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Process design optimization strategy to develop energy and cost correlations of CO_2 capture processes

Laurence Tock[a], François Maréchal[a]

[a]*Industrial Energy Systems Laboratory, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland, laurence.tock@epfl.ch*

Abstract

Within the global challenge of CO_2 emissions reduction, the process removing CO_2 from the flue gas by chemical absorption with monoethanolamine is analyzed in detail. The influence of the operating conditions on the thermo-economic performance and on the optimal thermal integration within a power plant is studied by applying process integration and multi-objective optimization techniques, with the aim of developing simpler parameterized models to be used to perform the overall process optimization. For different flue gas compositions and flows, a multi-objective evolutionary algorithm computes a set of optimal solutions. By fitting the Pareto fronts, correlations are defined to predict accurately the thermo-economic performances with regard to the capture rate, the flue gas flowrate and the CO_2 concentration. The substitution of the complex first-principle MEA unit model with a compact blackbox model applying these correlations reduces the optimization time of the overall process considerably without penalizing the overall power plant model quality. The developed approach allows to predict accurately the optimized state of the separation unit and the optimal performance and process integration of the global problem. Applied to process design of systems including a CO_2 capture unit like post- or pre-combustion processes, this approach is promising for the preliminary design and evaluation of process options.

Keywords: CO_2 capture, Chemical absorption, Blackbox model, Multi-objective optimization, Process design

1. Introduction

For power production, CO_2 capture and storage is considered as a promising option for mitigating climate change. The most common technology to capture CO_2 is chemical absorption with amines requiring however a significant amount of energy for solvent regeneration and therefore penalizing the efficiency of the electricity production. The impact of CO_2 capture on the process performance can be assessed by thermo-economic analysis including heat and power integration of the capture process and the related investment. Changing the design conditions of the ab- and desorption columns together with the flow of amines reveals to be sensitive to convergence and heavy in computation time, especially when the optimization is to be done together with the variation of the CO_2 concentration and with the purpose of finding the best economical design from the CO_2 capture point of view. Recent studies investigate the potential of replacing complex unit models of highly non-linear processes by compact yet accurate surrogate models (Henao and Maravelias [2010, 2011], Sipocz et al. [2011]) reproducing the results of the rigorous model in a fraction of the simulation time without losing accuracy.

This paper presents an approach to develop a blackbox model of the CO_2 capture unit predicting the investment, as well as the heat demands and their temperature levels required for the combined heat and power integration model by using correlations and neural networks that are drawn from the optimization results of the complex first-principle MEA unit model. The advantage of this approach with regard to the optimization problem formulation is that the optimized CO_2 capture subproblem can be introduced in a larger process to perform optimizations of the global problem, and with regard to energy integration that information about the heat demand and temperature levels are conserved. This approach is applied to study a gas turbine combined cycle process with flue gas recirculation and CO_2 capture.

2. Methodology

The approach to develop a simpler parameterized model of the CO_2 capture unit (i.e. subproblem) to be used in overall process design optimizations (i.e. global problem) (Figure 1) is implemented using process design techniques combining process modeling with established flowsheeting tools, and process integration in a multi-objective optimization framework as explained in Gassner and Maréchal [2009].

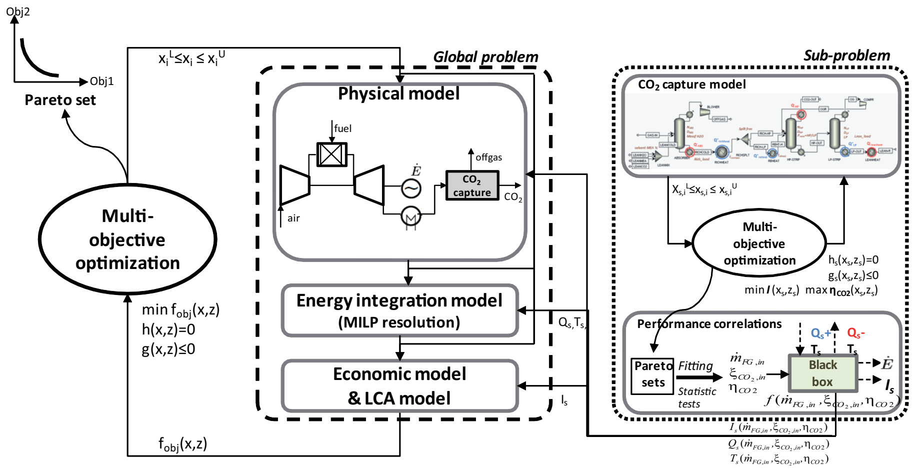

Figure 1: Illustration of the process optimization strategy.

The flowsheet of the CO_2 capture process (Figure 2) described in Bernier et al. [2010] is based on the Aspen-Plus rate-based model adapted from the default model available from *AspenTech*. CO_2 compression is not included in the capture unit. A CO_2 purity over 98%wt is targeted. The CO_2 capture unit performance is expressed by the investment cost I, the CO_2 capture rate $\eta_{CO2} = \frac{\dot{n}_{CO2captured}}{\dot{n}_{CO2,inFG}}$ and the energy demand (i.e. reboiler duty $\dot{Q}_{LP}$, electricity ($\dot{W}$)) and is essentially influenced by the decision variables given in Table 1. For the parameterized blackbox model reflecting the process behaviour, the selected input variables are the flue gas mass flow $\dot{m}_{FG}$ and the CO_2 concentration in the flue gas ξ_{CO2}. The absorber inlet temperature and pressure are kept constant by a blower and heat exchanger. The only decision variable is the CO_2 capture rate η_{CO2}. Consequently, the number of variables of the overall process is smaller than the one for the sub-problem since some parameters are internal to the black box system.

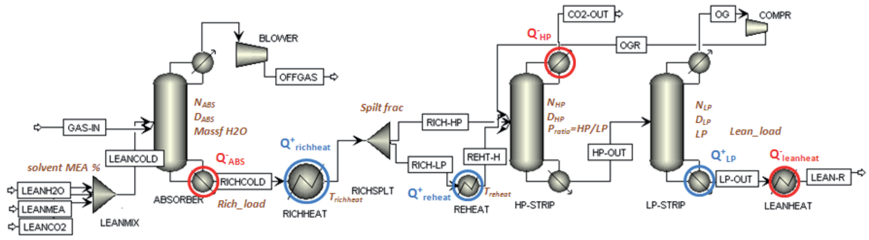

Figure 2: Flowsheet of the CO_2 capture unit implemented in Aspen Plus.

Table 1: Decision variables and feasible range for optimization.

Operating parameter	Range	Operating parameter	Range
Lean solvent CO_2 loading [kmol/kmol]	[0.18-0.25]	Split fraction [-]	[0-0.7]
Rich solvent CO_2 loading [kmol/kmol]	[0.4-0.5]	Nb stages absorber	[10-17]
Rich solvent pre-heat T [^oC]	[95-105]	Nb stages HP stripper	[8-15]
Rich solvent re-heat T [^oC]	[115-125]	Nb stages LP stripper	[6-10]
LP stripper pressure [bar]	[1.7-2.1]	Absorber diameter [m]	[6-12]
HP / LP pressure ratio [-]	[1-1.5]	HP stripper diameter [m]	[3-6]
MEA % in solvent [-]	[0.3-0.35]	LP stripper diameter [m]	[2-5]
Absorber steam out [kg_{H2O}/t_{FG}]	[306-309.5]		

2.1. *Sub-problem optimization*

For different flue gas compositions and flows of the CO_2 capture sub-problem, a multi-objective evolutionary algorithm described by Molyneaux et al. [2010] computes a set of optimal solutions in the form of a Pareto front (Figure 3). The objectives are to maximize the CO_2 capture rate and to minimize the investment with regard to the decision variables in Table 1. It is assumed that the objectives are not influenced by the pressure drop and heat load. It has been demonstrated by sensitivity analysis that minimum pressure drops and heat loads are correlated with the maximal CO_2 capture rate. Consequently, the assumption is valid and the optimum of the subproblem is contained in the optimum of the global problem.

2.2. *Surrogate model development*

By fitting the generated Pareto fronts (Figure 3), regression correlations and neural networks are defined to predict the thermo-economic performances with regard to η_{CO2} (x_1), $\dot{m}_{FG}$ (x_2) and ξ_{CO2} (x_3). Statistical tests are carried out to validate the proposed correlations. The F statistic is applied to test the model validity against the assumption that at least one coefficient of the correlation is significant. In addition the validity of each coefficient is verified by the t-test following a Student's t distribution, if the null hypothesis is supported. The approach is illustrated for the investment cost correlation.

2.2.1. *Investment correlation*

The goal is to develop a correlation of the investment with regard to the input variables I=f(η_{CO2},$\dot{m}_{FG}$,ξ_{CO2})=f(x_1,x_2,x_3). It is to note that the developed correlations for the investment cost do not follow the conventional cost estimation approach since it deals with the optimized investment computed from simulation with regard to certain decision variables. In a first attempt multi-dimensional polynomial correlations are set up. Therefore correlations are drawn for each data series with fixed ξ_{CO2} (I=$f_{\xi_{CO2}}(\eta_{CO2},\dot{m}_{FG})$) based on Eq.1 yielding for each one R^2 values around 0.98. According to the statistical tests, additional terms do not improve the goodness of fit. To include the variation with regard to ξ_{CO2} a linear variation of the coefficients in Eq.1 ($p_i = \kappa_{i,1} + \kappa_{i,2}\xi_{CO2}$) is first assumed. The statistical tests results reported in Table 2 show that some terms are not significant which leads to the final expression Eq.2. In a second attempt, a correlation related to the known physical relations in absorption/desorption columns is set up. The number of stages is related to the absorbed fraction through the Kremser equation assuming stage equilibrium instead of rate-based model, which allows together with the massflow to estimate the diameter and height through column design heuristics and consequently the costs. The parameters are defined by solving the minimization problem in the least-squares sense. A hybrid method combining mathematical programming and evolutionary algorithm for finding a good initial point has been used for this purpose. Finally, the neural network fitting tool from matlab using the Levenberg-Marquardt backpropagation algorithm for network training is also applied on the optimization results dataset (i.e. training 55% of data, validation 25%, testing 20%). The goodness of fit of these approaches is compared in Figure 4.

$$f_{x3}(x_1,x_2) = p_{00} + p_{10}x_1 + p_{01}x_2 + p_{20}x_1^2 + p_{11}x_1x_2 \quad (1)$$

$$f(x_1,x_2,x_3) = k_0 + k_1x_1 + k_2x_2 + k_3x_1x_2 + k_4x_1x_3 + k_5x_2x_3 + k_6x_1x_2x_3 + k_7x_1^2x_3 \quad (2)$$

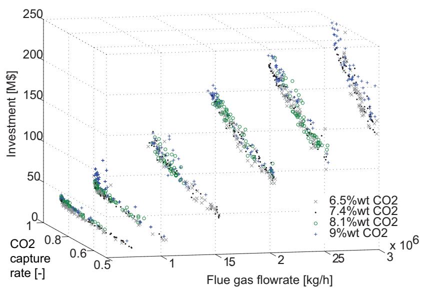

Figure 3: Pareto frontiers showing the trade-offs between investment and CO_2 capture rate for different $\dot{m}_{FG}$ and ξ_{CO2}.

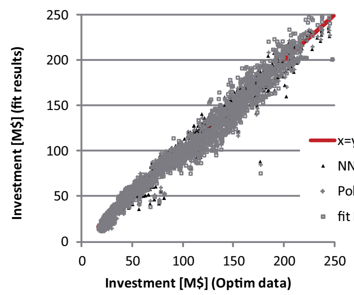

Figure 4: Fitted investment (polyfit Eq.2, fit Kremser fitK, neural network NN) versus optimization result.

Table 2: Regression results for the investment cost correlation leading to Eq.2. ($t_{0.95}$[1538]=1.96, $F_{0.95}$[7;1538]=3.23)

	cst	x_1	x_2	$\mathbf{x_3}$	x_1x_2	x_1x_3	x_2x_3	$x_1x_2x_3$	$\mathbf{x_1^2}$	$x_1^2x_3$	R^2	F-value
Coefficient	33.663	-117.33	-1.93E-5	**0**	1.2E-4	-366.04	4.7E-4	-4.5E-4	**0**	796.38	0.977	9565
t-value	-	-12.18	-3.38	**1.64**	14.4	-2.87	7.53	-4.7	**0.45**	6.2		

3. Application: NGCC with CO_2 capture

Similar to the investment, the correlations for the power demand, the reboiler duty and other heat loads have been obtained. These correlations are introduced in a blackbox model which is included in the natural gas combined gas turbine model with flue gas recirculation to optimize the process design with CO_2 capture (Figure 1). Compared to the optimization problem including the first-principle MEA unit model, the computation time is reduced (over 45%) (Figure 6), while the accuracy is nearly maintained as illustrated by the Pareto curves in Figure 5 generated by including the different balck-box models in the optimization. The fit including known physical relations performs the best.

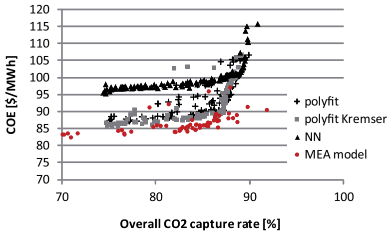

Figure 5: Pareto frontiers of the global problem optimization.

Scenario	time 1 run [h:mm:ss]	time moo [h:mm:ss]
MEA model	0:01:57	10:08:33
BB f2	0:01:05	4:54:32
BB fK	0:01:03	4:56:17
BB NN	0:01:04	4:59:11

Figure 6: Computation time comparison for multi-objective optimization with 400 evaluations and initial population of 30.

4. Conclusion

A strategy applying multi-objective optimization for developing energy and cost correlations of CO_2 capture process units is presented. Using the parameterized blackbox model of the chemical absorption unit in the optimization of a power plant with CO_2 capture reduces the complexity and computation time without loosing accuracy. The inclusion of predictions of each heat load and the corresponding temperature level is advantageous with regard to the overall process integration. This approach is promising for the preliminary design and evaluation of process options with CO_2 capture.

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