International Journal of Greenhouse Gas Control 10 (2012) 148–163

Contents lists available at SciVerse ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

CO_2 capture in power plants: Minimization of the investment and operating cost of the post-combustion process using MEA aqueous solution

Patricia Mores[a], Néstor Rodríguez[a], Nicolas Scenna[a,b], Sergio Mussati[a,b,*,1]

[a] CAIMI Centro de Aplicaciones Informáticas y Modelado en Ingeniería, Universidad Teconologica Nacional Facultad Regional Rosario – Zeballos 1341 – S2000BQA – Rosario, Argentina
[b] INGAR (CONICET-UTN) Instituto de Desarrollo y Diseño, Avellaneda 3657 – 3000 – Santa Fe, Argentina

ARTICLE INFO

Article history:
Received 19 January 2012
Received in revised form 30 May 2012
Accepted 4 June 2012

Keywords:
CO_2 capture cost
Mathematical modeling
Optimization NLP models
Greenhouse gas emissions
Post-combustion process

ABSTRACT

The post combustion process based on the CO_2 absorption using amine aqueous solution is one of the more attractive options to drastically reduce greenhouse gas emissions from electric power sector. However, the solvent regeneration is highly energy intensive affecting the total operating cost significantly. The CO_2 removal target depends on the absorption and desorption processes where the main parameters of both processes are strongly coupled. Consequently, the simultaneous optimization of the whole CO_2 capture process is essential to determine the best design and operating conditions in order to minimize the total cost.

This paper presents and discusses different cost optimizations including both investments and operating costs. The impact of different CO_2 emission reduction targets on the total annual cost, operating conditions and dimensions of process units is investigated in detail. Optimized results are discussed through different case studies.

1. Introduction

Over the last decades, amine gas sweetening has become a proven technology for the removal of CO_2 from natural gas. Certainly, CO_2 is efficiently captured in some large industrial plants such as natural gas processing and ammonia production plants. However, the CO_2 capture from large power plants is still under development.

There are three processes which have been shown to be technically feasible to CO_2 capture from flue gas of fossil-fueled power plants: post-combustion, pre-combustion and oxy-fuel combustion.

The post-combustion process using amine, which will be studied in this paper, is the most promising technology due to its capacity to treat large volumes of flue gas and it is well suited for retrofitting existing plants since this process is an end of the pipe treatment. However, it is still highly energy intensive due to the thermal energy requirement needed to regenerate the amine solution which increases the operating cost drastically. The loss of amine in the regenerator unit is another drawback of this method.

During the last years many research activities in CO_2 capture have been done in different lines from experimental studies at laboratory scale and pilot plants to the development and implementation of mathematical models in computers.

Much work on experimental studies at laboratory scale is being carried out by various workers in order to identify and determine the concentration of ionic species in the CO_2 capture process using amine aqueous solutions. One of the analytical methods used for studying the species distribution in solutions of carbon dioxide in aqueous monoethanolamine (MEA) and diethanolamine (DEA) is the nuclear magnetic resonance (NMR) (Choi et al., 2012; Böttinger et al., 2008; Yoon and Lee, 2003). The following are the major experimental variables investigated: the absorbed amount of CO_2 or CO_2 loading, ion concentrations and temperature. The results obtained in this research area not only improve the understanding of solution behavior associated with absorption and regeneration reactions but also provide the information needed to develop a model capable of describing the *L–V* equilibrium which is fundamental for simulation and optimization of CO_2 capture process using amines.

Particular emphasis is also placed on the study of reaction mechanisms between the different types of amines and CO_2 (Vaidya and Kenig, 2007, 2009; Xie et al., 2010). In addition, several researchers are focusing on the identification of oxidative and thermal degradations of amine solvents (Islam et al., 2011; Lawal and Idem, 2006;

Abbreviations: ABS, absorber; BLOW, blower; COMP, compressor; COND, condenser; ECO, economizer; I-COOL, inter stage cooler; LAC, lean amine cooler; MEA, monoethanolamine; REB, reboiler; REG, regenerator.

* Corresponding author at: Avellaneda 3657, 3000 Santa Fe, Argentina. Tel.: +54 342 4534451; fax: +54 342 4553439.
E-mail addresses: patricia_mores@hotmail.com (P. Mores), nestorhugo_r@yahoo.com (N. Rodríguez), nscenna@santafe-conicet.gov.ar (N. Scenna), mussati@santafe-conicet.gov.ar (S. Mussati).
1 Tel.: +54 342 4534451; fax: +54 342 4553439.

1750-5836/$ – see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijggc.2012.06.002

Nomenclature

ACC	annualized capital cost (million US$/year)
CRF	capital recovery factor
DC	direct cost (million US$)
G	flue-gas flow-rate (mol/s)
H	enthalpy (kJ)
I	cost index
i	interest rate
IC	indirect cost (million US$)
L	liquid flow-rate (mol/s)
n	compounding period
OLC	operating labor cost (million US$/year)
TO&MC	total operating and maintenance cost (million US$/year)
P	pressure (kPa)
PC	purchased cost (million US$)
SC	start-up cost (million US$/year)
T	temperature (K)
TAC	total annual cost (million US$/year)
TCI	total capital investment (million US$)
TPC	total purchased equipment cost (million US$)
TOLC	total operating labor cost (million US$/year)
TU&MUC	total utility cost including heating and cooling utilities, electricity, MEA and water make-ups and R&D costs (million US$/year)
U&MUC	total utility cost including heating and cooling utilities, electricity, MEA and water make-ups (million US$/year)
WC	working capital (million US$/year)
X	capacity: heat transfer area for heat exchangers (m^2); volume for absorber, stripper and tanks (m^3); real power for pumps, blower and compressors (kW)
y	mole fraction in vapor phase
K_{DC}	numerical constant used to compute the direct cost
K_{IC}	numerical constant used to compute the indirect cost
K_{WC}	numerical constant used to compute the working capital cost
K_{SC}	numerical constant used to compute start-up costs
α_{CO_2} loading	CO_2 loading factor (CO_2 mol/MEA mol)

Superscripts

0	reference value
1	current value

Subscripts

in	inlet
out	outlet
k	piece of equipment (ABS, REG, BLOW, RAP, LAC, ECO, MEA-TK, H_2O-TK, COND, REB, COMP, I-COOL)

Lepaumier et al., 2010). Knowledge of degradation products and main reactions allows a better understanding of amines chemical stability for CO_2 capture application.

In regards to the application of the mathematical modeling of CO_2 capture processes using amine, many articles focusing on the simulations and parametric optimizations in order to maximize the absorption efficiency have been published. A great number of authors employed process simulators such as: Aspen Plus (Cozad et al., 2010; Abu-Zahra et al., 2007a,b; Duan et al., 2012; Ali et al., 2005), HYSYS (Khakdaman et al., 2008; Aliabad and Mirzaei, 2009), and Aspen HYSYS (Oi, 2007), gProms (Kvamsdal et al., 2009; Lawal et al., 2009). Other authors proposed and developed in-house simulation algorithms (Rahimpour and Kashkooli, 2004; Sipöcz et al., 2011; Aroonwilas and Veawab, 2007). Freguia and Rochelle (2003) integrated a Fortran subroutine into Aspen Plus® to perform a rate-based calculation of CO_2 absorption into MEA. In these studies, key insights have been gained for the absorber and regenerator units. In most of these articles, the absorption column and regeneration unit have been studied separately. The effect of the pressure and temperature of absorber and different type of amines (primary, secondary and tertiary amines) on the CO_2 absorption efficiency was studied. In addition, the reboiler heat duty and operating conditions in the regenerator unit were also studied in detail. More specifically, many authors analyzed the effect of the different operating conditions for different types of amines in order to minimize the heat duty in the regenerator unit because it has a significant influence on the total operating cost (Oexmann and Kather, 2010; Nuchitprasittichai and Cremaschi, 2010).

On the other hand, several authors performed techno-economic evaluations of postcombustion processes (Karimi et al., 2011; Dave et al., 2011; Ho et al., 2011; Huang et al., in press; Kuramochi et al., 2010; Schach et al., 2010a,b; Oexmann et al., 2008; Peeters et al., 2007; Romeo et al., 2008; Singh et al., 2003, among others).

Karimi et al. (2011) investigated and compared five different configurations for aqueous absorption/stripping analyzing their energy requirements and capital costs and the best configurations were defined based on CO_2 avoided cost and total capture cost. The following are the configurations analyzed: (a) conventional process configuration, (b) split-stream configuration where the rich amine is split into two streams going to two sections of the stripper after preheating with two separate lean amine streams, (c) multi-pressure stripper configuration, (d) vapor recompression configuration and (e) compressor integration.

Unisim Design and ProTreat software were used for simulations, while for the cost calculations, data from Turton et al. (2008) and Sinnott et al. (2009) were considered. Results revealed that vapor recompression configuration is the best configuration because it has the lowest total capture cost and CO_2 avoided cost and the plant complexity does not increase very much compared to the benchmark. The split-stream configuration with cooling of semi-lean amine was the second best but this configuration increases the investment cost and plant complexity significantly.

Dave et al. (2011) performed a techno-economic comparative assessment for an amine based post-combustion capture (PCC) process applied to representative coal-fired power plants in Australia and China. The assessment is based on an in-depth analysis of the cost of generation. Aspen Rate-Sep, Steam-Pro, Steam-Master and PEACE software packages were used for process modeling and cost estimation of the integrated power and capture plants. According to the circumstances of both countries, the comparison reveals that post-combustion capture in China can benefit significantly from more energy efficient processes, whereas for the Australian circumstances the focus should be on reduction of capital costs. Development of more energy efficient PCC-processes will be most beneficial in China, whereas in Australia lower capital costs should be aimed for.

Kuramochi et al. (2010) compared the techno-economic performance of post-combustion CO_2 capture from industrial Natural Gas Combined Cycle (NGCC) Combined Heat and Power plants (CHPs) of scales from 50 MWe to 200 MWe with large-scale (400 MWe) NGCC for short-term (2010) future. The results have shown that the efficiency improvement by the better use of CHP capacity for meeting CO_2 capture energy demands and the long operation time can potentially overweigh the disadvantage of higher capital costs. It should be mentioned, however, that the study was based on a number of generalized relationships between the plant scale and technical and economic performances of NGCC-CHP and

CO_2 capture systems. In reality, industrial NGCC-CHPs are "tailor-made" for each industrial plant to meet plant-specific demands and conditions. The obtained results therefore only provide general indications about the techno-economic competitiveness of post-combustion CO_2 capture for medium scale industrial NGCC-CHPs.

Schach et al. (2010b) applied an exergoeconomic analysis for the following three different configurations: (a) a standard absorption/stripping cycle which was used as the base case and represents the benchmark, (b) absorber including an intercooler and (c) split-stream configuration. Aspen Plus was used to perform the simulations and RadFrac model was applied for the absorption and stripper columns. Configurations (b) and (c) show better results than the reference case. The matrix stripper configuration has the best exergetic efficiency and also the lowest energy demand. However, the cost of CO_2-avoided is higher than the cost of the configuration with intercooler. This is due to the higher investment cost for the matrix stripper. An additional stripper column and a second cross heat exchanger are needed, whereas for the intercooler configuration only an additional heat exchanger is required.

Oexmann et al. (2008) performed simulation campaigns in Aspen Plus in order to find the process parameters of the full CO_2-capture process for chemical absorption of CO_2 by piperazine-promoted potassium carbonate (K_2CO_3/PZ) and the subsequent CO_2-compression train that minimize the specific power loss. Subsequently, absorber and desorber columns are dimensioned to evaluate the corresponding investment costs. Regeneration heat duty, net efficiency losses and column investment costs are then compared to the reference case of CO_2-capture by monoethanolamine (MEA). The results showed that, for the parameter values assumed, the investment costs of the absorption and regeneration units using piperazine-promoted potassium carbonate are lower than the reference process which uses MEA. The enhanced reaction kinetics of the investigated K_2CO_3/PZ solvent lead to smaller column sizes.

Singh et al. (2003) conducted a techno-economic study of CO_2 capture from an existing coal-fired power plant adopting MEA scrubbing (post-combustion capture) and O_2/CO_2 recycle combustion. The results showed that both processes are expensive options to capture CO_2 from coal power plants. However, O_2/CO_2 recycle combustion appears to be a more attractive retrofit than MEA scrubbing due to a lower CO_2 emission.

Most of the mentioned articles focus on the parametric optimization of the process variables. To the knowledge of the authors, only few articles dealing with the simultaneous optimization of the whole post-combustion process involving detailed cost equations and rigorous modeling of the process-equipments have been discussed in the specific literature (Lawal et al., 2009; Fashami et al., 2009).

The development and implementation of detailed mathematical models of the post-combustion CO_2 process using amines in advanced optimization tools is often a complex task because it involves developing accurate and rigorous models to describe all pieces of equipments, including an absorber, stripper, liquid–vapor equilibrium of the system, CO_2 compression system and heat transfer units, among others. Moreover, the development of a systematic algorithmic procedure to find optimal solutions using realistic cost functions with process simulators is difficult due to the recycle structures contemplated in the flow-sheet (Oi, 2007; Vozniuk, 2010). In addition, the constraints needed to model the pieces of equipments are usually non-linear and non-convex which may lead to convergence problems.

This paper presents an optimization mathematical model consisting in the minimization of the process total annual cost subject to mass, energy and momentum balances where the process variables are optimized simultaneously. The proposed model used for optimization is an extension of previous models presented in Mores et al. (2011, 2012). Certainly, the previous models were used to study the absorption–desorption processes by solving several optimization problems considering different efficiency criteria. These models have now been extended to include the CO_2 compression stages and a complete cost model taking into account the investment and operating cost of each one of the pieces of equipments. The resulting model is deterministic in nature and highly non-linear. Temperature, flow-rate and composition profiles along the absorber and regenerator units, dimensions (height and diameter) and reboiler heat duty are some of the main variables which are simultaneously optimized.

Flue-gas specification coming from a combined cycle power plant, solvent concentration and CO_2 removal target are considered as model parameters (known values). General Algebraic Modeling System (GAMS) which is a high-level algebraic modeling system for large scale optimization is used for implementation and solving the resulting mathematical model. In general, mathematical programming environments such as GAMS, gPROMS, and AMPL have shown to be powerful tools, especially when the optimization problem is large, combinatorial and highly non-linear.

The paper is outlined as follows. Section 2 briefly describes the post-combustion process. Section 3 introduces the problem formulation. Section 4 summarizes the assumptions and the mathematical model. Sections 5 and 6 present and discuss the optimized results obtained from the developed NLP model. Finally, Section 7 presents the conclusions and future work.

2. Process description

Fig. 1 shows a schematic overview of the post-combustion process using MEA aqueous solution for CO_2 capture from a flue gas stream coming from a power plant.

As shown, the flue gas stream [G_{in}] mainly composed by CO_2, O_2, H_2O, N_2 coming from a coal fired power plants (or gas-fired combined cycle power stations) is fed into the bottom section of the absorber [ABS] while the lean MEA aqueous solution [L_{LC}] is fed into the top section of the absorber.

The CO_2 is chemically absorbed by the amine solvent as the flue-gas stream passes upward through the packing material inside the absorber. Then, the clean gas stream [G_{out}], with the most of the CO_2 removed, is emitted to the atmosphere. The CO_2 rich solution leaving the absorber [L_{RC}] passes through the rich-lean heat exchanger [ECO] where it increases temperature up to T_{RH} and enters at the top of the stripper [REG] for regeneration. The steam supplied in the reboiler [REB] placed at the bottom of the regenerator is used to heat the CO_2 rich solution up to the boiling temperature [T_{REB}].

Thus, the CO_2 captured in the absorber is released from the CO_2 rich-amine solvent in the regenerator. As shown, from the top of the stripper column, the stream mainly composed by CO_2 product, water vapor, and entrained amine enters at the reflux condenser [COND] where a partial condensation of the stream is carried out and the resulting stream accumulated in the reflux drum is pumped back to the top of the stripper column. The final CO_2 product is delivered to the compression section where it is dried and compressed through multi-stage compressors [COMP].

Finally, the lean solvent [L_{REB}] is pumped from the regenerator through the rich-lean heat exchanger [ECO] and the cooler [LAC] and is again fed into the absorber top.

The selection of type of the amine aqueous solvent plays an important role in the process efficiency. The following are some of the aspects that must be considered when selecting the type of solvent: corrosion, amine degradation, and energy needed to regenerate the amine solvent. In general, the absorption and desorption processes are affected in opposite way by all types of amines; higher absorption efficiency, higher energy requirement for regeneration.

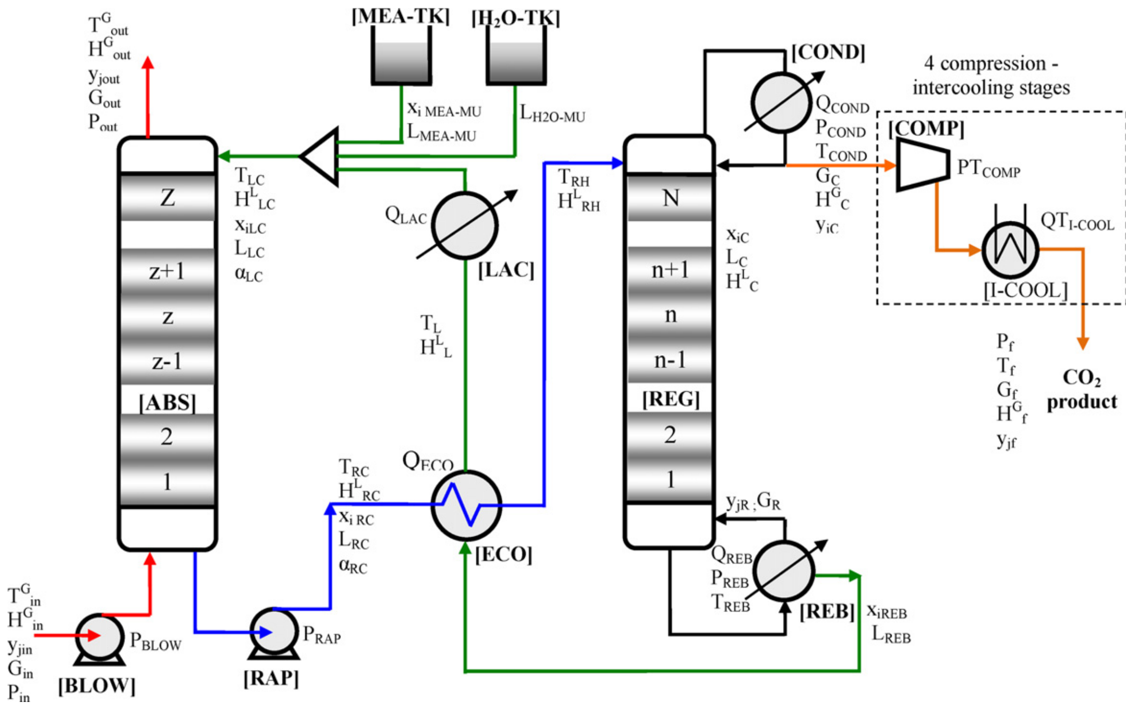

Fig. 1. Schematic diagram of the post-combustion CO_2 capture using amines.

The overall efficiency of the absorption–desorption process strongly depends on the type of amine used, steam temperature and pressure, CO_2 removal target, dimensions of the pieces of equipment (heaters, reboiler, condenser, absorber, stripper, pumps, compressors) and operating conditions (flow-rates, pressures, temperatures).

According to the above mentioned, it is easy to conclude that there exist many trade-offs between the process parameters and variables. Therefore, the simultaneous optimization of the process variables is essential to determine the best design of the entire CO_2 capture process.

3. Problem formulation

The optimization problem can be stated as follows. Given the flue gas conditions (composition, temperature and flow-rate) and the MEA solution concentration, the goal is to determine the optimal operating conditions and dimensions of the absorber/regenerator columns, compressors, pumps and heat exchangers in order to meet a given CO_2 emission reduction target at minimum total annual cost.

Mathematically, the numerical optimization problem stated in this paper can be written in the following general form:

$$\begin{aligned} &\text{Minimize} && F(x) \\ &\text{subject to:} && H_s(x) = 0 \quad \forall s \\ & && G_t(x) \leq 0 \quad \forall t \\ & && \text{Design specifications} \end{aligned}$$

where x is the vector of the model variables (heat duty in the reboiler, condenser and heat exchangers, electricity consumed by pumps and compressors, dimensions of absorber and regenerator units, H_2O and MEA make-up flow-rates). In addition, vector x also includes the following continuous decisions: temperature, composition and flow-rate profiles of aqueous solution and flue gas streams along the columns.

$F(x)$ refers to the objective function. In this model, the objective function is the total annual cost (TAC) and is computed by Eq. (1). $H_s(x)$ refers to equality constraints (mass and energy balances, correlations used to compute physical/chemical properties, pressure drops, investment and operating expenditures, among others). Basically, the equality constraints $H_s(x)$ of the economic model are given from Eqs. (2)–(17). The remaining constraints concerning the mass, energy and momentum balances can be found in Mores et al. (2011, 2012). On the other hand, $G_t(x)$ refers to inequality constraints which are used, for example, to avoid temperature crossover and to impose lower and upper bounds in some of the operating variables. Finally, design specifications refer to the model parameters (known and fixed values), e.g. the CO_2 removal target, flue-gas conditions and specific costs of heating and cooling utilities.

The investment and operating costs are computed in terms of the main process variables of each one of the pieces of equipment which are simultaneously optimized.

Finally, exploiting the robustness of the proposed model, the influence of the CO_2 removal target on the total annual cost is also investigated.

4. Assumptions and mathematical model

The complete mathematical model involves mass, energy and momentum balances (physical-thermodynamic model) and constraints used to compute investment and operating cost of each one of the pieces of equipments (cost model). As follows, the main assumptions and the mathematical model are presented.

- A low CO_2 concentration in flue gas stream is assumed. The main reason of this is that the developed model will be coupled into a combined cycle power plant in order to optimize the whole integrated plant. The CO_2 concentration in exhaust gases of such power plants is low.
- A maximum gas flow-rate that can be treated by one absorption train recommended in the literature is assumed in this

paper. According to the literature, the largest economic single train is approx. 4600 t per day from coal-fired flue gas or 2400 t per day from natural gas, based on a maximum column diameter of 12.8 m (Chapel et al., 1999). Therefore, it is considered that the whole process involves one absorption column and one regenerator unit. For larger flue gas flow-rates mentioned above, the number of absorbers and compressors should be increased. Based on the two previous assumptions, it is not necessary to specify the size of the reference power plant (MWe).

- Packed columns are considered for the CO_2 absorption and amine regeneration. As first approximation, random packing was assumed. The model will be further extended to also consider structured packing.
- For mathematical modeling purpose, the total height of absorber and regenerator columns is divided into N stages which allow to compute profiles of temperatures, flow-rates and compositions along the column. Ten stages ($N = 10$) are considered for absorption and regeneration columns. The first stage (Stage 1) refers to the bottom of the columns and the last stage (Stage 10) denotes the top of the columns.
- As first approximation, liquid and vapor phases are well-mixed. Thus, there is no concentration and temperature gradients in single liquid and vapor phases and point efficiency is equivalent to Murphree efficiency (η).
- Stage efficiency may be computed similarly to the tray efficiency. Dependence of stage efficiency with gas and liquid velocities and enhancement factor, among others, is considered.
- Non-ideal behavior in the gas phase is assumed. Fugacity coefficients are computed by using Peng–Robinson equations of state for a multi-component mixture (Peng and Robinson, 1976).
- As first approximation, ideal behavior in the liquid phase is assumed.
- An enhancement factor is used to introduce the effect of the chemical reaction on the CO_2 transfer.
- Aqueous MEA amine solution is used as the solvent (30 wt.%).
- As first approximation, thermal equilibrium is assumed between the liquid and gas phases.
- Pressure drop along the absorber and regenerator units is considered by using Robbins correlation (Robbins, 1991).
- Dimensions of both columns are considered as optimization variables. Certainly, the heights and diameters of both columns and the operating conditions are optimized simultaneously.
- CO_2 and H_2O are the only species transferred across the interface. This assumption is widely accepted in the literature (deMontigny et al., 2006).
- Dependence of densities, viscosities, diffusivities and enthalpies with the temperature and composition are considered (Greer, 2008).
- Dependence of transfer coefficient in liquid and vapor phases with the viscosity, density, nominal packing size and specific dry area and effective interfacial area for mass transfer are taken into account through Onda's correlations (Onda et al., 1968).
- An upper bound (1.225 kPa/m of packing) for the maximum allowable pressure drop is considered (Kister, 1992). Thus, the total pressure drop may be lower than the upper bound.
- Lower and upper bounds for the superficial gas velocity are also considered to avoid flooding problem and a bad gas–liquid distribution. Values suggested in literature range from 70 to 80% of the flooding velocity (Kister, 1992; Seider et al., 2009).
- It is assumed that absorber diameter should be ten times greater than the nominal diameter of packing (Seider et al., 2009). A maximum absorber diameter is adopted (13.0 m). This upper bound is suggested in the literature (Chapel et al., 1999).
- Six-tenths rule is used to compute the purchased equipment cost.
- Direct, indirect costs and working capital are considered and calculated as percentages of the purchase and installation cost (Abu-Zahra et al., 2007b).
- Chemical reactions take place at the liquid and vapor interface. The following reactions are considered:

$$2H_2O \leftrightarrow H_3O^+ + OH^- \tag{R1}$$

$$2H_2O + CO_2 \leftrightarrow H_3O^+ + HCO_3^- \tag{R2}$$

$$H_2O + HCO_3^- \leftrightarrow H_3O^+ + CO_3^{2-} \tag{R3}$$

$$H_2O + MEAH^+ \leftrightarrow H_3O^+ + MEA \tag{R4}$$

$$MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^- \tag{R5}$$

$$MEA + CO_2 + H_2O \leftrightarrow MEACOO^- + H_3O^+ \tag{R6}$$

$$CO_2 + OH^- \leftrightarrow HCO_3^- \tag{R7}$$

As mentioned earlier, the complete and detailed mathematical model used in this paper have been previously presented in Mores et al. (2011, 2012). For this reason, the cost mathematical model is only presented in the next section.

4.1. Cost mathematical model

4.1.1. Objective function

The objective function to be minimized is the total annual cost [TAC]. It is computed as the sum of the annualized capital cost [ACC] and the operating and maintenance cost [TO&MC]:

$$TAC = ACC + TO\&MC \tag{1}$$

4.1.2. Annualized capital cost [ACC]

The annualized capital cost is defined as the ratio between the total capital investment [TCI] cost and the capital recovery factor [CRF].

$$ACC = TCI\,CRF \tag{2}$$

The total capital investment [TCI] depends on the direct cost [DC], indirect cost [IC] and fixed capital investment [FCI]. Thus, TCI is computed by Eq. (3):

$$TCI = DC + IC + FCI \tag{3}$$

The direct cost DC is given by:

$$DC = K_{DC}TPC \tag{4}$$

where TPC refers to the total purchased equipment cost which is computed by Eq. (10). The constant factor K_{DC} (2.688) is taken from Abu-Zahra et al. (2007b) and includes the purchase and installation, instrumentation and control, piping, electrical installation, building and building services, yard improvements, service facilities and land. Table 1 lists the values assumed for each one of the items used to compute K_{DC}.

The indirect cost IC is given by:

$$IC = K_{IC}TPC \tag{5}$$

where the constant factor K_{IC} (1.0080) is also taken from Abu-Zahra et al. (2007b) and includes the engineering, construction expenses, contractors fees and contingency (Table 1).

The fixed capital investment [FCI] includes the working capital [WC] and start up cost [SC] which are computed as follows:

$$FCI = WC + SC \tag{6}$$

where WC and SC are computed as follows:

$$WC = K_{WC}TPC \tag{7}$$

$$SC = K_{SC}TPC \tag{8}$$

Table 1
Parameter values assumed to compute costs.

		Percentage of total purchased capital [TPC, Eq. (10)]
Direct costs (DC), K_{DC}		2.6880
1	Purchased equipment (C_P)	1.0000
2	Equipment installation	0.5280
3	Instrumentation and control	0.2000
4	Piping	0.4000
5	Electrical installation	0.1100
6	Building and building services	0.1000
7	Yard improvements	0.1000
8	Services facilities	0.2000
9	Land	0.0500
Indirect costs (IC), K_{IC}		1.0080
10	Engineering	0.2688
11	Construction expenses	0.2688
12	Contractor's fee	0.0134
13	Contingency	0.4570
Fixed capital investment (FCI)		1.2936
14	Working capital, K_{WC}	0.9240
15	Start-up cost plus MEA make-up cost, K_{SC}	0.3696
Total capital investment (TCI)		4.9896

Taken from Abu-Zahra et al. (2007b).

As indicated in Table 1, numerical values for K_{WC} and K_{SC} are, respectively, 0.9249 and 0.3696 (Abu-Zahra et al., 2007b).

The purchased equipment cost [PC] of the piece of equipment "k" is computed using the six-tenths rule ($m = 0.6$) as follows:

$$\mathrm{PC}_k = \mathrm{PC}_k^0 \left(\frac{X_k^1}{X_k^0}\right)^m \left(\frac{I_k^1}{I_k^0}\right) \tag{9}$$

where X and I are the capacity and cost index of the equipment k (absorber, stripper, reboiler, condenser, heaters, blower, storage tanks, pumps and compressors). The superscripts 0 and 1 refer to the base and current values, respectively. The base cost of equipment [PC_k^0] depends on the X^0 and is computed by correlations reported in Henao (2005) and Seider et al. (2009) and the base values used for X^0 and I^0 in Eq. (9) are listed in Table 1a. Table 2 lists the main investment items considered including the construction material of each one of them.

Then, the following constraint is used to compute the total purchased equipment cost (TPC):

$$\mathrm{TPC} = \sum_k \mathrm{PC}_k, \quad k = \mathrm{ABS, REG, BLOW, RAP, LAC, ECO, MEA\text{-}TK, H_2O\text{-}TK, COND, REB, COMP, I\text{-}COOL} \tag{10}$$

The capital recovery factor is computed by Eq. (11)

$$\mathrm{CRF} = \frac{i(1+i)^n}{(1+i)^n - 1} \tag{11}$$

where n and i are, respectively, the compounding periods (economic life of equipment) and the interest rate. It is assumed a project life of 25 years and 8% of interest rate.

4.1.3. Total operating and maintenance cost (TO&MC)

The total operating and maintenance cost [TO&MC] is computed as follows:

$$\mathrm{TO\&MC} = \delta_1\,\mathrm{TPC} + \mathrm{TU\&MUC} + \mathrm{TOLC} \tag{12}$$

As shown, it depends on the following cost-items: (a) TPC (total purchased equipment cost), (b) TU&MUC (heating and cooling medium costs, electricity, MEA and water make-up and R&D costs) and (c) TOLC (total operating labor cost). Factor δ_1 (0.3863) includes the following items: (a) local taxes, (b) insurances, (c) maintenance, (d) operating supplies, (e) plant overhead cost and (f) R&D cost. The contributions of each one of the mentioned items to the factor δ_1 are listed in Table 3 and were taken from Abu-Zahra et al. (2007b).

4.1.3.1. Utility costs including electricity cost and MEA and H_2O make-up costs (TU&MUC).

The utility cost "i" [UC_i] is computed by Eq. (13) where Y and P are the annual consumption computed from the mass and energy balances and the specific price of the utility

Table 1a
Base values used to compute PC^0.

Piece of equipment	X^0	I^0	Reference
Absorber/stripper packing: $[ABS]_P$, $[REG]_P$	182 m^3	381.7 (1996)	Henao, 2005
Absorber/stripper vessel: $[ABS]_V$, $[REG]_V$	234 m^2		
Reboiler [REB]	100 m^2		
Heater [ECO]	900 m^2		
Coolers and condensers: [LAC], [COND], [I-COOL]	900 m^2		
Pump [RAP]	250 kW		
Blower [BLOW]	745 kW		
Storage tank: [MEA-TK], [H_2O-TK]	100 m^3	499.6 (2006)	Seider et al., 2009
Compressor [COMP]	1400 kW		

Table 2
Pieces of equipments considered to compute the total capital investment including their construction material.

	Equipment type	Material of construction	Capacity (X)
Absorber	Vessel	CS	Superficial area
	Packing–Intalox Saddles, 5 in.	Ceramic	Packing volume
Stripper	Vessel	CS	Superficial area
	Packing–Intalox Saddles, 5 in.	Ceramic	Packing volume
Compressor interstage coolers	Floating head	SS (tubes)–CS (shell)	Exchange area
Condenser			
Lean amine cooler			
Rich/lean amine exchanger		SS (tubes)–SS (shell)	
Reboiler	Horizontal Kettle		
Amine storage tank	Roof tank	CS	Volumetric capacity
Water storage tank	Roof tank		
Flue gas blower and driver	Centrifugal (turbo)	SS	Brake horsepower
Compressor and drivers	Centrifugal		
Rich amine pump and driver	Centrifugal		

Table 3
Parameter values used to compute the total operating and maintenance costs.

	Percentage of total purchased capital [TPC, Eq. (10)]
δ_1	0.3863
Local taxes	0.0739
Insurance	0.0370
Maintenance	0.1478
Operating supplies	0.0222
Plant overhead cost	0.0887
R&D cost	0.0185
	Percentage of utility and make-up costs [U&MUC, Eq. (14)]
δ_2	1.0500
Raw material and utilities	1.0000
R&D cost	0.0500
	Percentage of total operating labor cost [OLC, Eq. (16)]
δ_3	2.4466
Operating labor	1.0000
Supervision and support labor	0.3000
Laboratory charges	0.1000
Administrative cost	0.1500
Plant overhead cost	0.7800
R&D cost	0.1165

Taken from Abu-Zahra et al. (2007b).

'i' (electricity, cooling water, low pressure steam, water make-up, MEA make-up and MEA inhibitors) respectively.

$$\mathrm{UC}_i = Y_i P_i^0 \left(\frac{I_i^1}{I_i^0} \right) \tag{13}$$

The total utility cost [U&MUC] is then computed as follows:

$$\mathrm{U\&MUC} = \sum_i \mathrm{UC}_i \tag{14}$$

The following cost-item, hereafter named [TU&MUC], takes into account the total utility cost [U&MUC] and R&D cost. Then, it is computed as:

$$\mathrm{TU\&MUC} = \delta_2 \mathrm{U\&MUC} \tag{15}$$

The numerical value used for δ_2 and the corresponding reference is detailed in Table 3.

Table 4
Stream specifications assumed for optimization.

Flue gas stream	
Gas flow-rate [mol/s]	10,000
Inlet temperature [K]	323.15
CO_2 [mol fraction]	0.0422
H_2O [mol fraction]	0.0845
O_2 [mol fraction]	0.1166
N_2 [mol fraction]	0.7567
Pressure [kPa]	101.3
MEA make-up stream	
MEA [mass fraction]	0.3
Temperature [K]	298.15
H_2O make-up stream	
Temperature [K]	298.15
Cooling water stream	
Inlet cooling water temperature [K]	298.15
Outlet cooling water temperature [K]	313.15
Reboiler pressure [kPa]	202.6
Compression pressure [kPa]	8600

Table 5
Parameter values assumed for the main pieces of equipment.

Heat exchangers	
Minimum temperature difference in cold and heat side [K]	1
Global energy transfer coefficient [KW/m^2 K]	
Condenser [U_{COND}]	0.3202
Interstage coolers [$U_{I\text{-}COOL}$]	0.2777
Lean amine cooler [U_{LAC}]	1.0050
Reboiler [U_{REB}]	1.3603
Economizer [U_{ECO}]	0.7608
Pumps, blower and compressor efficiency [%]	75
Hold up MEA make-up tank [days]	1
Hold up H_2O make-up tank [days]	30
Absorber and regenerator units	
Column type	Packed
Stages number	10
Packing specifications	
Type of packed	Ceramic Intalox Saddles
Specific area [m^2/m^3]	118
Nominal packing size [m]	0.05
Critical surface tension [N/m]	0.061
Void fraction	0.79
Dry packing factor [m^2/m^3]	121.4

Taken from Fisher et al. (2005), Henao (2005), United Technologies Research Center (1999), Perry and Green (1997) and Blauwhoff et al. (1985).

4.1.3.2. Total operating labor cost (TOLC). The operating labor cost (OLC) is computed as follows:

$$\mathrm{OLC} = \frac{\tau L_S}{L_{Yop}} S_{op} \tag{16}$$

where S_{op} is the annual operator salary (US$/year). τ refers to the number of operating shift per year (1000 shift/year; 8000 operating hours/year and 3 shifts/day have been considered). L_S refers to the number of operators per shift (3.5). L_{Yop} is the amount of shifts to be handled by one operator per year; in this paper 245 shift-op/year is assumed. The total operating and labor cost (TOLC) includes the following items: (a) supervision and support labor, (b) laboratory charges, (c) administrative cost, (d) plant overhead cost and (f) R&D.

Each one of these items is computed as a percentage of the operating labor cost (OLC) as indicated in Table 3. Thus, total operating and labor cost is given by:

$$\mathrm{TOLC} = \delta_3\,\mathrm{OLC} \tag{17}$$

Thus, Eqs. (1)–(17) are basically the main constraints used to compute investment and operating cost. In addition, several "intermediate" variables and equations were also defined in order to facilitate the model convergence. The complete mathematical model (physical-thermodynamic and cost models) involves approximately 3200 variables and constraints. It was implemented in General Algebraic Modeling System (GAMS; Brooke et al., 1996). The generalized reduced gradient algorithm CONOPT 2.041 was here used as NLP solver (Drud, 1992).

5. Results. Application of the NLP model

As mentioned earlier the models used in this paper to describe the L–V equilibrium of the CO_2–MEA–H_2O system and

Table 6
Specific costs of heating and cooling utilities, electricity.

Utility	Specific prices [P_i] used in Eq. (7)
H_2O make-up (Henao, 2005)	0.04 US$/t
MEA make-up (Rao and Rubin, 2002)	1250 US$/t
Cooling water	0.0329 US$/t
Steam (Henao, 2005)	3.66 US$/GJ
Electricity (Henao, 2005)	0.06 US$/kWh

Table 7
Distribution of the total operating and maintenance cost [TO&MC] for CO_2 removal = 80 and 95%.

	CO_2 removal = 80%; TO&MC = 35.06 million US$/year	CO_2 removal = 95%; TO&MC = 42.19 million US$/year
Heating and cooling utility costs, electricity cost, MEA and H_2O make-up costs, R&D cost [TU&MUC, %]	73.36	74.89
Total purchased equipment cost [δ_1TPC, %]	26.34	24.98
Total operating labor cost [TOLC, %]	1.12	0.93

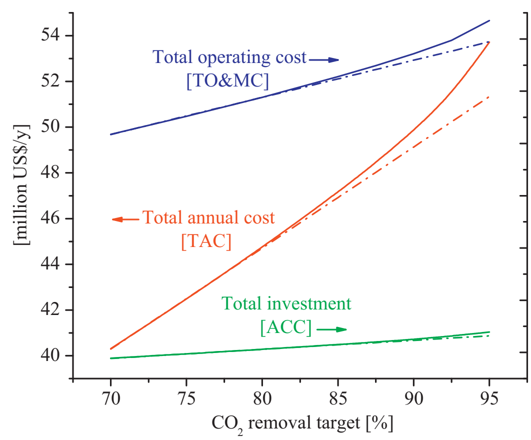

Fig. 2. Total annual cost including investment capital operating cost vs. CO_2 removal target.

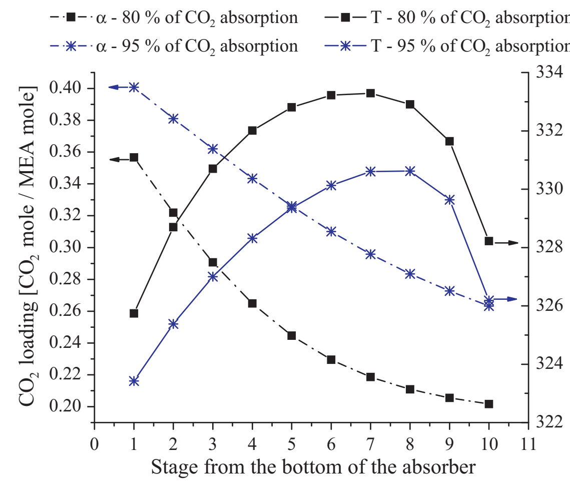

Fig. 4. CO_2 loading factor and temperature profiles along the absorber (80 and 95% of CO_2 removed).

the absorber and regenerator units have been successfully verified with experimental data in previous publications (Mores et al., 2011, 2012). In theses articles the models have been also used to optimize the whole CO_2 capture process from a thermodynamic point of view. For this reason, the comparison between predicted values by the proposed model (simulation mode) with experimental data is not presented in this paper.

According to Section 3, the goal of this paper is to simultaneously optimize the operating conditions and dimensions of the pieces of equipments in order to meet different CO_2 removal targets at minimum total costs.

As follows, the numerical results corresponding to the optimal operating conditions of each one of the pieces of equipments including their dimensions and heating/cooling utilities are presented and discussed separately in terms of CO_2 removal targets. Thus, the optimal solution set corresponding to each one of the fixed parameters is directly obtained from Figs. 2–5 and Tables 7–14.

Optimization problems have been solved using Intel Core 2 Quad Extreme QX9650 3 GHz 1333 MHz processor and 4 GB RAM and the parameters listed from Tables 4–6. The data listed in Table 6 were up-dated to 2011.

5.1. Optimal total cost values vs. CO_2 removal target

Figs. 2 and 3 show the influence of the CO_2 removal target on the total annual cost and how it is distributed in total investment and operating costs.

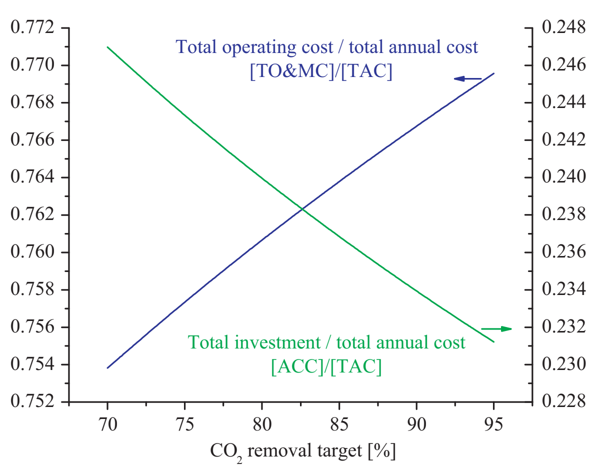

Fig. 3. Percentage of the investment capital operating cost vs. CO_2 removal target.

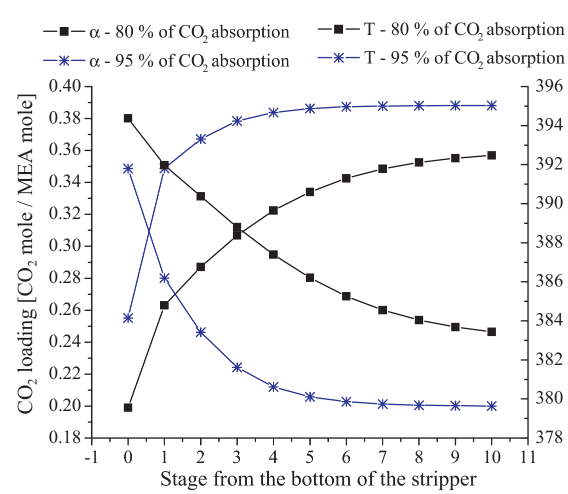

Fig. 5. CO_2 loading factor and temperature profiles along the stripper (80 and 95% of CO_2 removed).

Table 8
Distribution of the total utility costs [U&MUC] for CO_2 removal target = 80 and 95%.

	CO_2 removal = 80%; U&MUC = 24.38 million US$/year	CO_2 removal = 95%; U&MUC = 29.95 million US$/year
Steam [%]	57.36	58.05
Electricity [%]	28.64	27.67
Cooling water [%]	7.76	8.24
MEA make-up [%]	5.87	5.67
H_2O make-up [%]	0.38	0.36

5.2. Contribution of each one of the operating costs on the total operating cost (TO&MC)

Tables 7 and 8 show how the total operating cost is influenced by the CO_2 removal target for CO_2 removal target = 80 and 95%. Table 9 lists the operating costs of all cost-items for different CO_2 removal targets (70.0, 75.0, 80.0, 85.0, 87.5, 90.0, 92.5 and 95.0%).

5.3. Contribution of each one of the pieces of equipments on the total annual capital cost (ACC)

Tables 10 and 11 show the contributions of the investments of each one of the pieces of equipments on the total annual capital cost for different CO_2 removal targets (70.0, 75.0, 80.0, 85.0, 87.5, 90.0, 92.5 and 95.0%).

5.4. Optimal dimensions and operating conditions of each one of the pieces of equipment

Tables 12 and 13 compare the optimal dimensions and operating conditions of each one of the pieces of equipment for each one of the CO_2 removal targets.

5.5. Influence of the CO_2 removal target on the profiles of temperature and amount of captured CO_2 along the height of absorber and regenerator units

As mentioned in Section 1, the absorber and regenerator models are modeled by stages in order to obtain the optimal internal profiles of composition, temperature and flow-rate. Figs. 4 and 5 compare the CO_2 loading factor and temperature profiles along of absorber and stripper for 80 and 95% of CO_2 removal levels.

5.6. Comparison of optimal designs involving different objective functions

By exploiting the benefits of the proposed model, different optimal designs obtained by considering different objective functions are compared. Table 14 compares, the optimal solutions obtained for the following three objective functions: (a) total annual cost (min.), (b) total heat duty (min.) and (c) total heat duty/CO_2 recovery (min.) where the CO_2 recovery is here considered as an optimization variable.

5.7. Comparison between the output results predicted by the model and a solution reported by other authors

In order to verify the proposed model, Tables 15–18 compare the output results obtained by applying the proposed model with other reported costs (investment and operating costs).

6. Discussion of results

6.1. Optimal total cost values

Fig. 2 illustrates the total optimal costs [TAC] in terms of the CO_2 removal targets. It can be observed that the total cost [million

Table 9
Optimal values of TAC and TO&MC obtained for different CO_2 removal targets.

Cost-item	CO_2 removal target (%)							
	70.0	75.0	80.0	85.0	87.5	90.0	92.5	95.0
Total annual cost [TAC, million US$/year]	42.1379	44.0565	46.1367	48.3788	49.5813	50.8814	52.4142	54.8305
Total operating and maintenance cost [TO&MC, million US$/year]	31.7724	33.3652	35.0640	36.9300	37.9323	38.9981	40.2918	42.1939
(1) Total utility and amine cost [TU&MUC, million US$/year]	22.9965	24.3287	25.7214	27.2867	28.1289	29.0068	30.1096	31.5975
Utility and amine make-up cost [U&MUC, million US$/year]	21.7977	23.0604	24.3805	25.8642	26.6625	27.4946	28.5399	29.9502
Steam [UC_{Steam}]	12.9064	13.4371	13.9838	14.6868	15.0614	15.4232	16.0143	17.3865
Electricity [$UC_{Electricity}$]	5.7771	6.3716	6.9829	7.5712	7.8945	8.2588	8.5441	8.2864
Cooling water [UC_{Cwater}]	1.7815	1.8238	1.8908	1.9880	2.0409	2.0993	2.2205	2.4688
MEA make-up [$UC_{MEA\ mk}$]	1.2521	1.3416	1.4310	1.5205	1.5652	1.6099	1.6546	1.6993
H_2O make-up [$UC_{H_2O\ mk}$]	0.0804	0.0862	0.0919	0.0977	0.1006	0.1034	0.1063	0.1092
(2) Total purchase equipment cost [δ_1TPC, million US$/year]	8.6471	8.9188	9.2370	9.5507	9.7177	9.9132	10.1127	10.5416
(3) Total operating labor cost [TOLC, δ_3OLC, million US$/year]	0.3913	0.3913	0.3913	0.3913	0.3913	0.3913	0.3913	0.3913

Table 10
Distribution of the TPC for different CO_2 removal targets.

	CO_2 removal target = 80% (TPC = 23.69 million US$)	CO_2 removal target = 85% (TPC = 24.49 million US$)	CO_2 removal target = 95% (TPC = 27.03 million US$)
Compressors [%]	39.57	41.17	38.97
Absorber [%]	16.48	17.82	20.26
Lean-rich amine heat exchanger [%]	17.00	16.15	12.87
Reboiler [%]	7.00	7.13	7.41
Blower [%]	5.94	6.57	6.50
Condenser [%]	4.10	4.30	4.39
Desorber [%]	3.93	3.94	4.10
Lean amine cooler [%]	2.64	2.55	1.96
H_2O tank [%]	1.14	1.24	1.30
Interstage coolers [%]	1.19	1.23	1.17
MEA tank [%]	0.73	0.76	0.82
Pumps [%]	0.30	0.29	0.25

Table 11
Optimal values of total direct and indirect costs and fixed capital investment for different CO_2 removal targets.

Cost-item	CO_2 removal target [%]							
	70.0	75.0	80.0	85.0	87.5	90.0	92.5	95.0
Total annual cost [TAC, million US$/year]	42.1379	44.0565	46.1367	48.3788	49.5813	50.8814	52.4142	54.8305
Annualized capital cost [ACC, million US$/year]	10.3655	10.6913	11.0727	11.4487	11.6489	11.8832	12.1225	12.6366
Capital recovery factor [CRF][a]	0.093676	0.093676	0.093676	0.093676	0.093676	0.093676	0.093676	0.093676
Total purchased equipment cost [TPC, million US$]	22.1760	22.8729	23.6890	24.4935	24.9218	25.4231	25.9349	27.0347
Compressors [COMP]	8.7749	9.1295	9.4841	9.8340	10.0057	10.1769	10.3526	10.5365
Absorber [ABS]	3.6543	3.9528	4.2668	4.5568	4.7282	4.9392	5.0739	5.4761
Lean-rich amine exchanger [ECO]	3.7691	3.5817	3.4711	3.3247	3.2326	3.1632	3.1178	3.4800
Reboiler [REB]	1.5517	1.5805	1.6225	1.7020	1.7479	1.7968	1.8885	2.0035
Blower [BLOW]	1.3171	1.4564	1.5911	1.7089	1.7763	1.8563	1.9049	1.7566
Condenser [COND]	0.9098	0.9525	0.9942	1.0424	1.0680	1.0936	1.1352	1.1866
Desorber [REG]	0.8708	0.8734	0.8904	0.9289	0.9531	0.9732	1.0167	1.1083
Lean amine cooler [LAC]	0.5851	0.5648	0.5486	0.5287	0.5169	0.5059	0.4957	0.5310
H_2O tank [H_2O-TK]	0.2518	0.2751	0.2960	0.3201	0.3332	0.3454	0.3584	0.3515
Interstage coolers [I-COOL]	0.2634	0.2722	0.2820	0.2921	0.2971	0.3021	0.3080	0.3153
MEA tank [MEA-TK]	0.1622	0.1687	0.1772	0.1906	0.1985	0.2066	0.2194	0.2210
Pumps [RAP]	0.0658	0.0654	0.0649	0.0645	0.0642	0.0639	0.0637	0.0683
Direct cost [DC, million US$]	59.6092	61.4824	63.6760	65.8385	66.9897	68.3372	69.7130	72.6693
Indirect cost [IC, millionUS$]	22.3534	23.0559	23.8785	24.6894	25.1211	25.6265	26.1424	27.2510
Fixed capital investment [FCI, million US$]	28.6878	29.5893	30.6450	31.6857	32.2397	32.8883	33.5504	34.9732
Total Working Capital [WC]	20.4913	21.1352	21.8893	22.6326	23.0284	23.4916	23.9646	24.9808
Start-up and initial solvent costs [SC]	8.1965	8.4541	8.7557	9.0531	9.2114	9.3966	9.5858	9.9923

[a] Constant value.

US$/year] varies linearly with the CO_2 removal targets from 70.0 to 80.0% of CO_2 removal target and then from 80.0% the total cost increases a little more rapidly as the CO_2 removal target increases. Certainly, the total cost increases in 4.7 and 7.8% when the CO_2 removal target increases, respectively, from 75.0 to 80.0% and from 90.0 to 95.0%.

Fig. 3 shows how the total cost is distributed in operating cost [TO&MC] and investment [ACC] for each one of the CO_2 removal targets. The reported results clearly indicate that the total cost distribution in operating cost and investment is not significantly affected by the CO_2 recovery target. It can be seen that the ratio of [TO&MC]/[TAC] slowly decreases as the CO_2 removal target increases. Naturally, the ratio of [ACC]/[TAC] increases at the same rate that [TO&MC]/[TAC] decreases.

The average contributions of the operating cost and investment on the total cost for all CO_2 recovery targets are 76.2 and 23.8% respectively.

6.2. Contribution of each one of the operating costs on the total operating cost (TO&MC)

Table 7 illustrates the total contributions of each one of the cost-items (TU&MUC, purchased equipment and TOLC) on the total operating cost (TO&MC) for two CO_2 removal targets (80 and 95%). In addition, Table 8 shows how the total utility costs reported in Table 7 are distributed in heating and cooling utilities, total electricity consumed by pumps, blower and compressors and MEA and H_2O make-up costs. Table 9 presents a detailed description of the cost-items for the all CO_2 removal targets considered in Figs. 2 and 3.

As expected, it can be seen from Table 7 that, independently of CO_2 recoveries, the total operating and maintenance cost [TO&MC] is strongly influenced by [TU&MUC]. More specifically, it accounts for more than 73.0% of the [TO&MC]. The contributions of the total purchased equipment cost [δ_1TPC] and the total labor cost (TOLC) are, respectively, 26.0 and 1.0%.

Table 12
Optimal dimensions and operating conditions of absorption and regeneration units for different CO_2 removal targets.

	CO_2 removal target							
	70.0%	75.0%	80.0%	85.0%	87.5%	90.0%	92.5%	95.0%
Absorber [ABS]								
Packing height [H_{ABS}, m]	12.79	15.16	17.63	19.91	21.27	22.94	23.98	25.18
Diameter [D_{ABS}, m]	12.14	12.13	12.13	12.13	12.13	12.13	12.13	12.68
Total packing volume	1479.82	1752.01	2037.72	2301.62	2457.81	2650.24	2773.58	3181.13
Solvent inlet flow-rate [mol/s]	20,609.5	20,606.4	20,612.8	20,630.8	20,636.9	20,639.1	20,663.5	22,719.6
Solvent inlet temperature [T_{LC}, K]	315.47	316.48	317.36	318.57	319.34	320.09	320.85	320.48
Solvent outlet temperature [T_{RC}, K]	322.44	322.90	323.42	324.03	324.41	324.86	325.37	325.74
Inlet gas temperature [$T^{G_{in}}$, K][a]	323.15	323.15	323.15	323.15	323.15	323.15	323.15	323.15
Outlet gas temperature [$T^{G_{out}}$, K]	324.53	325.40	326.18	327.07	327.56	328.01	328.47	328.22
Pressure drop [ΔP_{ABS}, Pa/m]	466.46	467.24	467.31	467.77	468.20	468.39	468.44	387.81
Inlet CO_2 loading [α_{LC}]	0.2616	0.2610	0.2551	0.2413	0.2332	0.2246	0.2062	0.1989
Regenerator [REG]								
Packing height [H_{REG}, m]	4.91	4.96	5.21	5.49	5.64	5.71	5.84	6.31
Diameter [D_{REG}, m]	4.45	4.45	4.47	4.59	4.67	4.74	4.91	5.20
Total packing volume	76.54	77.40	82.23	91.20	96.84	101.22	110.83	134.52
Inlet liquid temperature [T_{RH}, K]	383.29	382.77	382.74	382.89	382.91	383.01	383.52	384.53
Outlet liquid temperature [T_{REB}, K]	391.42	391.45	391.79	392.54	392.94	393.34	394.10	394.37
Outlet gas temperature [T_C, K]	322.40	320.48	319.71	319.44	319.29	319.31	319.95	321.56
Pressure drop [ΔP_{REG}, Pa/m]	119.10	125.72	137.12	149.60	155.09	161.60	175.53	179.30
Inlet CO_2 loading [α_{RC}]	0.3883	0.3972	0.4007	0.3964	0.3931	0.3893	0.3756	0.3566

[a] Fixed value.

Table 13
Optimal dimensions and operating conditions of reboiler, condenser, heat exchanger units, compressors and pumps for different CO_2 removal targets.

	CO_2 removal target							
	70.0%	75.0%	80.0%	85.0%	87.5%	90.0%	92.5%	95.0%
Reboiler [REB]								
Temperature [T_R, K]	391.42	391.45	391.79	392.54	392.94	393.34	394.10	394.37
Area [A_{REB}, m^2]	2303.79	2375.53	2481.65	2687.62	2809.38	2941.81	3196.23	3526.97
Heat load [Q_R, kJ/s]	79,768.47	83,048.54	86,427.39	90,771.89	93,087.24	95,323.25	98,976.77	107,457.61
Driven force [DMLT_R]	25.45	25.70	25.60	24.83	24.36	23.82	22.76	22.40
Condenser [COND]								
Liquid flow-rate to stripper [mol/s]	404.402	404.604	422.717	463.317	486.937	514.767	590.019	713.834
Temperature [T_{COND}, K]	322.397	320.481	319.708	319.436	319.292	319.307	319.949	321.564
Heat transfer area [A_{COND}, m^2]	3217.010	3472.604	3729.924	4035.886	4202.738	4371.590	4652.617	5008.980
Heat load [Q_{COND}, kJ/s]	43,568.1	45,117.3	47,645.2	51,440.4	535,266	558,431	60,797.7	68,392.5
Driven force [K]	42.296	40.576	39.893	39.806	39.776	39.894	40.810	42.642
Lean-rich amine exchanger [ECO]								
Driven force [Δt_{ml}, K]	8.098	8.655	9.025	9.616	10.007	10.306	10.562	9.812
Heat transfer area [A_{ECO}, m^2]	18,545.50	17,034.89	16,167.27	15,046.27	14,358.65	13,848.36	13,518.53	16,236.34
Heat load [Q_{ECO}, kJ/s]	114,252.7	112,165.6	111,008.9	110,072.6	109,317.7	108,581.8	108,631.0	121,203.6
Lean amine cooler [LAC]								
Driven force [Δt_{ml}, K]	17.34	18.36	19.24	20.44	21.21	21.96	22.73	22.36
Heat transfer area [A_{LAC}, m^2]	1541.54	1453.33	1384.75	1301.96	1253.70	1209.74	1169.18	1311.36
Heat load [Q_{LAC}, kJ/s]	26,865.8	26,814.2	26,775.6	26,746.5	26,727.1	26,704.4	26,707.6	29,463.9
Interstage coolers [I-COOL]								
Average driven force [Δt_{ml}, K]	56.76	56.57	56.50	56.48	56.47	56.47	56.54	56.71
Total heat transfer area [$A_{I\text{-}COOL}$, m^2]	407.69	430.52	456.67	484.30	498.06	512.37	529.11	550.07
Total heat load [$QT_{I\text{-}COOL}$, kJ/s]	6439.5	6767.0	7169.2	7599.3	7813.0	8038.0	8313.3	8675.5
Compressors (4) [COMP]								
Total compression power [PT_{COMP}, kW]	4542.51	4852.33	5170.35	5492.13	5652.89	5814.97	5983.34	6161.79
Pump [RAP]								
Power [P_{RAP}, kW]	57.33	56.62	55.96	55.36	54.98	54.51	54.29	60.91
Blower [BLOW]								
Power [P_{BLOW}, kW]	2065.01	2441.71	2829.57	3187.10	3399.65	3658.37	3819.37	3336.97
Total electricity [kW]	6664.84	7350.65	8055.88	8734.58	9107.52	9527.86	9857.01	9559.67

Table 8 clearly shows that, independently of CO_2 recoveries, the total utility cost [U&MUC] is strongly influenced by the steam used in the reboiler [UC_{Steam}] and by the total electricity consumed by pumps, blower and compressors [$UC_{Electricity}$] and the corresponding contributions are about 57.7 and 28.15%, respectively. The costs of MEA make-up and cooling medium (water) represent approx. 13.5%. The cost of H_2O make-up is insignificant (0.38%).

As illustrated in Table 9, the ranking order of the cost distribution does not vary with the CO_2 removal target.

6.3. Contribution of each one of the pieces of equipments (PC_j) on the total purchased equipment cost (TPC)

Tables 10 and 11 clearly show the contributions of the investments of each one of the pieces of equipments on the total equipment purchased cost (TPC). As expected, TPC is significantly influenced by the compressors, the absorption unit and the lean-rich amine exchanger [ECO]. Indeed, these pieces of equipments represent more than 73.00% of the total capital investment. As is also shown in Table 10, the contributions of the blower (BLOW) and reboiler (REB) for CO_2 removal target = 85.0% are quite similar (approx. 7.0–8.0% each) and thus the ranking order may change as the CO_2 removal target and cost parameters vary. This also applies for the following groups of pieces of equipments: (a) [ABS] and [ECO]; (b) [COND] and [REG] and (c) [I-COOL] and [H_2O-TK].

A detailed comparison of the distribution of the each one of the cost-items on the TPC for the different CO_2 capture levels is shown in Table 11. The comparison shows that the ranking order from CO_2 removal target = 75.0–80% varies with respect to 70%. In addition, the ranking order from CO_2 removal target = 85.0–92.5% varies with respect to 95.0%. Certainly, from 75.0 to 80.0% of CO_2 removal the contribution of the water make-up tank [H_2O-TK] is greater than the inter-stage coolers [I-COOL], in contrast to that observed for 70.0%. Then, from CO_2 removal target = 85.0–92.5% the order between the blower [BLOW] and reboiler [REB] is also modified; the contribution of [BLOWER] becomes progressively more important than [REB], in contrast to that observed for 70.0% to 80.0% and 95.0%. Thus, it is possible to conclude that the contribution percentage of each one of pieces of equipments is slightly influenced by the CO_2 removal target but the effect is strong enough to vary the corresponding ranking order.

6.4. Optimal dimensions and operating conditions of each one of the pieces of equipment

Tables 12 and 13 compare the heat transferred driving force and dimensions of the main process-units to reach different CO_2 removal targets to minimize the total annual cost. The results listed in both tables correspond to those optimized results analyzed in the previous sections.

From the reported results, the following conclusions can be drawn:

- The volume of the packing material of the absorber for CO_2 removal target 95.0% (3181.13 m^3) is 115.0% greater than that required for 70.0%. Despite that the absorber diameter is an optimization variable, it remains almost constant as the CO_2 removal target increases (12.2 m). Thus, the absorber height and therefore the packing material volume considerably increase as the CO_2 removal target increases.
- The outlet gas temperature and the solvent inlet and outlet temperatures in the absorber slightly vary with the CO_2 removal targets.
- In order to meet the CO_2 emission target, the inlet CO_2 loading in the absorber slightly decreases as the CO_2 removal target increases.
- As expected, the higher CO_2 removal targets, the higher amount of CO_2 removed from the flue-gas stream and therefore the higher values of CO_2 loading leaving the absorber (α_{RC}).

Table 14
Optimal solutions for different optimization problems.

	P1. Minimizing TAC (CO_2 removal = 85%)	P2. Minimizing the total heat duty (CO_2 removal = 85%)	P3. Minimizing the total heat duty/CO_2 recovery (CO_2 removal "free")
CO_2 removal %	56,818.08	56,818.08	59,529.44
Amount of CO_2 captured [kg/h]	48.379	49.393	51.029
TAC [million US$/year]	10.366	11.533	11.915
TCI [million US$/year]	31.772	37.860	39.114
TO&MC [million US$/year]	56,818.08	56,818.08	59,529.44
Total purchased equipment cost [TPC, million US$]			
Compressors [COMP]	9.834	10.192	10.485
Absorber [ABS]	4.557	4.908	5.052
Desorber [REG]	0.929	0.896	1.229
Reboiler [REB]	1.702	1.640	1.708
Lean-rich amine exchanger [ECO]	3.325	2.874	2.817
Blower [BLOW]	1.709	1.951	1.910
Condenser [COND]	1.042	0.760	0.804
Interstage coolers [I-COOL]	0.292	0.345	0.355
Lean amine cooler [LAC]	0.529	0.494	0.484
H_2O Tank [H_2O-TK]	0.320	0.362	0.379
MEA tank [MEA-TK]	0.191	0.189	0.205
Total utility cost [U&MUC, million US$/year]			
Cooling water [UC_{water}]	1.988	1.856	1.975
H_2O make-up [$UC_{H_2O\ mk}$]	0.098	0.098	0.102
MEA make-up [$UC_{MEA\ mk}$]	1.520	1.520	1.593
Steam [UC_{Steam}]	14.687	14.649	15.225
Electricity [$UC_{Electricity}$]	7.571	8.560	8.684
Absorber			
Packing height [H_{ABS}, m]	19.91	23.34	23.92
Diameter [D_{ABS}, m]	12.13	11.94	12.10
Total packing volume [m^3]	2301.62	2614.08	2752.40
Solvent inlet temperature [T_{LC}, K]	318.57	335.88	336.71
Solvent outlet temperature [T_{RC}, K]	324.03	324.43	324.78
Outlet gas temperature [$T^{G_{out}}$, K]	323.15	327.83	328.47
Pressure drop [ΔP_{ABS}, Pa/m]	467.77	501.93	471.81
Inlet CO_2 loading [α_{LC}]	0.241	0.260	0.238
Desorber			
Packing height [H_{REG}, m]	5.49	5.07	9.71
Diameter [D_{REG}, m]	4.59	4.53	4.93
Total packing volume [m^3]	91.20	82.00	185.43
Inlet liquid temperature [T_{RH}, K]	382.89	380.02	380.73
Outlet liquid temperature [T_{REB}, K]	392.54	391.52	392.71
Pressure drop [ΔP_{REG}, Pa/m]	149.60	127.09	107.83
Inlet CO_2 loading [α_{RC}]	0.396	0.416	0.402
Reboiler, condenser and heat exchangers			
Heat load in reboiler [kJ/s]	90,771.89	90,537.31	94,101.44
Specific heat load in reboiler [MJ/kg of CO_2]	5.751	5.736	5.691
Heat transfer area in reboiler [m^2]	2687.6	2526.7	2703.2
Heat load in condenser [kJ/s]	51,440.4	42,597.8	47,203.0
Heat transfer area in condenser [m^2]	4035.9	2384.6	2616.2
Heat load in lean-rich amine heat exchanger [kJ/s]	110,072.6	103,013.0	103,812.7
Heat transfer area in lean-rich amine heat exchanger [m^2]	15,046.3	11,799.9	11,413.5
Heat load in lean amine cooler [kJ/s]	26,746.5	26,551.4	26,565.0
Heat transfer area in lean amine cooler [m^2]	1302.0	1163.7	1123.1

- In regards to the dimensions of the MEA regeneration unit, it is possible to conclude that the optimal volume of the packing material increases as the CO_2 removal target increases. The height and diameter increase, respectively, 29.5% and 16.8% from 70.0 to 95.0 CO_2 capture % resulted in an increase of the volume of the packing material in about 75.8% (58.0 m^3).
- The CO_2 removal target does not affect the outlet temperatures of liquid and vapor in the regenerator.
- By comparing the optimal values for the reboiler, it is concluded that the reboiler temperature and the driving force do not vary with the CO_2 removal target.
- As expected, the heat transfer areas and their heat loads in the reboiler, condenser, lean-rich amine heat exchanger and

Table 15
Comparison of the dimensions for absorption and regeneration units obtained from the proposed model and reported data.

	Column dimensions			
	Fisher et al. (2005)		This work	
	Absorber	Regenerator	Absorber	Regenerator
H [m]	15.00	10.00	17.68	11.03
D [m]	9.70	5.50	8.84	5.66
Vol [m^3]	1108.47	237.58	1085.78	277.75
dP [kPa]	10.30	10.30	8.83	2.42

Table 16
Comparison of the capacities of the main piece of equipments obtained from the proposed model and reported data.

Piece of equipment	Equipment sizing	
	Fisher et al. (2005)	This work (2011)
Flue gas blower [kW]	9200.0	7128.0
Absorber (4) [m^3]	4433.9	4343.1
Rich amine pump [kW]	1732.0	278.0
Stripper (4) [m^3]	950.3	1111.0
Condenser [m^2]	15,272.0	21,809.2
Reboiler [m^2]	30,436.0	48,751.9
Rich/lean amine exchanger [m^2]	101,136.0	87,686.5
Lean amine cooler [m^2]	35,972.0	31,023.5
Amine storage tank [m^2]	276.0	1259.6
Water storage tank [m^2]	628.3	3198.1
CO_2 compresors [kW]	34,845.0	40,306.7
CO_2 compresors interstage coolers [m^2]	Not included	3933.2

lean amine cooler increase significantly as CO_2 removal target increases. However, the corresponding driving forces are not affected.

- The CO_2 removal target has a strong influence on the total electricity consumed by compressors and pumps. Certainly, the total electricity necessary to remove 95.0% of CO_2 from flue-gas stream is 43.0% higher than that required to remove 70.0%.

6.5. *Influence of the CO_2 removal target on the profiles of temperature and amount of CO_2 captured along the height of absorber and regenerator units.*

Figs. 4 and 5 illustrate the outlet temperature and CO_2 loading factor in each one of stages of the absorber and stripper.

Fig. 4 clearly shows that, the profiles of temperature along the stages of the absorber for CO_2 removal target = 95% reach greater values than those predicted for 80%. Both temperature profiles follow qualitatively similar trends and exhibit maximum values in different parts of the absorber. Certainly, for 95% of removal the temperature increases from 328.4 (inlet temperature as indicated in Table 9) to 333.3 K in Stage 7 (maximum value) and then it gradually decreases to 325.7 at the bottom of the absorber (Stage 1). The temperature drop at the bottom of the absorber results from the cold gas entering to the bottom and contacting the hot liquid flowing downwards. In regards to the temperature drop, it is important to mention that the proposed model assumes, as a first approximation, thermal equilibrium between the liquid and vapor phases. Then, the temperature profiles obtained under non-thermal equilibrium condition may be similar or slightly different to those illustrated in Figs. 4 and 5. This aspect will be further investigated in detail.

As is also shown in Fig. 4, the CO_2 loading factor (CO_2 mol/MEA mol) monotonically increases from the top to the bottom of the column, as expected.

Finally, Fig. 5 shows the corresponding temperature and CO_2 loading profiles along the stripper. It can be seen how the CO_2 loading decreases from the top to the bottom of the stripper. The optimal values corresponding to the leaving CO_2 loading for 80% and 95% of CO_2 recovery are 0.26 and 0.20, respectively. Moreover, the optimal values of reboiler temperature (Stage 0) are 391.8 and 394.3 K, respectively.

Again, as in the case of the absorber, the corresponding temperature and CO_2 loading profiles for both CO_2 removal targets follow similar trends. In addition, these trends have been also obtained for the remaining CO_2 removal targets.

6.6. *Comparison of optimal designs involving different objective functions*

As mentioned earlier, by exploiting the benefits of the proposed model, different optimal designs obtained by considering different objective functions are compared. Thus, it is interesting to compare how much the design of the capture plant is affected when considering cost in the objective function, as opposed to the heat duty and specific heat duty as well. Precisely, the optimal solutions obtained for the following three objective functions are minimized

Table 17
Comparison of the purchasing equipment costs obtained from the proposed model and reported data.

Piece of equipment	Purchased equipment cost (million US$)		
	Fisher et al. (2005)	Fisher et al. (2005) updated to 2011	This work (2011)
Flue gas blower	2.040	2.553	1.005
Absorber	16.320	20.423	12.193
Rich amine pump	0.272	0.340	0.120
Stripper	3.760	4.705	6.015
Condenser	1.880	2.353	3.071
Reboiler	4.600	5.756	8.049
Rich/lean amine exchanger	11.200	14.016	13.561
Lean amine cooler	4.012	5.021	4.828
Amine storage tank	0.058	0.073	0.338
Water storage tank	0.097	0.121	0.591
CO_2 compresors	16.048	20.082	23.348
Interstage coolers (CO_2 compression)	0.749	0.937	1.099
Others: Cooling tower, filtration, CO_2 compressor separator, reflux accumulator and pumps	7.797	16.688	Not included
Total	74.371	93.067	74.217

Table 18
Comparison of the operating costs obtained from the proposed model and reported data.

	Fisher et al. (2005)	Fisher et al. (2005) updated to 2011	This work (2011)
MEA make-up [million US$/year]	6.95	8.70	8.79
H_2O make-up [million US$/year]	2.57	3.21	3.46
Solid waste disposal [million US$/year]	0.05	0.06	Not included
Cooling water [million US$/year]	Not included	–	3.42
Total utility cost [TU&MU, million US$/year]	9.57	11.98	15.68

and compared: (1) total annual cost (hereafter named P1), (2) total heat duty (hereafter named P2) and (3) total heat duty/CO_2 recovery (hereafter named P3) where the CO_2 recovery is here considered as an optimization variable. The parameters used to solve the three problems are listed Tables 4 and 5.

As it is clearly shown in Table 14, similar optimal solutions are obtained by solving P1, P2 and P3 problems. The total annual costs predicted by the three objective functions are fairly similar. Therefore, the detailed comparison in Table 14 reveals that the objective functions involved by P2 and P3 problems can be used as alternative optimization criteria for the cost-optimal design of post-combustion CO_2 capture processes using amines. This aspect is valuable from a solution strategy point of view, because the optimal solutions obtained by solving P2 or P3 can be efficiently used as initialization to solve P1. Certainly, according to the comparison of the values predicted for P1 and P2, it is easily to conclude that solutions of P2 or P3 problems are not only initial feasible points but also they are in the neighborhood of the optimal solutions for P1. Therefore, a feasible solution can be easily obtained for P1 after a few iterations if the solution corresponding to P2 or P3 is used as starting point.

6.7. A comparison between the output results predicted by the model and data reported by other authors

It is also interesting to compare the output results obtained by applying the proposed model with costs reported by other authors (operating cost and investment). The reference case is taken from Fisher et al. (2005) and, for a valid comparison, the reported costs were properly updated to 2011. It should be mentioned, however, that the process configuration of the reference case is slightly different in comparison to the configuration considered in this article. For instance, in contrast to this article, Fisher et al. (2005) included a cooling tower, filtration, CO_2 compressor separator and reflux accumulator and are considered to compute the total purchased equipment cost. In this article, the cost of cooling water used as cooling medium is considered to compute the total operating cost.

For a more detailed comparison, the complete cost solutions are compared and discussed from Tables 15–18. Therefore, the results presented in these tables correspond to an unique optimal solution.

Tables 15–17 compare the dimensions, capacities and purchased equipment costs of the main piece of equipments. For the dimensions of the absorber and regenerator columns, Table 15 clearly shows that the predicted values are in good agreement with the published data.

From the results presented in Table 16, it can be seen that the capacities of some of the piece of equipments predicted by the model are close to the values reported by Fisher et al. but the capacities predicted for some of the process-units are different. The differences could be explained by several factors not taken into account in Fisher et al. but considered in this work and/or vice versa. For example, the assumptions considered to derive the mathematical models (mass, energy and momentum balances) may influence the solutions. Other aspect to be mentioned is that, as opposed to this work, the solution reported by Fisher et al. was obtained by simulations instead of optimizations and consequently the results may be different.

Table 17 compares the predicted and the published values of the purchased equipment cost of each one of the piece of equipments. Despite the fact that the cost equations used in this work are different to those used in Fisher et al., the predicted values are in good agreement. It should be noted that the total purchased equipment cost reported by Fisher et al. is 76.379 million US$ if the costs involved by the cooling tower, filtration, CO_2 compressor separator, reflux accumulator and pumps are not considered. Also, Table 17 clearly shows that the purchased costs estimated by Fisher et al. increased 25.0% from 2005 to 2011.

Table 18 compares the distribution of the total utility cost. It should be stressed here that the cooling water cost was not included by Fisher et al. (2005) in contrats to this work. Certainly, the values listed in Table 18 corresponds to a cooling water cost of 0.01 US$/t. In addition, it should also be mentioned that, for a valid comparison, the costs of electricity to run compressors and pumps and steam used in the reboiler of the regeneration section are not included in Table 18.

Basically, if the cooling water cost is not considered the total variable O&M cost predicted by the proposed cost model is quite similar to that reported by Fisher et al. (2005).

7. Conclusions. Future works

A non-linear and predictive mathematical model for the simultaneous optimization of the reactive CO_2 absorption into aqueous MEA solutions has been presented. The proposed model is a valuable tool not only to optimize the process but also to simulate the absorption process if the degree of freedom of the equation system is zero. The model variables are simultaneously optimized. A detailed objective function including the total annualized capital cost and operating and maintenance costs has been used for minimization. Output results provide the optimal profiles of temperature, composition and flow-rate of liquid and gas streams along the height of the absorption and regeneration units. In addition, the capacities of compressors, pumps, heat transfer areas including the heat loads and consumption of heating and cooling utilities are also obtained.

The effect of the CO_2 removal target on the total annual cost and the contributions of each one of the pieces of equipments have been investigated. From the obtained results, it is concluded that, from CO_2 removal target = 70.0–80.0% the total cost (investment and operating costs) varies linearly and then, from 80.0 to 95.0%, it increases exponentially. The total operating cost, which is strongly influenced by the utilities and electricity, represents more than 75% of the total annual cost. The contribution of the steam used in the reboiler and the electricity consumed by pumps and compressors on the total operating cost are approx. 57.0% and 28.0%, respectively.

The ranking order of the contributions of the steam, electricity, cooling water, MEA and H_2O make-ups on the total operating and maintenance cost is not affected by the CO_2 removal target.

In regards to the total purchased equipment cost, it was found that the compressors and the absorption unit are the pieces of equipments with the first and second largest impact, respectively, on the total annual cost for all CO_2 removal targets analyzed. From the obtained results, it is possible to conclude that the contribution percentage of each one of pieces of equipments is slightly influenced by the CO_2 removal target but the effect is strong enough to vary the corresponding ranking order of some of them (blower [BLOW], reboiler [REB], inter-stage coolers [I-COOL] and water tank [H_2O-TK]). From 75.0 to 80% of CO_2 removal the contribution of the water make-up tank [H_2O-TK] is greater than the inter-stage coolers [I-COOL], in contrast to that observed for 70.0%. Then, from CO_2 removal target = 85–92.5% the order between the blower [BLOW] and reboiler [REB] is also modified; the contribution of [BLOWER] becomes progressively more important than [REB], in contrast to that observed for 70.0% to 80% and 95%.

It is interesting and essential to investigate the best alternative integration between the CO_2 capture processes and power-electricity generation plants in order to reduce the total annual cost. In fact, part of the steam generated in the power plant can be used in the reboiler of the regeneration section. Also, the electricity generated can be efficiently used to drive pumps and compressors. Thus, the mathematical model presented in this paper will be coupled to a previous one which has been developed to study a combined cycle power plant (CCPP). The resulting model will also consider the entire configuration of the process (number and arrangement of pieces of equipments) as optimization variable. Discrete decisions will be used to model different alternative integrations between the CO_2 capture process and the combined cycle power plant. Pressure levels, number and type of steam turbines (back-pressure, extraction–condensation turbines) and the design of the heat recovery steam generator including number of tubes in economizer, evaporator and super-heater are some of the optimization variables for the CCPP.

Finally, the extension of the proposed steady state model to a dynamic model in order to optimize the start-up and shut-down phases of the process study start-up operation is also another interesting point to be addressed in future works. Non-thermal equilibrium between liquid and vapor phases will be also considered.

Acknowledgements

The following two organizations are gratefully acknowledged for their financial support: Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET, Argentina) and the Universidad Tecnológica Nacional Facultad Regional Rosario (UTN-FRRo, Argentina).

References

Abu-Zahra, M.R.M., Schneiders, L.H.J., Niederer, J.P.M., Feron, P.H.M., Versteeg, G.F., 2007a. CO_2 capture from power plants. Part I. A parametric study of the technical performance based on monoethanolamine. International Journal of Greenhouse gas control 1, 37–46.

Abu-Zahra, M.R.M., Schneiders, L.H.J., Niederer, J.P.M., Feron, P.H.M., Versteeg, G.F., 2007b. CO_2 capture from power plants. Part II. A parametric study of the economical performance based on mono-ethanolamine. International Journal of Greenhouse gas control 1, 135–142.

Aliabad, Z., Mirzaei, S., 2009. Removal of CO_2 and H_2S using aqueous alkanolamine solutions world academy of science. Engineering and Technology 49, 194–203.

Ali, C., Backham, L., Croiset, E., Douglas, P., 2005. Simulation of CO_2 capture using MEA scrubbing: a flowsheet decomposition method. Energy Conversion and Management 46, 475–487.

Aroonwilas, A., Veawab, A., 2007. Integration of CO_2 capture unit using single- and blended-amines into supercritical coal-fired power plants: implications for emission and energy management. International Journal of Greenhouse Gas Control 1 (2), 143–150.

Blauwhoff, P.M.M., Kamphuis, B., Van swaaij, W.P.M., Westerterp, K.R., 1985. Absorber design in sour natural gas treatment plants: impact of process variables. Chemical Engineering and Processing 19, 1–25.

Böttinger, W., Maiwald, M., Hasse, H., 2008. Online NMR spectroscopic study of species distribution in MEA–H_2O–CO_2 and DEA–H_2O–CO_2. Fluid Phase Equilibria 263 (2), 131–143.

Brooke, A., Kendrick, D., Meeraus, A., 1996. GAMS – A User's Guide (Release 2.25). The Scientific Press, San Francisco, CA.

Chapel, D., Ernst, J., Mariz, C., 1999. Recovery of CO_2 from flue gases: commercial trends. Originally presented at the Canadian Society Chemical Engineers Annual Meeting, October 4–6, Saskatoon, Saskatchewan, Canada.

Choi, J.H., Oh, S.G., Kim, Y.E., Yoon, Y., Nam, S.C., 2012. Carbon dioxide absorption characteristics of aqueous alkanolamine using nuclear magnetic resonance spectroscopy. Environmental Engineering Science 29 (5), 328–334.

Cozad, A., Sahinidis, N., Miller, D.C., 2010. Optimization of power plant simulations with integrated carbon capture systems using black-box algorithms. In: 2010 Annual Meeting Conference Proceedings, November 7–12, Salt Lake City, UT.

Dave, N., Do, T., Palfreyman, D., Feron, P.H.M., Xu, S., Gao, S., Liu, L., 2011. Post-combustion capture of CO_2 from coal-fired power plants in China and Australia: an experience based cost comparison. Energy Procedia 4, 1869–1877.

deMontigny, D., Aboudheir, A., Tontiwachwuthikul, P., Chakma, A., 2006. Modelling the performance of a CO_2 absorber containing structured packing. Industrial & Engineering Chemistry Research 45, 2594–2600.

Drud, A.S., 1992. CONOPT, A GRG Code for Large Scale Nonlinear Optimization. Reference Manual. ARKI Consulting and Development A/S, Bagsvaerd, Denmark.

Duan, L., Zhao, M., Yang, Y., 2012. Integration and optimization study on the coal-fired power plant with CO_2 capture using MEA. Energy 3, http://dx.doi.org/10.1016/j.energy.2011.12.014.

Fashami, S.Z., Edgar, T.F., Rochelle, G.T., 2009. Texas Wisconsin California Control Consortium Meeting , February 3rd, 2009.

Fisher, K.S., Beitler, C., Rueter, C., Searcy, K., Rochelle, G., Jassim, M., Figueroa, J., 2005. Integrating MEA regeneration with CO_2 compression to reduce CO_2 capture costs. In: Fourth Annual Conference on Carbon Capture and Sequestration DOE/NETL, May 2–5.

Freguia, S., Rochelle, G.T., 2003. Modeling of CO_2 capture by aqueous monoethanolamine. AIChE Journal 49, 1676–1686.

Greer, T., 2008. Modeling and simulation of post combustion CO_2 capturing. PhD Thesis. Telemark University College, Faculty of Technology, Porsgrunn, Norway.

Henao, C., 2005. Simulación y evaluación de procesos químicos, 1st edition. Universidad Pontificia Bolivariana, Medellín.

Ho, M.T., Allinson, G.W., Wiley, D.E., 2011. Comparison of MEA capture cost for low CO_2 emissions sources in Australia. International Journal of Greenhouse Gas Control 5 (1), 49–60.

Huang, Y., Wang, M.H., Stephenson, P., Rezvani, S., McIlveen-Wright, D., Minchener, A.J., Hewitt, N., Dave, A., Fleche, A. Hybrid coal-fired power plants with CO_2 capture: a technical and economic evaluation based on computational simulations. Fuel, in press.

Islam, M.S., Yusoff, R., Ali, B.S., Islam, M.N., Chakrabarti, M.H., 2011. Degradation studies of amines and alkanolamines during sour gas treatment process. International Journal of the Physical Sciences 6 (25), 5877–5890.

Karimi, M., Svendsen, H.F., Hillestad, M., 2011. Capital costs and energy considerations of different alternative stripper configurations for post combustion CO_2 capture. Chemical Engineering Research and Design 89 (8), 1229–1236.

Khakdaman, H.R., Zoghi, A.T., Abedinzadegan, M., Ghadirian, H.A., 2008. Revamping of gas refineries using amine blends. IUST International Journal of Engineering Science 19 (3), 27–32.

Kister, H.Z., 1992. Destillation Design. McGraw Hill, USA.

Kuramochi, T., Faaij, A., Ramírez, A., Turkenburg, W., 2010. Prospects for cost-effective post-combustion CO_2 capture from industrial CHPs. International Journal of Greenhouse Gas Control 4 (3), 511–524.

Kvamsdal, H.M., Jakobsen, J.P., Hoff, K.A., 2009. Dynamic modeling and simulation of a CO_2 absorber column for post-combustion CO_2 capture. Chemical Engineering and Processing: Process Intensification 48, 135–144.

Lawal, O.A., Idem, R.O., 2006. Kinetics of the oxidative degradation of CO_2 loaded and concentrated aqueous MEA–MDEA blends during CO_2 absorption from flue gas streams. Industrial & Engineering Chemistry Research 45, 2602–2607.

Lawal, A., Wang, M., Stephenson, P., Yeung, H., 2009. Dynamic modelling of CO_2 absorption for post combustion capture in coal-fired power plants. Fuel 88 (12), 2455–2462.

Lepaumier, H., Martin, S., Picq, D., Delfort, B., Carrette, P., 2010. New amines for CO_2 capture. III. Effect of alkyl chain length between amine functions on polyamines degradation. Industrial & Engineering Chemistry Research 49, 4553–4560.

Mores, P., Scenna, N., Mussati, S., 2011. Post-combustion CO_2 capture process: equilibrium stage mathematical model of the chemical absorption of CO_2 into monoethanolamine (MEA) aqueous solution. Chemical Engineering Research and Design 89 (9), 1587–1599.

Mores, P., Scenna, N., Mussati, S., 2012. A rate based model of a packed column for CO_2 absorption using aqueous monoethanolamine solution. International Journal of Greenhouse Gas Control 6, 21–36.

Nuchitprasittichai, A., Cremaschi, S., 2010. Optimization of CO_2 capture process with aqueous amine using response surface methodology. In: AIChE Annual Meeting, Conference Proceedings.

Oexmann, J., Hensel, C., Kather, A., 2008. Post-combustion CO_2-capture from coal-fired power plants: preliminary evaluation of an integrated chemical absorption process with piperazine-promoted potassium carbonate. International Journal of Greenhouse Gas Control 2 (4), 539–552.

Oexmann, J., Kather, A., 2010. Minimising the regeneration heat duty of post-combustion CO_2 capture by wet chemical absorption: the misguided focus on low heat of absorption solvents. International Journal of Greenhouse Gas Control 4 (1), 36–43.

Oi, L.E., 2007. Aspen HYSYS simulation of CO_2 removal by amine absorption from a gas based power plant. In: SIMS 2007 Conference, Gosteborg.

Onda, K., Takeuchi, H., Okumoto, Y., 1968. Mass transfer coefficients between gas and liquid phases in packed columns. Journal of Chemical Engineering of Japan 1, 56.

Peeters, A.N.M., Faaij, A.P.C., Turkenburg, W.C., 2007. Techno-economic analysis of natural gas combined cycles with post-combustion CO_2 absorption, including a detailed evaluation of the development potential. International Journal of Greenhouse Gas Control 1 (4), 396–417.

Peng, D.Y., Robinson, D.B., 1976. A new two constant equation of state. Industrial Engineering Chemical Fundamentals 15, 59–64.

Perry, R.H., Green, D.W., 1997. Perry's Chemical Engineers' Handbook, 7th edition. McGraw Hill.

Rahimpour, M.R., Kashkooli, A.Z., 2004. Modeling and simulation of industrial carbon dioxide absorber using amine-promoted potash solution. Iranian Journal of Science & Technology, Transaction B 28 (B6), 653–666.

Rao, A.B., Rubin, E.S., 2002. A technical, economic, and environmental assessment of amine-based CO_2 capture technology for power plant greenhouse gas control. Environmental Science and Technology 36, 4467–4475.

Robbins, L.A., 1991. Improve pressure-drop prediction with a new correlation. Chemical Engineering Progress 87 (5), 87–91.

Romeo, L.M., Bolea, I., Escosa, J.M., 2008. Integration of power plant and amine scrubbing to reduce CO_2 capture costs. Applied Thermal Engineering 28 (8–9), 1039–1046.

Schach, M.O., Schneider, R., Schramm, H., Repke, J.U., 2010a. Techno-economic analysis of postcombustion processes for the capture of carbon dioxide from power plant flue gas. Industrial & Engineering Chemistry Research 49 (5), 2363–2370.

Schach, M.O., Schneider, R., Schramm, H., Repke, J.U., 2010b. Exergoeconomic analysis of post-combustion CO_2 capture processes. Computer Aided Chemical Engineering 28, 997–1002.

Seider, W.D., Seader, J.D., Lewin, D.R., Widagdo, S., 2009. Product and Process Design Principles: Synthesis, Analysis and Evaluation, 3rd edition. John Wiley & Sons Inc.

Singh, D., Croiset, E., Douglas, P.L., Douglas, M.A., 2003. Techno-economic study of CO_2 capture from an existing coal-fired power plant: MEA scrubbing vs. O_2/CO_2 recycle combustion. Energy Conversion and Management 44 (19), 3073–3309.

Sinnott, R.K., Towler, G., Coulson, J.M., Richardson, J.F., 2009. Chemical Engineering Design, 5th edition. Elsevier.

Sipöcz, N., Tobiesen, A., Assadi, M., 2011. Integrated modelling and simulation of a 400 MW NGCC power plant with CO_2 capture. Energy Procedia 4, 1941–1948.

Turton, R., Bailie, R.C., Whiting, W.B., Shaeiwitz, J.A., 2008. Analysis, Synthesis and Design of Chemical Processes, 3rd edition. Prentice hall.

United Technologies Research Center, 1999. Combustion, 2000 Phase II, Progress report DE-AC22-95PC95144—25.

Vaidya, P.D., Kenig, E.Y., 2007. CO_2–alkanolamine reaction kinetics: a review of recent studies. Chemical Engineering & Technology 30 (11), 1467–1474.

Vaidya, P.D., Kenig, E.Y., 2009. Kinetics of carbonyl sulfide reaction with alkanolamines: a review. Chemical Engineering Journal 148 (2–3), 207–211.

Vozniuk, I.O., 2010. Aspen HYSYS process simulation and AspenICARUS cost estimation of CO_2 removal plant. FMH606 Master's Thesis. http://teora.hit.no/dspace/bitstream/282/975/1/Master%20ThesisIevgeniia%20Vozniuk.pdf.

Xie, H.B., Zhou, Y., Zhang, Y., Johnson, J.K., 2010. Reaction mechanism of monoethanolamine with CO_2 in aqueous solution from molecular modeling. Journal of Physical Chemistry A 114 (43), 11844–11852.

Yoon, S.J., Lee, H., 2003. Substituent effect in amine–CO_2 interaction investigated by NMR and IR spectroscopies. Chemistry Letters 32 (4), 344.