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Effect of Uncertainties in Solvent Properties on the Techno-Economic Performances of a CO_2 Absorber

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The use of computational models and simulation tools is vital for design and optimisation of CO_2 absorption processes. When developing these tools, mathematical submodels such as models for physical properties and mass and heat transfer models are prerequisite as they are employed to make inferences about the absorption process performance. Although these models are meant to represent and predict the system behavior accurately, they will be compromised due to uncertainties and lack in our knowledge of all the detailes of the physical system. With this motivation, a systematic framework to uncertainty quantification and global sensitivity analysis is presented in this paper in order to account for the uncertainties in solvent properties on a rate-based absorber model (density, viscosity, solubility, surface tension, vapour-liquid equilibrium, chemical reaction and reaction kinetics, heat of reaction, specific heat capacity). In this work, Monte Carlo simulation and Sobol's indices methodology are applied for the uncertainty quantification. The process chosen for this case study is 30 wt % MEA CO_2 capture from the flue gas of a natural gas combined cycle power plant delivering net power output of 830 MWe without capture. The study is based on simultaneously propagating uncertainties in solvent properties and it confirms that the packing height and capital cost of an absorber column might significantly increase in order to achieve a certain CO_2 capture ratio with a high level of confidence. Results of the sensitivity analysis also indicate that the reaction rate constant showed the largest impact on the uncertainties in absorber packing height and capital cost followed by viscosity, vapour-liquid equilibrium, density, solubility, heat of absorption, heat capacity and surface tension.

1. Introduction

Post combustion CO_2 capture by absorption in chemical solvents is the most technologically mature and commercially-ready alternative for effective mitigation of global CO_2 emissions. It has been implemented commercially on existing large-scale power plants in recent years. However, a broad large-scale deployment is still not taking place at satisfactory pace. The main drawback of the process is the high-energy requirement of the solvent regeneration step and so the associated costs for the capture unit (Papadopoulos and Seferlis, 2017). In order to improve the process design and to explore the potential of new solvents for energy and cost reduction, efficient and robust modelling tools for the process performance prediction as well as process optimization are essential.

In practice, no physical system studied can be described precisely by the mathematical models used in predictive computational tools. Assumptions and simplifications lead to uncertainty which ultimately affects the accuracy of the prediction and the evaluation of process performance. To analyse these uncertainties, uncertainty quantification (UQ) study is a suitable tool. UQ is a research area that deals with methodologies and approaches to characterize and quantify the different sources and effects of uncertainties. As such, UQ should be incorporated as inherent part of the process modelling activity in the early process design phase. By incorporating UQ, the model predictions can be evaluated over the entire range of uncertain parameter space and uncertainty bounds can be provided. UQ provides valuable insights to process decision makers on the level to which uncertainty affects the key process parameters. Qualified feedback can be also provided as to where more experimental information should be acquired so that the associated uncertainty in the model outcomes could be reduced.

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UQ has gained attention and has been employed in recent years within several chemical engineering applications. Goyal and Pepiot (2018) applied UQ technique for analysis of the validity of a biomass pyrolysis model in comparison with experimental measurements and to seek future experimental targets for model predictions improvement. Behrooz and Hoseini (2018) studied the uncertainties in the thermodynamic model parameters of a benzene-toluene distillation column and hydrocarbon mixture separation via distillation to be addressed in the chemical process design. Rossi et al. (2019) investigated the use of UQ technique for four aspects of the process system engineering applications; dynamic optimization, predictive maintenance, soft-sensor systems and risk assessment. Within the solvent-based capture technologies, only relatively limited number of studies have been reported so far. Bahakim and Ricardez-Sandoval (2015) studied how uncertainties in CO_2 content, temperature and flow rate of the flue gas stream influence the optimal design and equipment sizes using power series expansion (PSE) approximations. Mathias and Gilmartin (2014) applied perturbation method to evaluate uncertainties in chemical equilibrium, reaction kinetics and viscosity parameters on the performance of the simulation of CO_2–AMP system. Morgan et al. (2015) developed generalized UQ methodology using Bayesian inference and Monte Carlo sampling to determine the effect of parametric uncertainty in the property models on the percentage of CO_2 captured and on reboiler duty. Morgan et al. (2017) also applied similar methodology to determine the effect of uncertainty in the thermodynamic model parameters. As a continuation of these two previous works, Soares Chinen et al. (2018) performed UQ analysis of the effect of hydraulic and mass transfer sub-models on the percentage of CO_2 captured and on the lean solvent loading for the CO_2-MEA system. Despite these efforts, to the best of the authors' knowledge, there is no reported study that would systematically and explicitly analyse the overall impact of uncertainties in solvent properties on the key techno-economic performance parameters of the absorption process by propagating several model parameter uncertainties simultaneously as similarly shown by (Gkouletsos et al., 2019) by propagating multiple thermodynamic property parameters to study absorption refrigeration process performance.

Due to the influence of the chemical reaction in the liquid phase, the CO_2 absorption process is a relatively complex system to model. The process involves many fundamental physical phenomena and thermo-physical properties namely internal column hydraulics, phase equilibria, heat and mass transfer, chemical reaction kinetics, viscosity, density, surface tension and heat of reaction. Reliable and adequate submodels for the description of the physical phenomena and predictions of the thermo-physical properties are required in order to simulate the behaviour of the CO_2 absorber process. Modelling the absorber column, is important as it is one of the major equipments of the process with a significant effect on the economics of the capture process.

The presented work aims at developing a systematic uncertainty quantification framework with incorporated solvent based CO_2 absorber process model. The study includes a global sensitivity analysis (SA) and identifies the parameters with the most influence on the variability of the model output. Overall, the study will provide analyses of (1) where the uncertainty associated to the specific sub-models are produced, (2) what are the current ranges and magnitudes of sub-models uncertainties, and (3) how these sub-model uncertainties propagate through and affect the overall process simulation outcomes. In addition, confidence limits will be established on the predictability of key performance indicators of the absorber column in terms of equipment design and associated costs.

2. Methodology

2.1 Uncertainty quantification and sensitivity analysis framework

The framework illustrated in Figure 1 is applied to perform the UQ study for CO_2 capture with chemical solvent absorption. Since MEA solution (30 wt %) is generally considered to be the benchmark solvent system with a comprehensive literature database, the UQ framework is first applied for UQ analysis of this solvent system. First, sources of uncertainties in the key solvent property models are identified. These uncertainties are then quantified by prescribing statistical characterization. The characterization of the uncertain parameters is typically performed in a probabilistic framework typically represented as a probability distribution function (PDF) in which marginal distribution of uncertain parameter and the type of distribution are defined. Next, these uncertainties are propagated through the absorber model by drawing samples from the uncertain parameter space and performing tens to hundred of thousands simulations with the aim of obtaining probabilistic context of the output quantities. In this work, a non-intrusive Monte Carlo simulation is used. Monte Carlo approach is relatively simple, straightforward and can be used for highly nonlinear and complex models. 10,000 sample runs are performed in this case study to achieve an acceptable level of accuracy of the model outputs. Once propagation is completed, the impact of the uncertainties on the prediction of the absorber model performance parameters can be analysed and statistical analysis of the results provided. This work focuses specifically on investigating the effect of parameter uncertainties in the property sub-models and on establishing the confidence limits on the percentage CO_2 capture ratio (CCR) with respect to the absorber packing height and its capital cost. In the final step of this framework, sensitivity analysis is performed. For the purpose of this study, Monte Carlo based

Sobol' Indices method is chosen. This method is a global sensitivity analysis which is also known as variance-based sensitivity analysis. This is different from local sensitivity method since the sensitivity indicators of the model output are assessed by accounting the entire domain of possible input parameter space while the local sensitivity indicators are only applied around the selected base value. An open-source UQ software developed by ETH Zurich (UQLab) is used to perform the UQ and the sensitivity analysis (Marelli and Sudret, 2014).

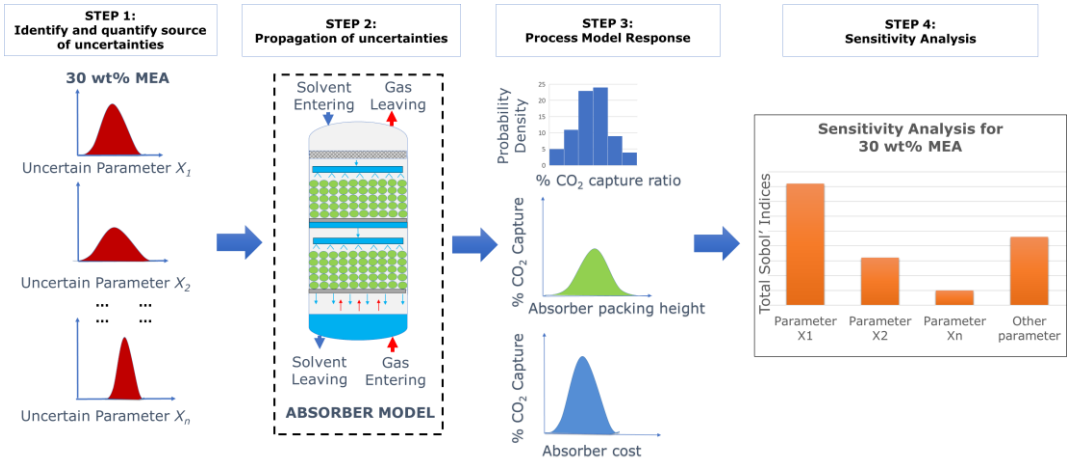

Figure 1: Framework of uncertainty quantification and sensitivity analysis methodology

2.2 Case study design

In order to estimate the effect of the model parameter uncertainties on the absorber simulation performances, an in-house MATLAB based absorber model was developed and applied to simulate the absorption of CO_2 from the flue gas of a natural gas power plant delivering net power output of 830 MWe without capture (Force, 2011). The model is validated against steady state pilot plant data for 30 wt % MEA (Flø, 2015). The approach used in this work for the absorption process simulation is a rate-based approach based on adapted two-film theory model presented by Flø (2015). Table 1 provides a summary of the input process variables for the absorber model simulation in which the inlet CO_2 concentration in the flue gas is 3.96 mol %.

Table 1: Input process specifications for absorber model simulation

	Simulation input data
Flue gas flow rate (kg/s)	665
No. of absorber	2
Inlet CO_2 concentration (% mol)	3.96
Inlet gas temperature (K)	321.4
Rich solvent flow rate (m^3/s)	0.87
Lean solvent temperature (K)	314.8
Lean loading (mol CO_2/mol MEA)	0.25
Rich loading (mol CO_2/mol MEA)	0.45
Packing type	Mellapak 250Y

The analysis of uncertainty propagation through the absorber model in this case study was carried out in two steps, (1) initially setting 90 % removal of CO_2 from the flue gas as a requirement on the absorber simulation performance and (2) simulating the absorber performance at various CCR to determine packing height and capital cost.

Table 2 presents a list of the specific submodels that are applied for MEA system and that are considered to be the sources of uncertainties for the rate-based absorber model investigated in this study. Uncertainty in most of the experimental data are reported as maximum absolute percent deviation (MAD) and average absolute deviation (AAD) which is the measure of model capacity over its predictions against the experimental dataset used in the model fitting. Therefore whenever the MAD value is available or reported in the literature this is considered as the uncertainty range. Otherwise, the uncertainty range is selected based on the reported AAD values or based on expert judgement. In this study, the distribution type for the following uncertain properties is represented by normal (Gaussian) distribution.

Table 2: Source of uncertainties ranges for 30 wt % MEA

Submodel	Source	Uncertainty Range (%)	Uncertainty Source	Distribution Type
Density	(Hartono et al., 2014)	± 8.6	MAD	Normal
Viscosity	(Hartono et al., 2014)	± 8.5	MAD	Normal
Solubility	(Hartono et al., 2014)	± 11.6	MAD	Normal
Surface tension	(Jayarathna et al., 2013)	± 5	AAD	Normal
Heat capacity	(Cheng et al., 1996)	± 6	MAD	Normal
Heat of absorption	(Kim et al., 2014)	± 11	Expert	Normal
Kinetic rate constant	(Luo et al., 2015)	± 25	Expert	Normal
Vapour-liquid equilibrium	(Brúder et al., 2012)	± 20	Expert	Normal

In the present work, the effect of model parameter uncertainty on the capital cost of the absorber was evaluated using EU H2020 CEMCAP cost evaluation methodology which included the direct cost of "standard" equipment assessed using Aspen Process Economic Analyzer (Gardarsdottir et al., 2019).

3. Results and discussion

The Monte Carlo simulation was applied to simultaneously propagate all 8 uncertainty sources and 10000 random sample runs were performed with the simulation model. The simulation model in this case was set to remove 90 % of CO_2 from the flue gas. The results are presented in Figure 2 in terms of distribution predictions on CCR in the form of histogram when the uncertainty are included. The PDF describes the density of probability at each point in the range of an uncertain variable. The red line in the figure shows the fitted normal (Gaussian) distribution. Although the deterministic value is roughly the same as the predicted mean value at 89.5 % CCR, the absorber model predicts the CCR as low as 82 % and as high as 96 % which is about 8.4 % lower and 7.3 % higher with respect to the deterministic value of 90 %. This demonstrates that by considering uncertainties in the model input, the predictive performance of the model is not 100 % even for a system so well defined as 30 wt % MEA. Increasing the understanding of the possible sources and ranges of discrepancies in the model outcomes by applying uncertainty quantification analysis will lead to better informed decisions.

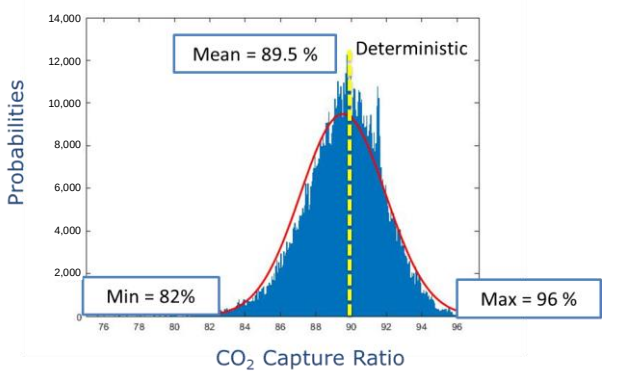

Figure 2: Histogram of percentage CO_2 capture ratio with the effect of uncertainties propagation

The results showing impact on the packing height when simulating model input uncertainties at different CCR is illustrated in Figure 3a. The results are shown with the comparison to the deterministic prediction of the simulation model. The figure can be used as a guidance to study the design performance for an absorber at different CCR. Based on Figure 3a, for instance, if 85 % CCR as a strict constraint need to be achieved for an absorber design with high confidence and certainty, the prediction on the packing height will be between the range of 10.6 m and 13.6 m at 50 % confidence interval instead of 12 m as the deterministic value. In this case study, the solvent is MEA that have numerous literature data on the solvent properties for, the outcome will be different with even more wider interval when uncertainty analysis will be performed for absorber performance with a novel solvent due to much less of available empirical data in such a case.

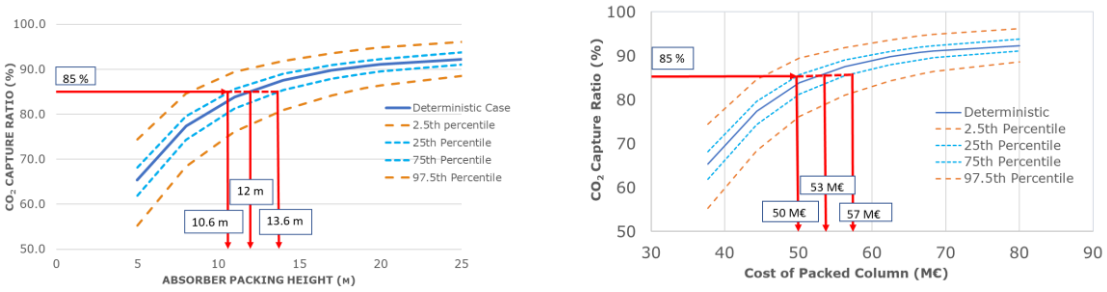

Figure 3: CO_2 capture ratio at different (a) absorber packing height and (b) capital cost of absorber packed column

The uncertainty in the absorber performance in terms of packing height can be translated into the uncertainty in the capital cost prediction for the absorber column as well as shown in Figure 3b. Based on the predictions on the range of packing height for 85 % CO_2 capture ratio as shown in Figure 3a, Figure 3b shows the deterministic prediction of the absorber capital cost and the range of cost values when the uncertainties are incorporated. In the case of 85 % CCR, the cost of absorber will be in the range of 50 MEUR and 57 MEUR when the deterministic value is 53 MEUR. This exemplifies the benefit of performing this type of study especially for novel solvent systems with limited data sets, as it will provide better understanding of prediction ranges for process performance under the presence of uncertainty and as such it will also provide a better basis for the evaluation of the technology potential and so allow for a more informed decisions making. Figure 4 shows the results of the sensitivity analysis in terms of sensitivity indices based on Sobol's method for the case of 90 % CO_2 capture ratio. The total sobol' indices is a measure of the contribution of input variable to the output variance in addition to all variances caused by its interactions with other input variables. The results for this case study show that the reaction rate constant contributed the most to the uncertainties in the absorber packing height followed by viscosity, vapour-liquid equilibrium (VLE), density, solubility, heat of absorption, heat capacity and surface tension.The results of the global sensitivity analysis provide an understanding of the model input-output relationships over the whole range of multi-dimensional parameter space and they help to highlight the parameters that contribute the most to the uncertainty in the model outputs.

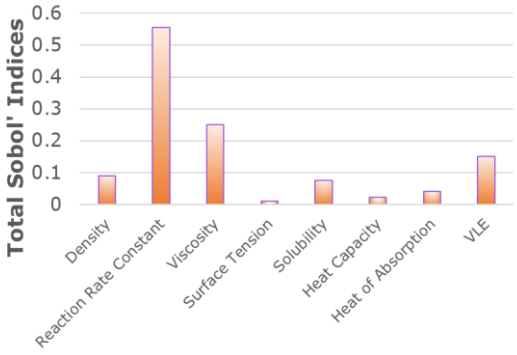

Figure 4: Monte carlo sobol' sensitivity analysis for simulation case at 90 % CO_2 capture ratio

4. Conclusions

A systematic uncertainty quantification and sensitivity analysis was performed on the process simulation of a MEA based CO_2 absorber. The results showed significant uncertainty ranges on the predictions of CCR, absorber packing height and capital cost under the presence of 8 uncertainty sources. The CCR prediction in this study was within 10 % uncertainty with respect to the deterministic value of 90 % CCR. The uncertainty in the different CCR predictions propagates into uncertainty in the packing height prediction and the associated capital cost. Among the 8 uncertain model parameters analysed in this case study, reaction rate constant has the most significant effect on the prediction of absorber column height and cost. Incorporating a systematic uncertainty quantification and sensitivity analysis in the solvent based CO_2 capture process modelling proved to be an additional source of useful information. UQ can lead to a wide range of possible outcomes and become a key to a more reliable predictions of process performances in terms of equipment design and associated costs.

The applied global sensitivity analysis further helps to examine the dependence of model predictions on the uncertainties in the input parameters and to identify those which contribute the most to overall uncertainty in model outcomes. By excluding insignificant parameters from the future analysis, computational requirements can be lowered and experimental research efforts can be directed to those parameters where reduction in uncertainty would improve the predictive capability of the models the most. This methodology can be also successfuly applied for novel solvent systems to obtain more reliable process performance and cost predictions and so more reliable estimations of novel solvents potential to reduce the energy requirements and costs.

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