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Optimal steady-state design of a post-combustion CO₂ capture plant under uncertainty

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Abstract

This paper presents a study on the effect of process uncertainty on the optimal design of a CO₂ capture plant. A recent method in the optimal design of large-scale chemical processes under uncertainty, which employs Power Series Expansion (PSE) models to approximate the process constraints, has been used in this work due to its computational benefits. Uncertainty in the CO₂ content in the flue gas stream entering the plant is assumed; the problem under analysis aims to find the most economically feasible design, by sizing the plant’s process equipment, as well as obtaining its optimal operating conditions, in the presence of uncertainty. The results show that process uncertainty have a direct effect on the sizes of the absorber and stripper columns and operation of the reboiler duty, whereas the cross heat exchanger and condenser’s heat transfer areas are not significantly affected.

1. Introduction

Among all the greenhouse gases, carbon dioxide is considered to have the most impact on global warming [1–4]. CO₂ capture and storage is a strategy that has been adopted in chemical industries for controlling CO₂ emissions [5–7] where post-combustion using chemical absorption [8–11] is a developed method for capturing CO₂ from flue gas. An MEA-based post-combustion CO₂ capture unit consists of an absorption tower where the amine solvent comes into contact with the entering flue gas (rich in CO₂), a stripping column to regenerate the amine solvent using heat supplied by reboiler steam, along with other heat transfer equipment. There have been numerous studies to obtain the

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optimal design and operation of MEA-based post-combustion CO₂ capture plants [12–19]. These studies were conducted at steady-state operation and assume that all the model parameters are completely known. However, uncertainty in the input variables or parameters is almost inherent in every process due to errors in measurements or lack of accurate process knowledge. Therefore, optimal designs of the CO₂ capture plant obtained using steady-state calculations may not be feasible while operating under process uncertainty. Studies of optimal design under uncertainty have been widely reported in the field of process systems [20–24]. With respect to CO₂ capture plants, there have been several studies that have accounted for uncertainty in the prices of economic parameters (such as fuel, CO₂, electricity) to obtain the optimal timing of investments or technology selection for power generation plants coupled with CO₂ capture units [25–32]. Nevertheless, those studies have not analyzed the effect of process-level uncertainties on the optimal design and operation of the CO₂ capture plant flowsheet, which, to the authors’ knowledge has not yet been reported in the open literature.

This article presents a study of the effect of process uncertainty on the optimal design of a CO₂ capture plant. A recent ranking-based approach for optimal design under uncertainty proposed by Bahakim et al [33] uses a Power Series Expansions (PSE)-based model to approximate large-scale nonlinear chemical processes has been used in this work to address the optimal design. The approach is efficient because it does not require simulating the plant model many times. Flue gas from power plants represents the main input to amine-based CO₂ capture plants, and thus uncertainty in this stream will be considered while designing the main process equipment of the plant. The organization of this paper is as follows: Section 2 describes the PSE-based method in approximating actual nonlinear models, along with the optimal design under uncertainty formulation. An explanation of the CO₂ capture process along with the implementation and formulation of the problem is presented in Section 3. Results and discussions are presented in Section 4. Concluding remarks are presented in Section 5.

2. Optimal process design under uncertainty: PSE-based method

A process model \( J \) of the system under analysis is assumed to be available for simulations and is represented as follows:

\[
J(d, \kappa, x, \gamma, u, \delta) = 0
\]  

(1)

where the model outputs and inputs of the process are denoted by \( \gamma \) and \( u \), respectively, \( \kappa \) is the model parameters, \( x \) represents the state variables, and \( d \) is the vector of design variables. Uncertainty in the model inputs or parameters is denoted by \( \delta \) and is assumed to follow a certain probability distribution function (PDF) with distribution parameters \( \psi \), i.e.,

\[
\delta_c \sim \text{PDF}(\psi_c) \quad c = 1, 2, \ldots, C
\]  

(2)

where each of the \( c \) uncertain variables will be assigned a specific PDF with its own distribution parameters \( \psi_c \). The choice on the PDF usually comes from process heuristics or process experience or plant data analysis. Typically, normal or uniform distributions are considered reasonable assumptions as they fit well most of the engineering applications [34]. Once the PDF description of the uncertainties are set, \( N \) random Monte Carlo sampling from each PDF can be generated to obtain a set of \( N \) uncertain realizations for each uncertain parameter. To accommodate the input uncertainties, the optimal design need to satisfy the process constraints to become feasible. The process constraints are formulated as follows:

\[
h(\kappa, x, \gamma, u, \delta) \leq 0
\]  

(3)

where \( h \) represent the set of process restrictions such as environmental, operational or safety constraints. In the present method, the actual process constraints \( h \) are approximated by PSE-based models (\( h_{\text{PSE}} \)) as follows:
where $S^{(i)}$ refers to the $i^{th}$ sensitivity term of constraint function $h$, i.e., the first and second terms represent the Jacobian and Hessian matrices of the process constraint function $h$, respectively; $\delta$ are the steady-state values of the uncertain variables. $h_{PSE}$ is an approximation to the actual nonlinear process constraint $h$; a thorough discussion on the approximation used by the present method is presented in [33]. In this method, a probabilistic ranking-based approach has been adopted, where each constraint will be assigned a user-defined probability of satisfaction ($Pr_h$) value which will act as the minimum probability that particular constraint is expected to remain feasible when operating under uncertainty. From the process constraint histogram obtained by evaluating the PSE-based model for all sampled uncertainty realizations, an extreme possible value $\omega_{h_{PSE}}$ with respect to the input probability ($Pr_h$) can be calculated as shown in Figure 1.

![Process constraints' distributional analysis](image)

**Figure 1** Schematic representation of the process constraints' distributional analysis.

The extreme possible value $\omega_{h_{PSE}}$ refers to the highest possible value that the constraint will attain ($Pr_h$ %) of the time when operating under input uncertainties. Therefore, the probabilistic form of the process constraints can be expressed as follows:

$$P(h(\mathbf{k}, \mathbf{x}, \gamma, \mathbf{u}, \delta) \leq 0) \geq Pr_h \quad \iff \quad \omega_{h_{PSE}} (Pr_h) \leq 0$$

(5)

The choice of the user-defined $Pr_h$ values is an engineering decision that constitutes a tradeoff between reduced constraint violations and increased plant costs. Critical (safety) constraints are usually assigned very high values to ensure safe operation of the process. When the process constraint is assigned a probability limit close to unity ($Pr_h \to 1$), conservative designs are obtained and this is called the worst-case approach. Based on the above explanations, the optimal design of a process system under uncertainty can be formulated as follows [33]:
The above optimization formulation minimizes the objective cost function $\Phi$, typically described in terms of the capital (CAP) and operating (OP) costs, by selecting feasible process designs $d$ and operating conditions or model inputs $u$, which are aimed to satisfy the process constraints, at minimum cost, under process uncertainty. More details about the ranking-based method used in this work can be found in [33].

3. Optimal design of a post-combustion CO$_2$ capture plant

Figure 2 presents a schematic diagram of a typical amine-based carbon capture unit. Flue gas rich in CO$_2$ enters the absorber column where a solvent, typically monoethanolamine (MEA), absorbs the CO$_2$. To regenerate the amine solvent (now rich in CO$_2$), this is heated with steam from a reboiler inside a stripping column, resulting in a CO$_2$ product at the top of the stripper column whereas the regenerated amine solvent at the bottom is recycled back to the absorber to continue removing CO$_2$. In addition, the process includes a cross heat exchanger, which maintains the process temperatures within limits, and a condenser unit at the top of the stripper to ensure high CO$_2$ product purity is achieved.

The problem considered in this work aims to optimize the design of the main process equipment and the operation of the CO$_2$ capture (CC) plant, i.e., the heights and diameters of both packed columns, the heat transfer areas of both the cross heat exchanger and the condenser, and the heat duty of the reboiler. Thus, the decision variables for this problem are as follows:

$$
\begin{align*}
\eta_{cc} &= [d_{abs}, d_{abs}, D_{abs}, D_{strip}, A_{HX}, A_{cond}] \\
u_{cc} &= [Q_{reb}] \\
\theta_{cc} &= [\eta_{cc}, u_{cc}]
\end{align*}
$$
Moreover, the following process constraints have been considered for the present analysis:

\[
0.95 - \varphi \leq 0 \quad (8)
\]
\[
0.95 - \zeta \leq 0 \quad (9)
\]
\[
T_{\text{reb}} - 383 \leq 0 \quad (10)
\]
\[
393 - T_{\text{reb}} \leq 0 \quad (11)
\]
\[
T_{\text{lean}} - 313 \leq 0 \quad (12)
\]
\[
315 - T_{\text{lean}} \leq 0 \quad (13)
\]

The first two constraints are performance constraints for minimum CO\(_2\) removal rate and CO\(_2\) product purity, respectively. The rest are operational constraints that are aimed to maintain the feasible operation of the process, e.g., the temperature constraint on the reboiler aims to prevent solvent degradation. All of the above constraints have been reformulated as in (5), i.e., in a probabilistic form. For example, constraint (8) has been formulated as follows:

\[
\omega_{\text{constraint}(8)} \leq 0 \iff P(0.95 - \varphi \leq 0) \geq Pr_{\text{constraint}(8)} \quad (14)
\]

In addition to compliance with the constraints, the optimal design of a CO\(_2\) capture (CC) plant aims to minimize the economic costs consisting of the capital (CAP) and operating (OP) costs:

\[
\Phi_{\text{CC}} = \text{CAP}_{\text{CC}} + \text{OP}_{\text{CC}}
\]
\[
\text{CAP}_{\text{CC}} = C_{\text{abs}} + C_{\text{strp}} + C_{\text{HX}} + C_{\text{cond}}
\]
\[
\text{OP}_{\text{CC}} = C_{\text{reb}}
\]

where the capital costs include the costs of the main process equipment, i.e., absorber \(C_{\text{abs}}\), stripper \(C_{\text{strp}}\), cross heat exchanger \(C_{\text{HX}}\) and condenser \(C_{\text{cond}}\), whereas \(C_{\text{reb}}\) denotes the operating costs associated with the reboiler heat duty \(Q_{\text{reb}}\). The detailed expressions for these cost functions are presented [35].

In this study, the pilot plant presented by Dugas [36] on a CO\(_2\) capture plant using MEA has been used as the base plant, which design and operation is presented in Table 1. The cost of this plant is evaluated using the capital and operating cost functions shown in (14). Detailed equipment specification and operating conditions of the CO\(_2\) plant can be found in [5,6,36]. The CO\(_2\) capture process has been modeled in Aspen HYSYS and validated with the base-case pilot plant of Dugas [36]. Since in this work the effect of uncertainty on the optimal design will be analyzed using this Aspen HYSYS model, a base design that has also been obtained from the same source model for comparison purposes. Therefore, the steady-state optimization (without uncertainty) of the CO\(_2\) plant has been performed and also presented in Table 1.

4. Effect of uncertainty on the optimal design of CO\(_2\) capture plant

In this work, the effect of uncertainty in the CO\(_2\) content in the flue gas stream (%CO\(_2\)), on the design of the plant is studied. The uncertainty in this input variable is assumed to follow a normal distribution with the following distribution parameters:

\[
\%\text{CO}_2 \sim N(17.5\, \text{mol\%}, 0.175\, \text{mol\%})
\]
As mentioned in Section 2, the PSE-based method gives the user an extra degree of freedom in selecting the minimum probability of satisfaction $Pr_k$ for each constraint. In the current study, a value of 0.85 will be chosen for each of the constraints shown in (8)-(13), meaning that these constraints will be satisfied at least 85% of the time when operating under the uncertainty described in (16). PSE-based approximation models as shown in (4) were used to obtain the distributions of each constraint as a result of $N$ randomly sampled uncertain realizations in %CO$_2$. In order to select which expansion order $q$ in the PSE approximation is most suitable for this problem and to demonstrate the convergence property of this method, the problem was solved several times using different expansion orders from $q=1$ to $q=6$. Figure 4 shows the PSE approximated fitting (in blue) to the actual distribution (histogram) of the CO$_2$ capture rate constraint (8), which was obtained by random Monte Carlo simulations, and the optimal designs obtained using the different expansion orders are presented in Table 2.

Table 2 Optimal steady-state plant designs under uncertainty.

<table>
<thead>
<tr>
<th>Decision variables</th>
<th>$q=1$</th>
<th>$q=2$</th>
<th>$q=3$</th>
<th>$q=4$</th>
<th>$q=5$</th>
<th>$q=6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reboiler duty, $Q_{reb}$ (kW)</td>
<td>184.5000</td>
<td>195.4961</td>
<td>194.2464</td>
<td>194.5281</td>
<td>197.2880</td>
<td>196.1544</td>
</tr>
<tr>
<td>Absorber height, $H_{abs}$ (m)</td>
<td>6.1</td>
<td>6.1</td>
<td>6.1</td>
<td>6.1</td>
<td>6.1</td>
<td>6.1</td>
</tr>
<tr>
<td>Absorber diameter, $D_{abs}$ (m)</td>
<td>0.3950</td>
<td>0.3794</td>
<td>0.3401</td>
<td>0.3390</td>
<td>0.3345</td>
<td>0.3371</td>
</tr>
<tr>
<td>Stripper height, $H_{strp}$ (m)</td>
<td>3.05</td>
<td>5.3375</td>
<td>5.3375</td>
<td>5.3375</td>
<td>5.3375</td>
<td>5.3375</td>
</tr>
<tr>
<td>Stripper diameter, $D_{strp}$ (m)</td>
<td>0.3150</td>
<td>0.4322</td>
<td>0.6365</td>
<td>0.6377</td>
<td>0.6382</td>
<td>0.6379</td>
</tr>
<tr>
<td>Heat trans. area, $A_{HX}$ (m$^2$)</td>
<td>10.7991</td>
<td>10.8259</td>
<td>10.8553</td>
<td>10.8260</td>
<td>10.8259</td>
<td>10.8262</td>
</tr>
<tr>
<td>Heat trans. area, $A_{cond}$ (m$^2$)</td>
<td>19.7984</td>
<td>19.7987</td>
<td>20.3930</td>
<td>20.3932</td>
<td>20.3935</td>
<td>20.3928</td>
</tr>
<tr>
<td>Cost</td>
<td>$CC$ ($/y)$</td>
<td>3.76E+04</td>
<td>4.12E+04</td>
<td>4.43E+04</td>
<td>4.44E+04</td>
<td>4.44E+04</td>
</tr>
<tr>
<td></td>
<td>$OC$ ($/y)$</td>
<td>7.42E+03</td>
<td>7.86E+03</td>
<td>7.81E+03</td>
<td>7.82E+03</td>
<td>7.93E+03</td>
</tr>
<tr>
<td></td>
<td>Total ($/y$)</td>
<td>4.50E+04</td>
<td>4.91E+04</td>
<td>5.21E+04</td>
<td>5.22E+04</td>
<td>5.22E+04</td>
</tr>
<tr>
<td></td>
<td>CPU Time (h)</td>
<td>1.489</td>
<td>2.031</td>
<td>2.934</td>
<td>3.832</td>
<td>5.089</td>
</tr>
</tbody>
</table>

Figure 3 show that, as the expansion order is increased, the more accurate the PSE approximation seems to fit the actual distribution. By inspecting the results shown in Table 2 it shows that the computational time increases rapidly as higher expansion order is used, thus discouraging the use of high-order PSE approximations if unnecessary. Table 2 also shows that the optimal designs converge at $q=3$, i.e., the maximum difference in the total costs with respect to the design obtained when $q=6$ is less than 1%. Therefore, a PSE expansion order $q=3$ is justified for this problem as it is 23% faster than $q=4$ and 54% faster than $q=6$ in obtaining the optimal designs.
From Table 2, it is clear that the effect of uncertainty in the flue gas stream’s CO2 composition has a significant effect on the optimal design previously obtained without considering uncertainty (see Table 1). Larger absorber and stripper columns (both diameters and heights) as well as higher reboiler duty were obtained when compared to the optimal steady-state design without uncertainty (Table 1). With uncertainty in the flue gas stream’s CO2 composition, there will be instances when the CO2 composition is higher than the nominal steady-state value. Therefore, to maintain the same plant performance, larger absorber is needed to maintain the CO2 removal rate, and larger stripper and reboiler heat duty is required to maintain the CO2 product purity on target, i.e., a minimum of 95% purity. Although this larger plant is 5% and 24% higher in operational and capital costs than that obtained at nominal conditions (base-case in Table 1), respectively, that plant design satisfies the constraints of this process (8)-(13) according to the user-defined 85% probability of satisfaction (Figure 4a). On the other hand, the optimal steady-state design that did not consider uncertainty at the design stage was found infeasible when operating under uncertainty with more than 80% violations (Figure 4b). Note that the cross heat exchanger and condenser areas obtained from the present uncertainty analysis and shown in Table 2 remained relatively unchanged in the presence of uncertainty.
5. Conclusions

This study evaluates the effect of process uncertainty on the optimal design of a post-combustion CO₂ capture plant using a novel ranking-based method has been presented. The search for the optimal plant’s design is carried out by searching for the sizes of the key process units included in the CO₂ capture plant (e.g., packed column’s height and diameters, heat exchanger and condenser areas) that minimizes the process economics in the presence of uncertainty in the flue gas stream conditions. The optimal designs obtained under uncertainty yielded a larger sized plant and needed more utility (i.e., reboiler duty). As a result, these designs were more expensive than the actual plant’s design and the design obtained from optimization (without considering uncertainty) with higher operational and capital costs. However, while the present method yielded larger and thus more expensive designs, it ensures that the environmental and operational constraints are satisfied according to the user-defined probability of satisfaction, whereas the base-case design did not meet the CO₂ removal rate target most of the time when operating under uncertainty. Therefore, the designs presented in this study will potentially lead to savings since the plant’s CO₂ removal rate may not need to be reduced, or the plant itself may not need to be shut down, when changes in the flue gas stream’s conditions may occur. Instead, the proposed designs will ensure that the plant can continuously operate at its design specifications since it can accommodate the potential changes that may occur in the fossil-fired power plant’s operation due to varying changes in the electricity demands.

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