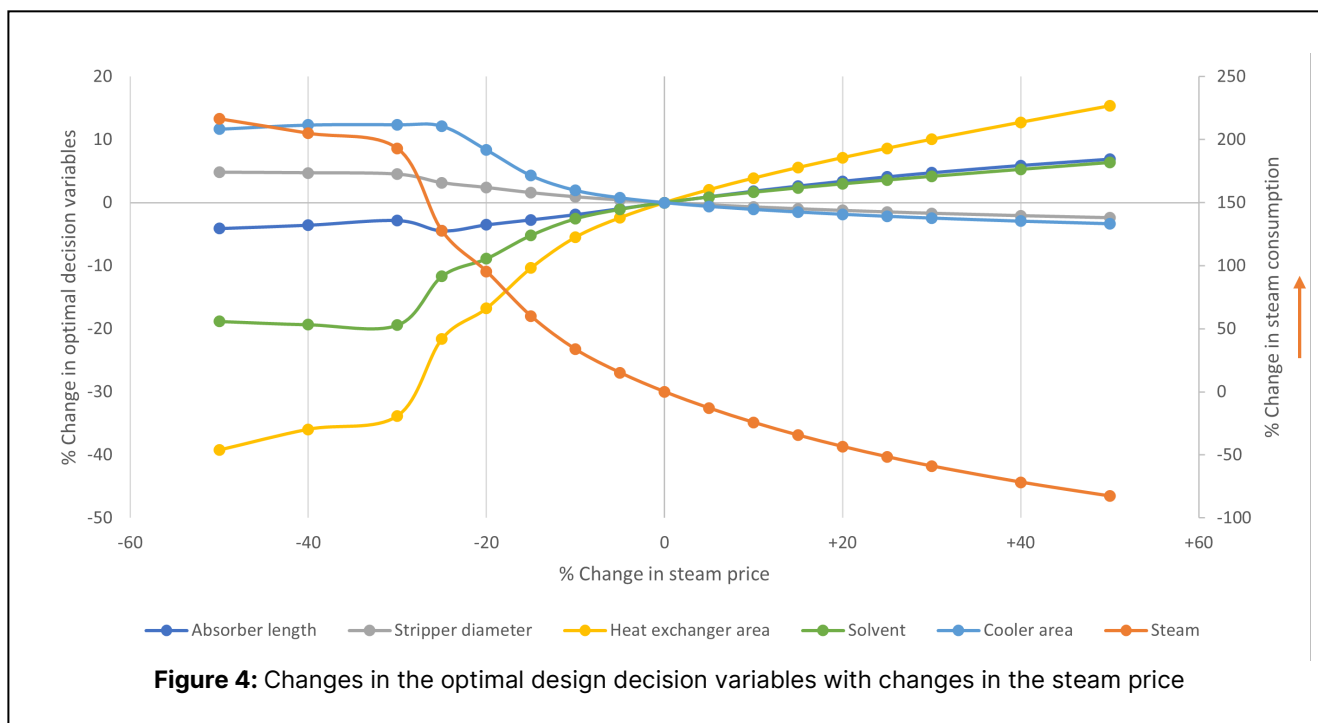


Figure 3: Percentage reduction in TAC by redesigning for different steam prices

The change in the values of the other decision variables given the steam price changes are shown in Fig 4. Once again, we observe the jump to a better solution at the -30% price change point. The cooler area and the stripper diameter have a similar trend with the steam consumption where they decrease with increasing steam prices. Using more steam increases the temperature of the lean solvent being pumped back to the absorber. Therefore, a bigger cooler and a higher cooling water consumption is needed when more steam is used as the system would now need more cooling. Usage of more steam also decreases the lean loading since more CO_2 is flashed from the rich solvent at a higher temperature. Moreover, since more water and CO_2 are flashed with increased steam usage, the gas flowrate within the stripper column increases, leading to a need for larger diameter. However, its change from the nominal solution is around 10%.

The packed absorber length, solvent flowrate and the total heat exchanger area show an opposite trend with steam consumption. Since more steam and cooling water are used, there is less of a need for the heat exchangers. Thus, at low steam prices, there is a significant (reaching up to 40%) reduction in the total heat exchanger area needed. Cooling improves the absorber performance since absorption is exothermic. As discussed above, using more steam leads to more cooling water consumption therefore, we can use a shorter column when steam prices are low. However, the change in absorber packing height is less significant. Similarly, since increased cooling water improves absorption and more steam improves stripping, less solvent may be used



to achieve the same capture target. Indeed, we can see that 20% less solvent is used for the cheapest steam price case.

CONCLUSIONS

We leveraged the optimization capabilities of the equation-oriented model of a novel solvent-based PCC process that we had previously developed to find cost-optimal solutions considering variation in economic parameters. This was done through a series of parameter sweeps on the price of cooling water, steam, electricity, and the solvent. The prices were perturbed in steps up to a range of $\pm 50\%$. Piperazine had the most significant effect on the change of cost of capture while electricity had the least effect. Upon comparing the nominal solutions obtained for each price change from the baseline with those solutions obtained on re-optimizing for each price change, it was observed that only changes in steam price had a significant impact. Thus, we infer that the optimal solution for the nominal case is robust to changes in the price of cooling water, electricity and piperazine. In contrast, for steam, an optimal value with significant differences from that of the nominal solution was obtained for different prices. This change was significant for cheaper steam prices, where yearly savings of 3.8% were obtained when reoptimizing for 50% cheaper steam. For this case, a bigger cooler and a larger stripper diameter was chosen, while savings were achieved through using a shorter absorber column, lesser solvent amount, and smaller heat exchangers. So, if this plant was to be

implemented at different locations where different steam prices apply, it is worth changing the design accordingly, whereas for the other utilities this may not be a concern.

There are many more parameters in this model that could be considered uncertain. When transitioning into an optimization under uncertainty framework, it is important to pre-screen the parameters with the highest impact through sensitivity analyses as shown in this work. In the future, more parameters relating to epistemic and operational uncertainty should be investigated and the sensitivity of the total cost to said parameters should be ranked in a systematic way. Another future direction could be to assess the flexibility of a design by optimizing solely over the decision variables related to operation.

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