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CO₂ Capture Cost Reduction: Use of a Multiscale Simulations Strategy for a Multiscale Issue

L. Raynal*, A. Gomez, B. Caillat and Y. Haroun

IFP Energies nouvelles, Rond Point de l'échangeur de Solaize, BP 3, 69360 Solaize - France
e-mail: ludovic.raynal@ifpen.fr - adrien.gomez@ifpen.fr - benjamin.caillat@ifpen.fr - yacine.haroun@ifpen.fr

* Corresponding author

Résumé — Réduction du coût du captage de CO₂ : mise en œuvre d'une stratégie de simulations multi-échelle pour un problème multi-échelles — Le captage et le stockage de CO₂ est un moyen important en vue de la réduction des émissions de CO₂ (International Energy Agency, 2009). Les procédés de captage en post-combustion utilisant des amines sont considérés parmi les options préférées pour le CSC (Captage et Stockage du Carbone). Cependant, le coût du CO₂ évité est très important et doit être réduit. Cet article a pour objectif de montrer que la combinaison de différents outils de simulations réalisées à différentes échelles permet une analyse fine des coûts du CO₂ et des paramètres associés responsables de ces coûts à différentes échelles. Il est tout d'abord montré, à partir d'une analyse technico-économique à l'échelle globale du procédé, que les coûts d'investissements représentent près de la moitié du coût du CO₂ total. En se focalisant sur ce dernier coût, une analyse de sensibilité basée sur des simulations Aspen à l'échelle intermédiaire de l'absorbeur, permet d'identifier les paramètres clés régissant le transfert de matière et le dimensionnement de la colonne. On montre que le paramètre le plus important est l'aire interfaciale, les coefficients de transfert de masse en phase gaz et en phase liquide n'ayant que très peu d'influence. Enfin, des simulations CFD (*Computational Fluid Dynamics*) réalisées à grande et petite échelles permettent d'orienter l'optimisation du design des colonnes *via*, d'une part, l'étude de l'interaction entre distributeurs et lit de garnissage, et d'autre part, la détermination à l'échelle locale de la perte de charge ou de paramètres de transfert de masse. Une discussion porte sur l'utilisation couplée de ces différents moyens de simulations qui permettront à terme d'aller plus loin dans le développement de technologies et la réduction des coûts de captage du CO₂.

Abstract — CO₂ Capture Cost Reduction: Use of a Multiscale Simulations Strategy for a Multiscale Issue — Carbon Capture and Storage (CCS) is one important option for CO₂ mitigation (International Energy Agency, 2009). Post-combustion capture processes using amines are considered one of the preferred options for CCS. However, the cost of avoided CO₂ is very large and must be reduced. The present article aims to show that combining different simulation tools used on different scales makes possible a fine analysis of CO₂ capture costs and the associated parameters responsible for these costs on different scales. It is first shown, from a macro-scale techno-economic analysis, that investments represent about one half of the total CO₂ cost. Focusing on this cost, a sensitivity analysis, via Aspen calculations performed on a meso-column scale, enables one to identify key mass-transfer parameters that control absorption column design. It is shown that the most important mass-transfer parameter is the interfacial area, the gas and liquid mass transfer coefficients having almost no

influence. Finally, from CFD (Computational Fluid Dynamics) simulations performed both on a large and on a local scale, some insights are given in order to optimize column design, first via the determination of large-scale distributor/packed bed interactions, and second via the determination of local pressure drop or local mass transfer parameters. It is also discussed how simulations should be performed on different scales in a two-way coupling approach in order to ensure fruitful results in the development of new technologies and further in CO₂ capture cost reduction.

NOMENCLATURE

a_e	Effective or interfacial area (m ⁻¹)
CAPEX	Capital expenditure (€)
CFB	Circulating Fluidized Bed (boiler technology)
D	Column diameter (m)
$Diff$	Diffusivity (m ² /s)
DNS	Direct Numerical Simulation
E	Acceleration coefficient (-)
e	Liquid film thickness (m)
$F_S = \sqrt{\rho_G} V_{SG}$	F-factor or gas capacity factor (Pa ^{1/2})
H	Height of the packed bed (m)
He	Henry coefficient (-)
HETP	Height Equivalent to a Theoretical Plate (m)
K_{Ga}	Overall mass transfer coefficient (s ⁻¹)
k_G	Gas-side mass transfer coefficient (m.s ⁻¹)
k_L	Liquid-side mass transfer coefficient (m.s ⁻¹)
LES	Large Eddy Simulation
MEA	Mono-Ethanol-Amine
MWe	Electric power produced by the power plant (MW)
NUT	Number of Unit Transfer (-)
OPEX	Operational expenditure (€)
$Pe = U_L e / Diff$	Peclet number (-)
Q_L	Liquid load (m ³ .m ⁻² .h)
REU	Representative Elementary Unit
U_L	Liquid film velocity (m/s)
VOF	Volume Of Fluid
V_{SG}	Gas superficial velocity (m.s ⁻¹)
$We = \rho_L U_L^2 e / \sigma$	Weber number (-)
y_{CO_2}	Percentage of CO ₂ molar fraction in the gas (%)
$\Delta P/L$	Pressure drop per unit length of packing (Pa/m)

GREEK LETTERS

θ	Contact angle (°)
μ_G	Gas viscosity (kg.m ⁻¹ .s ⁻¹)

μ_L	Liquid viscosity (kg.m ⁻¹ .s ⁻¹)
ρ_G	Gas density (kg.m ⁻³)
ρ_L	Liquid density (kg.m ⁻³)
σ	Surface tension (N/m)

INTRODUCTION

In the context of climate change and CO₂ mitigation, it is now well known that Carbon Capture and Storage (CCS) is one important solution to develop (International Energy Agency, 2009). On the one hand, the development of this technology must go fast enough to meet environmental targets; on the other hand, CO₂ capture cost has to be reduced. Indeed, since capture has a cost with no direct added value but CO₂ mitigation, and in order to avoid too great an increase in the electricity cost, the deployment of CO₂ capture processes will be possible only for those whose costs have been optimized, both in terms of energy demand and investment requirements. It is thus of great importance to identify the key parameters that affect the avoided CO₂ costs in order to determine the subjects on which research and development must focus.

The Castor EU project has shown that Post-Combustion Capture (PCC) processes based on the use of chemical solvents can meet the requirements of 90% recovery of CO₂ from flue gas while delivering a high-purity CO₂ for storage or for chemical use. However, the reference case, the 30wt% MEA process, is known to be energy-demanding. Indeed, it has been determined that about 3.7 GJ/ton_CO₂ are required for solvent regeneration (Knudsen *et al.*, 2009; Abu-Zahra *et al.*, 2007), which represents a major part of the operating costs, as discussed later. While a lot of work is now under way to identify new original solvents, requiring in particular less energy for their regeneration (*e.g.* Puxty *et al.*, 2009; Ma'mum *et al.*, 2007; Porcheron *et al.*, 2011), far less work dealing with absorber design and linked investments is being conducted. Some recent studies have presented either new packings (Alix *et al.*, 2011; Duss and Menon, 2010) or interaction between packing and gas distributors (Duss and Menon, 2010; Raynal and Royon-Lebeaud, 2007) but, to our knowledge, there is no fully detailed study that

explicitly gives the cost repartition linked with the design parameters and their respective impact. This is the goal of the present study.

The main purpose of this work is, indeed, to show where R&D efforts should be made, which is where cost sensitivity is high. Particular attention is dedicated to absorber design. The second purpose is to show that efficient process development must rely on different simulation tools used on different scales, one simulation on a given scale giving insights into the other in a two-way coupling approach.

The retained multiscale simulations strategy is described in Section 1, while Section 2 is dedicated to the different results obtained on different scales. Section 3 ends the paper, focusing on what is missing for going one step further; that is, full absorber design from simulation tools.

1 MULTISCALE SIMULATIONS DESCRIPTION

The present strategy involves three different types of simulations. First, a techno-economic simulation is performed on a process global scale in order to determine the avoided CO₂ cost repartition. Second, process simulations are performed on a reactor scale in order to study the main parameters that impact absorber design, which represents the main investment costs. Finally, CFD simulations are used for simulations performed on two scales with two different approaches. On a meso-scale, CFD is used with a macro-porous approach to study how internals may interact with gas and liquid flows within the packed bed. On a small scale, CFD is used, *via* more demanding models, to determine local characteristics in terms of hydrodynamics and mass transfer for a given packing geometry. All these three types of simulations are described in the following sub-chapters.

1.1 Simulations for Process Evaluation

To evaluate the impact of a design on the economics of a process, one has to consider the repartition of operating costs (OPEX) as well as the repartition of the investment costs (CAPEX). So far, most of the studies have focused on the energy consumption and processes are often compared with each other in terms of required GJ of steam per ton of avoided CO₂ or consider that energy requirement is the main key parameter for future developments (Knudsen *et al.*, 2009; Mathias *et al.*, 2010; Darde *et al.*, 2010). The aim of the present process evaluation is to precisely determine all costs both in terms of operating costs and also in terms of investment costs for

the standard MEA 30wt% process. The capture unit considered corresponds to the treatment of 90%vol. of the CO₂ emitted by a 630 “MWe equivalent” CFB coal power plant. The “MWe equivalent” designation comes from the fact that the present process evaluation considers an integrated plant. In such a case, steam and electricity are directly taken from the power plant, which further results in a loss of efficiency of the latter. To provide the same amount of electricity to the market as an existing 630 MWe without capture, one consequently requires a more powerful power plant. For the MEA 30wt% process, the present process simulations show that this 630 “MWe equivalent” power plant corresponds to a 840 MWe power plant with capture. Corresponding flue gas characteristics in terms of flow rate and composition and a simplified process flow diagram are shown in Figure 1. The present approach thus differs from what is discussed in Raynal *et al.* (2011). In the latter study, a non-integrated approach was considered, where electricity and steam were bought on the market. Such an approach is convenient for comparing two processes with each other, since the power plant is not directly impacted by the capture plant; however, it is not well adapted when, for a given process, one wants to identify and quantify each parameter impact with further design optimization, which is the goal of the present study. The present approach thus corresponds to the case of a full grass-root integrated project (power plant + capture unit).

The approach used to evaluate the cost of a given process consists of three steps, which are described in the following subsections.

1.1.1 Process Simulations

The first step of the process evaluation consists of simulations of the absorption/desorption loop, using the Aspen Plus 7.2 commercial software. The boundary limits considered in the study are the same as described by Raynal *et al.* (2011). It includes treatment of flue gas at atmospheric pressure and delivery of CO₂ at high pressure (110 bar abs.). The simulation obtained is used to determine the heat and material balances of the capture unit. First, it makes possible the determination of almost all OPEX costs and, second, it gives the inputs for the next step, consisting of process design.

1.1.2 Process Design of Main Equipments

Using the results of the process simulation, the main equipments are designed *via* process simulations using both Aspen Plus® RateSep™ and IFP Energies nouvelles (IFPEN) in-house software. The Aspen Plus software is used for absorber and desorber packed bed

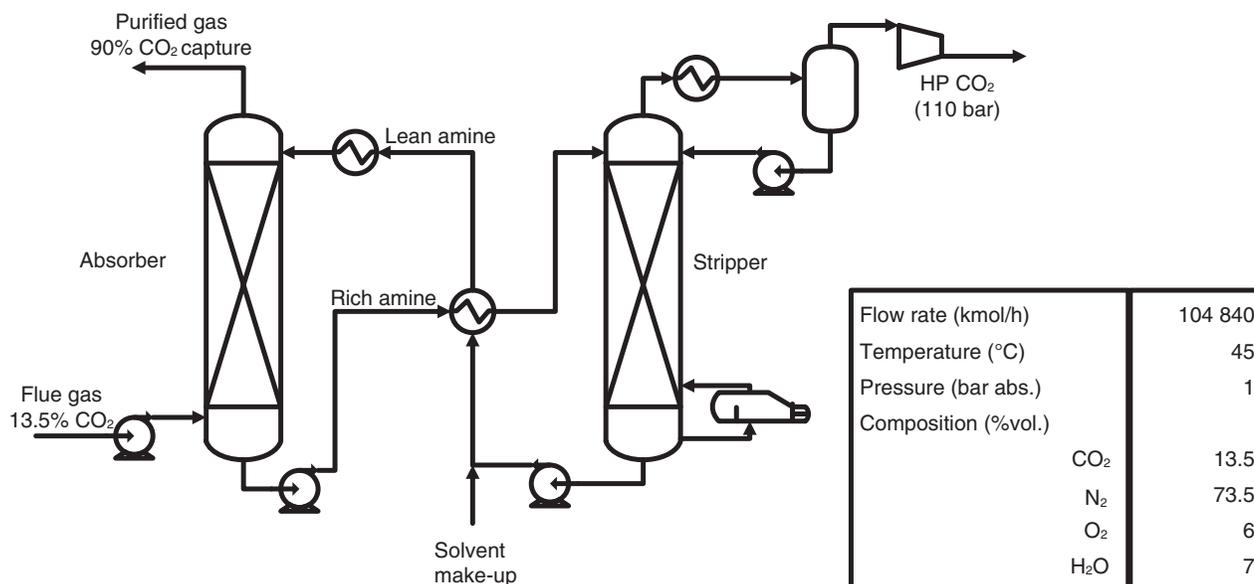


Figure 1

Simplified process flow diagram of the MEA process and flue gas characteristics.

design (see details in Sect. 1.2); the in-house software is used for further detailed column designs (including number of beds, washing section, space for internals, etc.) and other equipment designs. Only the main equipments are considered here (columns, heat exchangers, pumps, blower, compressors, etc.).

1.1.3 Cost Evaluation

The main equipments designed in the previous step are then cost-evaluated using IFPEN in-house software that determines investment budgets with a $\pm 30\%$ precision (preliminary quotation for InSide Battery Limits – ISBL). To determine CAPEX, one must first deduce OSBL (OutSide Battery Limit) from ISBL, which includes costs such as storage, engineering and contingencies, and second, must take into account financial assumptions. The main economic parameters considered for the cost analysis are reported in Table 1. With this procedure, one ends up with a first estimation of the process cost. Different modifications of the design can then be quickly evaluated, allowing in particular a cost comparison for different absorption tower designs.

1.2 Simulations for Absorber Design

During the EU Castor project, the Castor pilot plant of Dong Energy was equipped with the Koch-Glitsch

TABLE 1
Economic evaluation parameters

Reference year	2010
Capital allowances (yr)	25
Depreciation (yr)	10
Discount rate (%)	10
Cost of debt (%)	7
OSBL (storage, utilities, buildings, contingencies, etc.)	Percentage of ISBL
Time of construction (month)	36
Project life years (yr)	25
Tax rate (%)	30
Coal price (€/t)	87 (3.4 €/GJ)

third-generation random packing IMTP-50 (Knudsen *et al.*, 2009), as can be seen in Figure 2a. Since the design of the absorber is directly linked to the packing, it is of great interest to determine the sensitivity of the design toward it. The choice of the most adequate packing is linked to its performances in terms of pressure drop and mass transfer efficiencies, a compromise between capacity and efficiency being looked for. The capacity

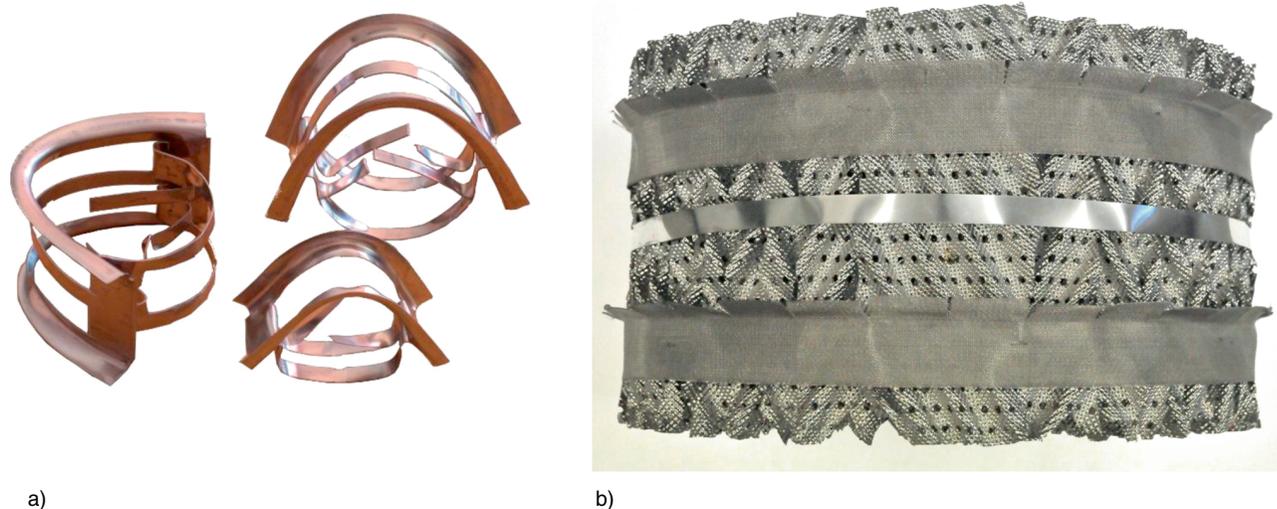


Figure 2

Pictures of the packings considered in the present study; a) IMTP-40 and IMTP-50 random packings, b) Mellapak 250.X structured packing.

of the packing, which is further used to determine the diameter of the column, can easily be determined from packing manufacturer software. The efficiency, which is further used to determine the height of the column, is much more difficult to determine. The overall mass transfer coefficient, $K_G a$, often linked to HETP or NUT values for distillation applications (Billet, 1995), is commonly given, for absorption with chemical reaction, by five parameters (Danckwerts, 1970). Three parameters correspond to mass transfer performances linked with gas/liquid operating conditions and packing; the liquid-side mass transfer coefficient, k_L , the gas-side mass transfer coefficient, k_G , and the effective area, a_e . Two parameters correspond to thermodynamic and kinetic performances of the solvent; the Henry coefficient, He (-) and the acceleration coefficient, E (-), both varying with pressure and temperature conditions and with solvent loading. All these parameters are linked in the following relationship:

$$\frac{1}{K_G a_e} = \left(\frac{1}{K_G} + \frac{He}{E k_L} \right) \times \frac{1}{a_e} \quad (1)$$

It has been shown that, when comparing simulations with the results of the Castor pilot plant, detailed simulators such as AspenTech Aspen Plus 2006.5 software with Aspen RateSep can accurately simulate the absorber performances provided that appropriate thermodynamics and kinetics corresponding to the 30wt% MEA

solvent are used (Dugas *et al.*, 2009; Tobiesen *et al.*, 2007). RateSep is a detailed model that takes into account heat and mass transfer transport equations in both gas and liquid phases, equipment hydrodynamics and chemical reaction mechanisms to predict column performance. With such a model the enhancement factor, E in Equation (1), is determined *via* the resolution of a transport equation solving chemical species diffusion and reaction in the liquid diffusion film, the thickness of which being mainly determined from the liquid mass transfer characteristics. The simulations performed in the present study are similar to those of Dugas *et al.* (2009) in terms of thermodynamics and kinetics. However, here, we considered the mass transfer parameters as variables. These parameters were modified *via* in-house Fortran model routines in order to correspond to different packing performances. Packing choice is indeed the main possibility for column design optimization once the solvent and associated heat and mass balances are given.

The work performed here was done in two steps. First, a sensitivity analysis toward all three parameters, k_L , k_G and a_e , was conducted. In this case, each one of the three previous parameters is varied, with all other parameters, flow conditions and design being kept constant. The simulations give the respective CO₂ capture performances. Second, a comparison between IMTP packings (25, 40, 50 and 70) at two levels of flooding percentage, 50 and 80%, was made. The determination of the flooding

percentage is done with the commercial software KG-Tower 4.0 for flow conditions at the bottom of the absorber. The determination of the height is made using Aspen calculations with IFPEN in-house correlations for mass transfer parameters. Mass transfer correlations are based on either IFPEN internal data or literature data (Alix and Raynal, 2009; Nakov *et al.*, 2007; Billet, 1995). All the calculations are carried out for a constant CO₂ capture rate of 90%.

1.3 CFD Simulations for Detailed Column Design

CFD is more and more used to calculate flow characteristics in packed beds. Raynal and Royon-Lebeaud (2007) have shown how simulations using different types of approaches could complement each other in order to simulate gas/liquid flow in packed columns. Two main types of modeling can actually be considered on two different scales.

On a small or local scale, that is, on the scale of the smallest periodic element or Representative Elementary Unit (REU), one can determine local parameters both in terms of hydrodynamics and mass transfer. One can indeed determine pressure drop, liquid film thickness and liquid holdup; but also the liquid film velocity at the interface and the wetting quality.

For dry pressure drop (the gas phase only is considered) determination in structured packing, three-dimensional simulations were carried out considering a computational domain which corresponds to the smallest periodic REU of the Mellapak 250.Y structured packing (*Fig. 2b*). The computational method is based on Large Eddy Simulations (LES). This CFD approach is founded on the observation that the small scales of turbulent motion are characterized by a more universal character than the large scales, which transport the turbulent energy. Thus, the LES method accurately resolves the large eddies only, the effects of the small scales being determined by a subgrid-scale model. Since LES requires significantly less grid points than DNS, this method is well suited for detailed studies of complex turbulent flows in structured packing at high Reynolds numbers. More details on the LES method can be found in Blazek (2001) or Piomelli (1998), the subgrid model used in this work being based on the WALE model formulation as developed by Nicoud and Ducros (1999). The assumption of this model remains the same as in the Smagorinsky model but involves a local rotation rate in the expression of the turbulent viscosity; this is justified since dissipative scales are also characterized by a high rotation rate. The WALE model thus allows one to predict the

correct wall behavior with an implicit damping effect. The present LES simulations differ from previous calculations performed by Petre *et al.* (2003) or Raynal *et al.* (2004), who used more standard models (RANS $k-\varepsilon$ or laminar models) and are thus much more demanding in terms of mesh, solver, boundary condition definition and CPU time. However, as discussed in Raynal and Royon-Lebeaud (2007), the agreement between experimental and previous numerical results was good but not fully satisfactory. The observed disagreement is possibly due to the fact that the gas Reynolds number range of interest is in the range 400-2.10⁴, for which neither laminar nor fully turbulent flow models apply. It is thus believed that the LES approach should be considered since it can cover a very large range of Reynolds numbers.

Still on a local scale, the second type of CFD simulation deals with the Volume Of Fluid (VOF) approach. The VOF method consists of a Eulerian description of each phase on a fixed grid, the interface between the two phases being calculated using the transport equation of the local volume fraction of one phase. The Navier-Stokes equations are solved according to a standard one-fluid formulation. The purpose of the one-fluid formulation is to describe the physical parameters for both phases using only one equation valid in the entire computational domain (Scardovelli and Zaleski, 1999). Combined with appropriate turbulent modeling, this method has been used to simulate the gas/liquid flow on a liquid film scale within packings (Ataki and Bart, 2006; Raynal and Royon-Lebeaud, 2007; Haroun *et al.*, 2012). From local information, such as the liquid film thickness and liquid holdup but also the liquid film velocity at the interface and the wetting quality, one can further determine mass transfer parameters for different types of packings used in process simulations such as the liquid-side mass transfer coefficient and the effective area, respectively. In these types of calculations, the chemical species concentration equation is solved coupled to the Navier-Stokes equations, while thermodynamic equilibrium of chemical species at the interface is considered using Henry's law. This method has been proved to be able to simulate mass transfer simultaneously with the evolution of a deformed interface (Haroun *et al.*, 2010a,b).

On a large column scale, other types of approaches must be used. Large-scale simulations are performed *via* macroscopic approaches considering the packed bed as a continuous porous media, being isotropic or not depending on whether the packing is of random or structured type. Such simulations, performed here with the Fluent 6.0 commercial code with the standard $k-\varepsilon$ turbulent model, enable one to determine the quality

of the distribution and the internals/packed bed interaction. The details of the packing geometry are no longer solved but it is taken into account *via* closure laws for gas/liquid/solid interactions terms which are derived either from experiments, or from previous calculations performed on a small scale.

2 SIMULATIONS RESULTS

2.1 Process Simulations and Economic Evaluation

Here, the results from the process simulations are summarized. The results given below correspond to an optimized configuration of the process in terms of lean and rich CO₂ loadings, respectively equal to 0.24 and 0.48 (see the discussion in Raynal *et al.*, 2011), the column design being optimized for two types of packings, Mellapak 250.X structured packing for absorbers and IMTP-50 random packing for strippers:

- process specific energy consumption = 3.7 GJ/t_{CO₂},
- solvent flow rate = 10 800 m³/h,
- absorber design: 4 columns, $\varnothing = 9$ m; $H = 36$ m,
- stripper design: 2 columns, $\varnothing = 9$ m; $H = 30$ m,
- amine reboiler (24 Kettle type) = 25 MW_{th},
- CO₂ compressor = 56 MWe.

The corresponding cost analysis result is given in Table 2.

First, one observes that the obtained CO₂ penalty is 57 €/t_{CO₂}, which differs significantly from the figure given in Raynal *et al.* (2011) of 74 €/t. This difference comes essentially from the fact that the present evaluation considers an integrated plant while, in the previous analysis, utilities were bought on the market. It also comes from the fact that the technology for the CO₂ compressor has been changed to Integrally Geared Technology, more appropriate and more cost-effective than classical axial compressors. The total cost, but also the cost repartition, is strongly affected by this approach, which is more representative for a grass-root project. Since utilities are taken from the power plant and not bought on the market, the OPEX are consequently relatively less significant than in the case of the non-integrated plant. This turns into a CAPEX/OPEX ratio of 45/55 approximately, instead of about 30/70 in the non-integrated approach.

Second, one can decompose the cost into four main items which account for more than 90% of the total capture cost. In decreasing order, one obtains: reboiler (31%), columns (24%), CO₂ compressor (22%) and chemicals (14%). This latter value corresponds to the solvent make-up needed to compensate for MEA degradation evaluated at 1.4 kg_{MEA}/t_{CO₂} (Knudsen

et al., 2009). Note that this rather high value calls for the use of additives as proposed, for example, in the HiCapt+™ process developed by IFPEN (Lemaire *et al.*, 2011). The first way to decrease the CO₂ capture cost is, of course, the energy penalty reduction that is made possible *via* the use of new solvents requiring less regeneration energy at the reboiler, as discussed in the introduction of the present paper. The second main way to optimize the MEA process is clearly to decrease its CAPEX, which further calls for column design optimization, since columns account for almost 50% of the CAPEX. The need for R&D efforts in new packings and column designs is thus of high importance for CO₂ capture cost reduction. This is reinforced by the presence of a gas blower to overcome pressure drop, whose cost could also be decreased by using more efficient columns.

It is important to note that economic parameters may have a great impact on the analysis results. Since the scope of the present paper is not to focus on economic evaluation, all the results obtained in terms of sensitivity analysis are not reported here, although such calculations were realized internally at IFPEN. We nevertheless wish to underline this influence and to illustrate that one must be cautious when making direct comparisons between different studies from the literature. This is done with the two following examples, and illustrated in Figure 3. As a first example, comparing two processes without specifying the reference year may lead to important mistakes or misleading conclusions. Indeed, when performing calculations over a three-year period (2006-2009), a change in CO₂ capture cost of more than 10 €/t for the MEA process was calculated. Note that, if using an updated cost index, such as the IHS-CERRA or Nelson-Farrar, which can be found in the *Oil & Gas Journal*, for example, the difference obtained is less than 1 €/t_{CO₂}. As a second example, we can discuss the price of coal, which is the main cost that varies in time. In recent years, it has varied from a minimum of 60 €/t up to a maximum of 120 €/t. With the presently considered value of 87 €/t, it was determined that coal price may impact the CO₂ capture cost by a variation of about ± 5 €/t_{CO₂}. To complete this discussion on sensitivity analysis, the influence of other economic parameters is shown in Figure 3, where modifications of four economic parameters have been varied over a -50/+50% range around the reference values given in Table 1. One notes that, for a given ISBL, the resulting CO₂ capture cost varies roughly from 50 up to 65 €/t for a fully defined case.

In order to provide an easy document that summarizes this techno-economic study, the obtained respective cost repartition for both CAPEX and OPEX is reported in the simplified flow diagram in Figure 4, where capital

TABLE 2
Cost repartition

Repartition	CAPEX			OPEX			TOTAL (%)
	43.3%			56.7%			
	€/MWh	€/t	%	€/MWh	€/t	%	
Absorber	5.9	9.1	37				24.1
Regenerator	1.5	2.4	9.7				
Flue gas blower	0.3	0.4	1.6	1.2	1.8	5.6	
CO ₂ compressor	3.2	5.0	20.2	4.7	7.3	22.8	21.7
Reboiler	1.8	2.8	11.5	9.6	14.8	46.1	31.1
Chemicals	0.5	0.8	3.1	4.7	7.3	22.7	14.2
Pumps	0.7	1.2	4.7	0.6	0.9	2.8	8.9
Exchangers	1.7	2.7	10.8				
Miscellaneous	0.2	0.3	1.4				
Sub-total	15.8	24.6	100	20.8	32.1	100	
TOTAL	36.6	€/MWh					
	56.7	€/t					

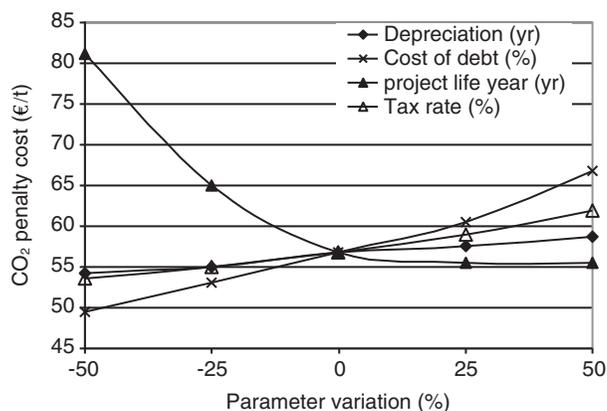


Figure 3
Sensitivity of the CO₂ capture cost toward economic parameters. The reference value for each parameter is given in Table 1.

letters correspond to OPEX costs, and lower-case letters correspond to CAPEX, respectively. Since from one estimation to another, one may use different cost estimation assumptions, as previously discussed, characteristic ranges are given.

2.2 Absorber Simulations

2.2.1 Mass Transfer Parameters Sensitivity Analysis

Figure 5 and Figure 6 show the results concerning the sensitivity analysis of mass transfer parameters. Figure 5 shows the dry molar fraction of CO₂ in the gas stream along the absorber for various interfacial area values, all other parameters being kept constant. The reference case corresponds to in-house values of a_e measured at IFPEN (Alix and Raynal, 2009), in good agreement with data deduced from the Intalox Packing brochure or given by Seibert *et al.* (2005) and Nakov *et al.* (2007) for random packings of IMTP type. One observes that moderate changes of 20% (squares) or 40% (triangles) around the reference values have a significant impact on the CO₂ profile, further impacting the total performance of the absorber. A change of $\pm 40\%$ in the effective area induces changes from 1.5% to 3.2% in the CO₂ molar fraction value at the absorber outlet. From our experience and from the discrepancies observed in the literature from one source to another, an uncertainty between $\pm 10\%$ and more certainly of $\pm 20\%$ in the effective area determination is typical (see previously cited sources and Billet, 1995). This means that, to make sure the required performance is achieved, one must

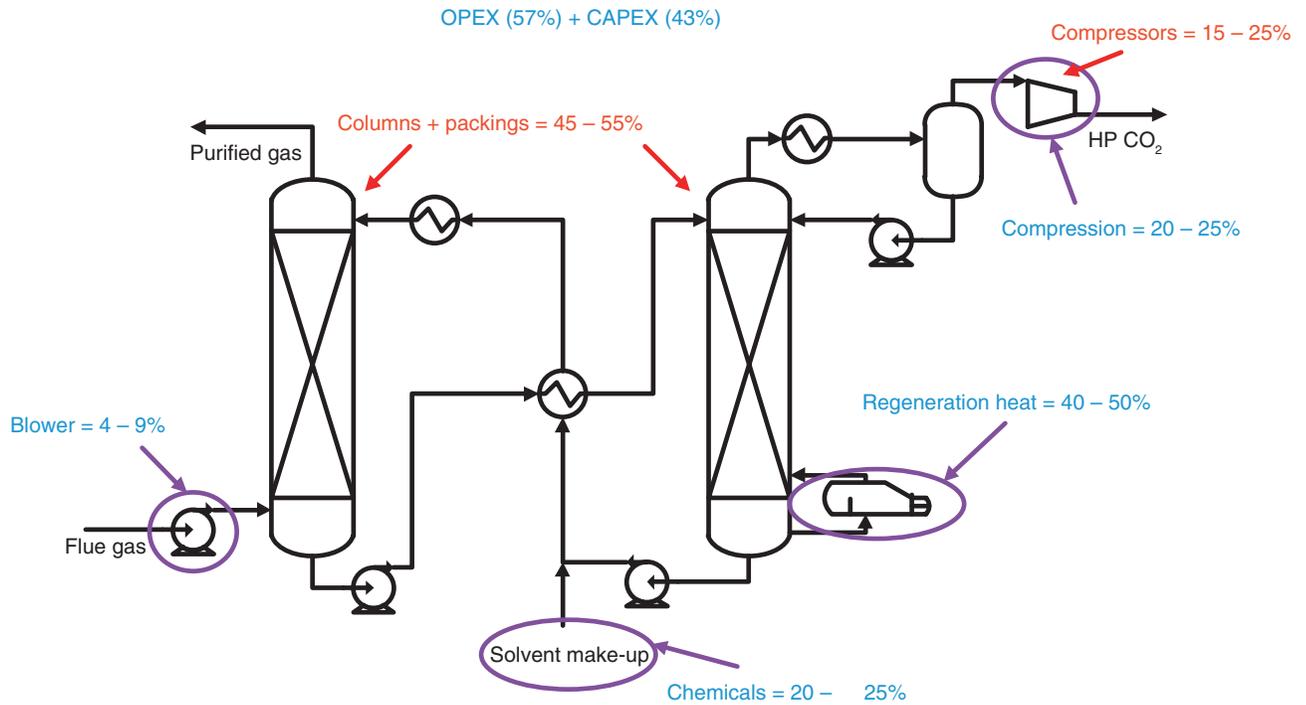


Figure 4
Sketch of the capture cost repartition for the MEA 30wt% process.

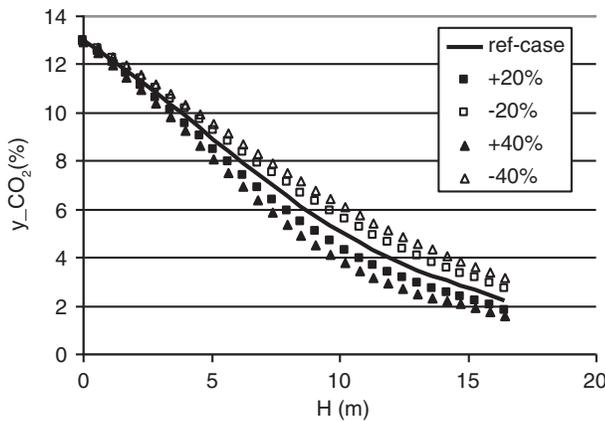


Figure 5
CO₂ gas concentration profiles along the absorber for different effective areas, a_e .

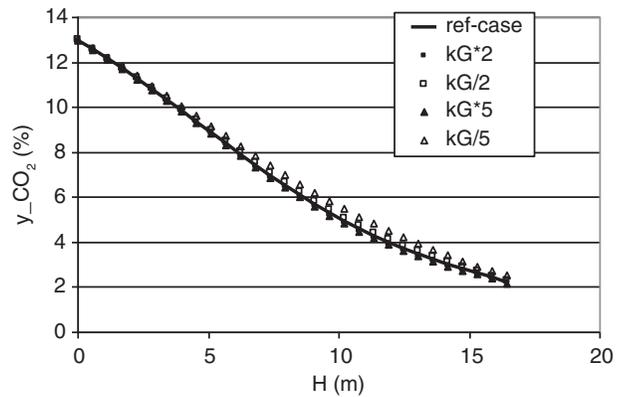


Figure 6
CO₂ gas concentration profiles along the absorber for different gas-side mass transfer parameters, k_G .

select a packed bed height that must take this sensitivity into account, which requires a well-defined simulation tool.

Figure 6 shows similar data but with changes in the gas-side mass transfer coefficient, k_G . One observes that the sensitivity toward this parameter is much less than

that observed toward the effective area. A change of a factor of 25 in the gas-side mass-transfer coefficient induces values for the CO₂ molar fraction at the absorber outlet ranging from 2.5% to 2.2% only. It can thus be concluded that this process is not gas-side controlled at all. Similar calculations were performed

to check the influence of the third mass transfer parameter, the liquid-side mass-transfer coefficient, k_L . The latter varied over a range from 1 to 7 around a reference value deduced from the correlation developed in Billet (1995) for similar random packing. For all tested values, the CO₂ molar fraction at the absorber outlet happens to vary only very little, from 2.2 to 2.3%.

The present sensitivity analysis clearly shows that the performance of the absorber, or the height required for the packed bed for a given CO₂ capture rate, is essentially given by the effective area. There is almost no gas-side resistance, the kinetics being not fast enough and the liquid-side mass transfer coefficient has almost no impact. This latter result enables us to conclude that the column operates in the pseudo-first-order regime in which the enhancement factor is equal to the Hatta number and the mass transfer rate is independent of the liquid-side mass transfer (Danckwerts, 1970). As discussed in Raynal *et al.* (2011), similar sensitivity toward the effective area could already be deduced from the work of Tobiesen *et al.* (2007), even if it was not within the scope of their study. Prediction of mass transfer characteristics or packing efficiency is thus entirely given by the effective area, which calls for precise experimental or numerical determination of this parameter.

2.2.2 Packing Influence

From previous results, we can anticipate that the change from one packing to another will impact the height of the column *via* its interfacial area. Besides, a change in packing will impact the absorber diameter design *via* its capacity and the required percentage to flooding design, usually close to 70%. Note that a change in packing will not only affect the investment costs, but also, at a lower level, operational costs *via* the bed pressure drop. Figure 7 and Figure 8 show a comparison, for the diameter and for the packing bed height, respectively, between the different packings of IMTP types for two different values of flooding percentage, all other parameters being kept constant. One first observes that small-sized packings, IMTP 25 or 40, induce significantly larger diameters than larger-sized packings, IMTP 50 or 70. They would thus not be selected *a priori* for such an application that treats huge quantities of gas. However, they induce a much smaller height of the packed beds. One also observes a relatively significant impact of the flooding percentage on the diameter values, while having little effect on the corresponding height. With such curves and with the economic methodology given in Section 2, one can determine the balance between capacity and efficiency, transposing them into economic terms (cost of the column and power required for the

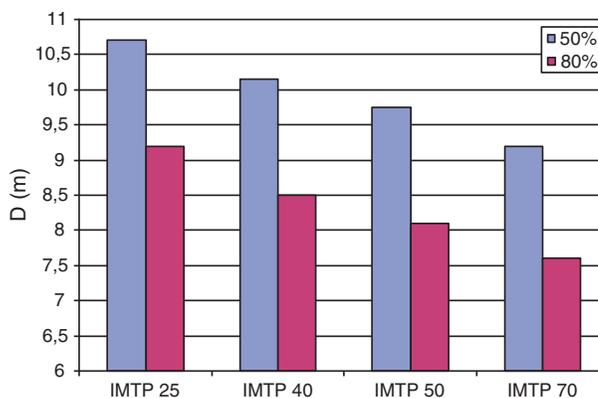


Figure 7

Design values needed, respectively, for the diameter for two flooding percentage values, 50 and 80%, for the different IMTP packings while achieving a constant CO₂ capture rate of 90%.

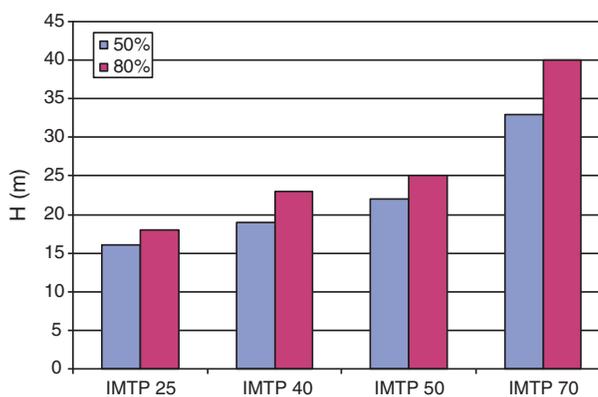


Figure 8

Design values needed, respectively, for the height for two flooding percentage values, 50 and 80%, for the different IMTP packings while achieving a constant CO₂ capture rate of 90%.

blower). From such an analysis, it is possible to properly choose the packing that corresponds to minimum costs.

2.3 CFD Simulations

2.3.1 Simulations on a Large Scale

In all previous simulation steps, one assumes perfectly distributed flow, which is quite easy to do on a laboratory scale or assumed in process simulators but which is no longer obvious on a large scale, in particular when

low gas pressure drop values are required and when dimensions are so huge. Figure 9 shows experimental bed pressure drop results obtained on a 1 000-mm-diameter column operating with air and water and equipped with IMTP-40 packing. Two curved pipe gas distributors were used, one with a baffle (D1) and one without (D2). One observes that the change from one distributor to another has little impact far from flooding but may dramatically influence the gas/liquid flow at a high gas flow rate, with a change in the flooding limit of about 15%. In the case of the distributor with the baffle (D1 – closed symbols and continuous lines), one observes that flooding occurs at lower gas flow rates than when the D2 distributor without baffles is used. Such an impact can be explained *via* CFD simulations performed with identical conditions to those in experiments. Indeed, as shown in Figure 10, the D1 distributor induces high velocities at the periphery of the column where higher local liquid retention is known to appear due to wall effects (Olujić *et al.*, 2006). These two combined effects thus induce early flooding. On the contrary, distributor D2, while far from being perfect, induces high velocities at the core of the packed bed, avoiding zones with high liquid concentrations.

Such CFD simulations performed on a large scale can thus be used both for designing gas distributors, in particular in non-conventional columns such as a square-shaped column (Duss and Menon, 2010) but also for determining the distance between the gas distributor

and the packed bed inlet for detailed design purposes, or for choosing the best packing arrangements, as discussed in Raynal and Royon-Lebeaud (2007).

2.3.2 Simulations on a Small Scale

Concerning pressure drop determination, the CFD results obtained with the LES-Wall method are shown in Figure 11, where they are compared with the experimental data of Spiegel and Meier (1992). One observes that the agreement between the simulated and experimental dry pressure drop is very satisfactory for all gas F-factors used. The relative error between CFD and experimental data is about 10%.

Concerning mass-transfer determination, the CFD results obtained with the VOF method are shown in Figure 12. Figure 12a shows the CO₂ concentration contours in the gas-liquid flow down a two-dimensional slice of the structured packing at steady state. Figure 12b shows a comparison between the non-dimensional local liquid-side mass transfer coefficient, that is a Sherwood number, with the Higbie (1935) theory (line). One observes that the liquid-side mass transfer coefficient is well reproduced provided that adequate velocity and length scales are considered for exposure time determination. It is found that the exposure time of the fluid element at the interface corresponds to the ratio between the curvilinear distance between two periodic corrugation contact points and the interface velocity, as further discussed in Haroun *et al.* (2010b).

So far, such simulations, taking into account both hydrodynamics and mass transfer, have not been performed in a fully representative 3D element as used for pressure drop calculations due to CPU requirement limitations. However, as shown in Figure 13, it is nevertheless possible to study wetting efficiency and then determine the interfacial area from VOF simulations in a REU. The results are presented using non-dimensional Weber numbers defined as the ratio of fluid's inertia to surface tension ($We = \rho_L U_L^2 e / \sigma$) and the contact angle θ . Based on visual observation, this figure shows qualitatively that for conditions corresponding to a MEA flow with two different wetting conditions in terms of surface tension or contact angle, the interfacial area differs significantly. One obtains an interfacial area which is either very close to the geometrical area, as observed in experimental measurements for such a high liquid flow rate (Rocha *et al.*, 1996; Repke *et al.*, 2006), or significantly less than the geometric area when “default” VOF parameters are used. This disagreement calls for intensive work on this type of modeling.

These simulations on a small scale are so far used to complement experimental work or used for developing

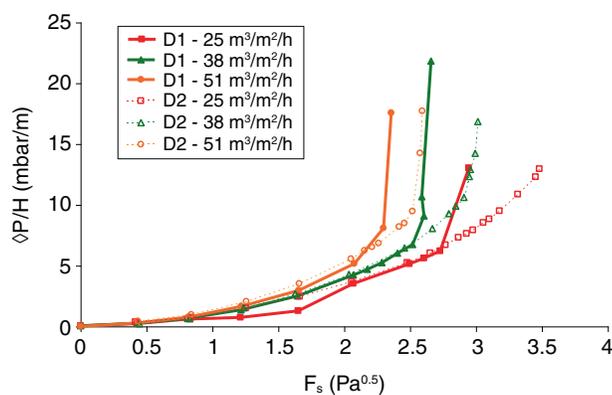


Figure 9

Influence of the gas distributor. Experimental pressure drop curves versus gas load for three values of liquid load for two types of R&D gas distributor, column of 1 m in diameter at ambient pressure, gas is air, liquid is water (distributor D1: curved pipe with baffles – closed symbols with continuous lines; D2 curved pipe without baffles – open symbols with dotted lines).

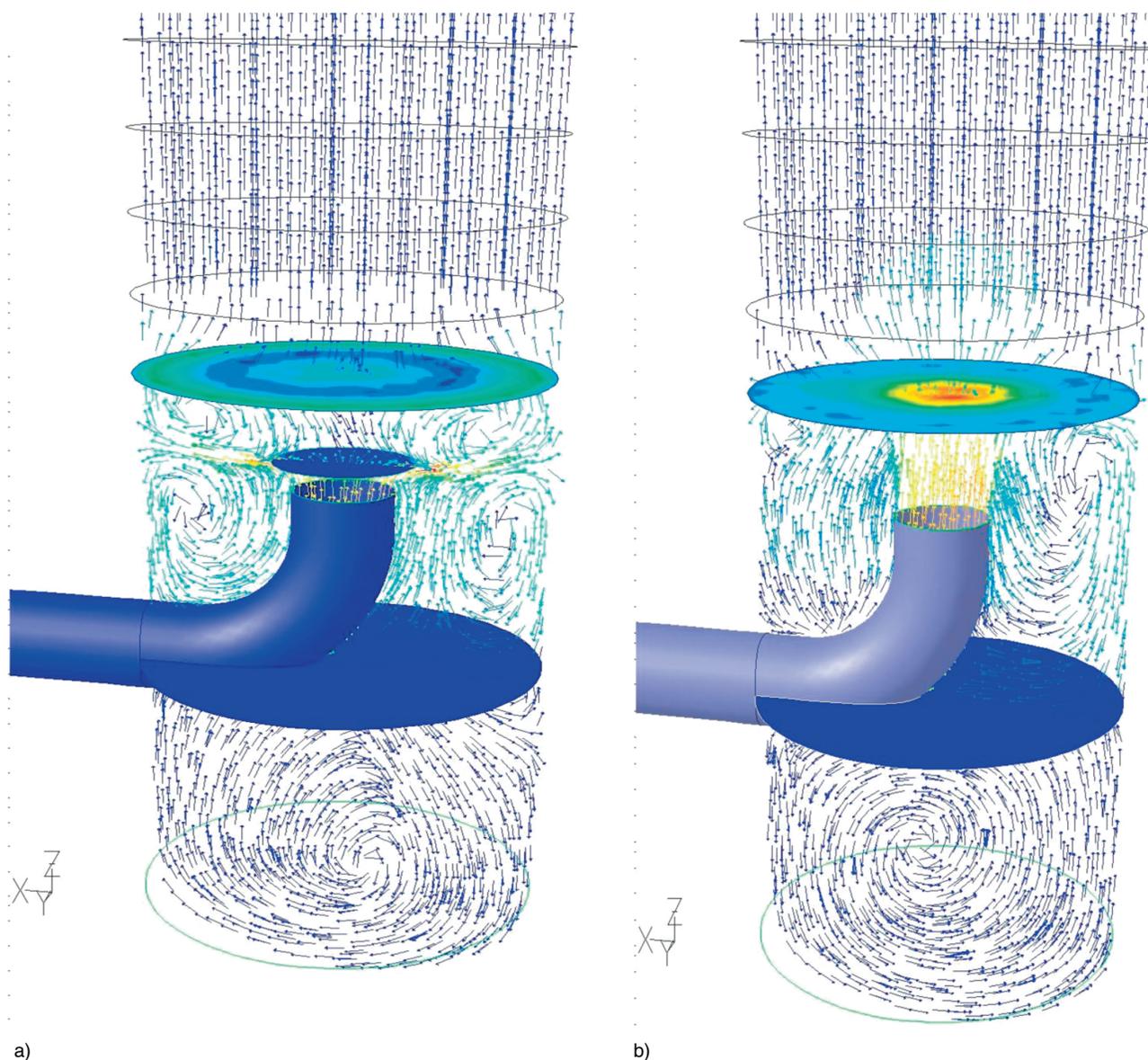


Figure 10

Influence of the gas distributor. CFD pressure contours at bed inlet and velocity field in the $y = 0$ plane for the same gas and liquid flow conditions, only the gas distributor differs. a) D1: curved pipe with baffles, b) D2: curved pipe without baffles.

a more comprehensive knowledge of what happens in this complex two-phase flow in packed beds. They could be further used to develop and perform preliminary tests of new and original geometries for packings. Since CCS may be a very large market, new packings have indeed recently been proposed for this application (Alix *et al.*, 2011; Menon and Duss, 2011). However, the cost of development of new packings is very large since it

requires intensive experimental work, which cannot be considered for a large variety of geometries. The present simulations could be of great help at least for a pre-screening or pre-design step. This step would be performed before any development experimental test phase, since simulations allow one to test any virtual geometry for a very large range of operating conditions.

3 DISCUSSION

It is shown here that a strategy implying different simulation tools on different scales enables one to identify the key parameters that impact CO₂ capture cost. It is thus

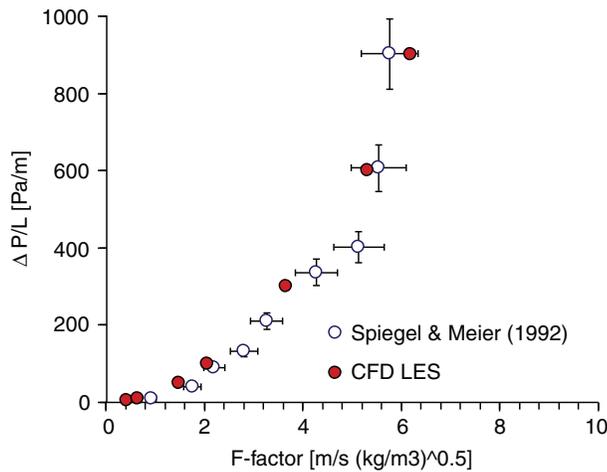


Figure 11
Dry pressure drop versus gas flow capacity factor in the REU corresponding to the Mellapak 250.Y. Comparison between numerical results and experimental data.

of great interest to combine economic estimation tools with process simulations and CFD simulation tools to be able to achieve the most optimized design in terms of choice of packing and adapted corresponding internals. It is indeed very important to understand that the present multiscale strategy is efficient only if the different simulation tools are used in a two-way coupling approach. Simulations on a large scale will help to identify parameters to focus on; local simulations will help to determine new values for the latter parameters, which will be included in meso-scale simulations that will further end with macro-scale process evaluation. The possibility of mastering all simulation tools will ensure optimized solution developments. Indeed, since flue gas quantities are so huge, one would *a priori* change the reference IMTP-50 packing to a more capacitive packing. This is what has been done within the EU Cesar project where the Dong Energy pilot has been equipped with Mellapak 2X (Knudsen, 2009) in replacement of the previously tested IMTP-50. However, what is really needed is a complete quantitative sensitivity analysis that compares full costs induced by different packings, as illustrated here. This must be done in terms of CAPEX, which are more related to the total packing volume installed than to the diameter only and in terms of OPEX, which must take into account not only the characteristic linear pressure drop

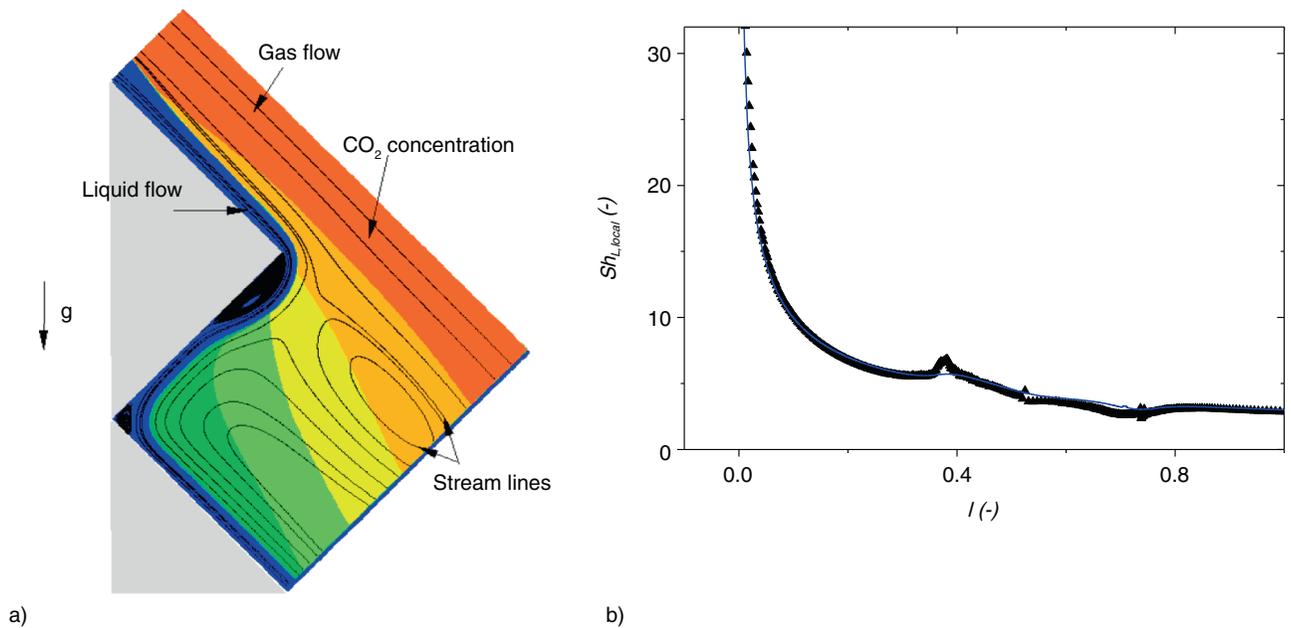


Figure 12
a) CO₂ concentration contours in gas/liquid flow on structured packing. b) Local evolution of the liquid-side Sherwood number with the dimensionless distance from the inlet. Comparison between numerical results and Higbie solution. Physical properties and operating conditions : $\rho_L/\rho_G = 780$, $\mu_L/\mu_G = 50$, $Fr = 5$, $We = 8$, $Pe_L = 10^4$, $Q_L = 45 \text{ m}^3/\text{m}^2/\text{h}$.

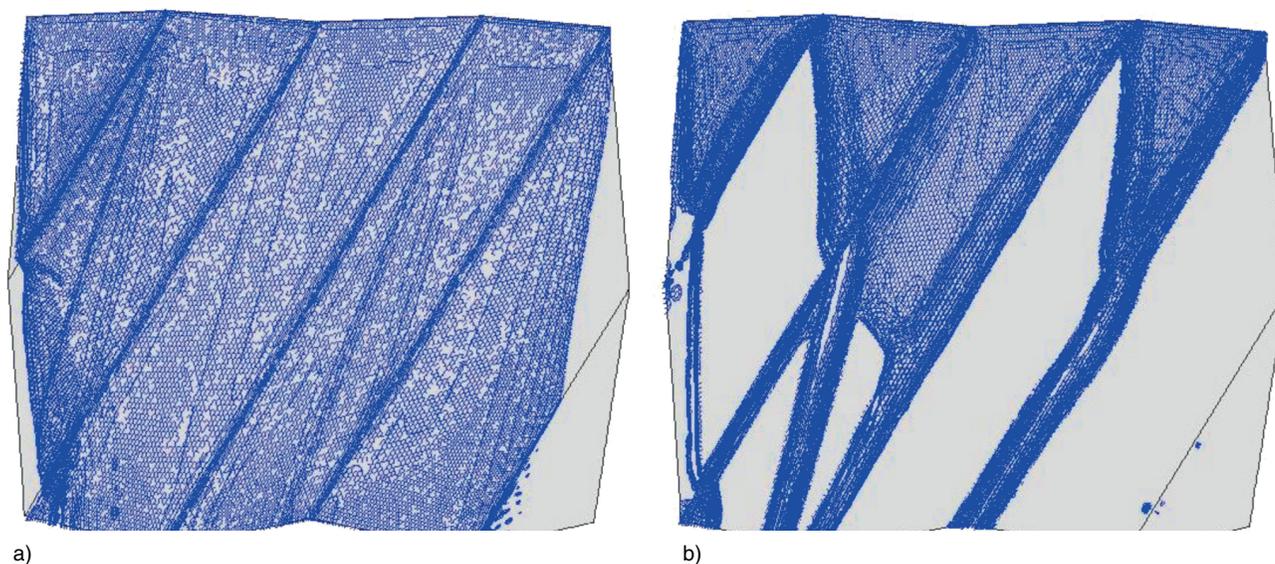


Figure 13

MEA flow on Mellapak 250.X structured packing with two different wetting conditions. $Q_L = 130 \text{ m}^3/\text{m}^2/\text{h}$; $F_s = 2.4 \text{ m/s (kg/m}^3)^{0.5}$.
 a) $We = \infty$; b) $We = 1$, contact angle $\theta = 90^\circ$.

of a packing but also the total height installed. In the case of structured packings, which offer high interfacial area and low pressure drop, it would thus be interesting to perform a similar study using the well-known Mellapak 250 or equivalent, and compare it not only with high capacity packing such as the Mellapak 2X but also with less capacitive but more efficient packings such as Mellapak 350 or 500.

This paper also aims to show that from simulations only, one would be able to develop new technologies (distributor or more importantly, new packing) or new detailed design rules for the column equipped with the latter and evaluate the corresponding gain. This possibility is unfortunately not true for quantitative extrapolation yet. Only insights can be given. Indeed, important phenomena on both the local and meso-scales still need developments in closure laws for precise quantitative CFD simulations. On the local scale, it has been shown, for example, that the wall texture on packing may influence liquid-side mass transfer (Kohrt *et al.*, 2011), which has not been reproduced by CFD tools. On a large scale, a two-phase flow Euler/Euler approach is required if one wants to take into account liquid dispersion and its two-way coupled interaction with gas distribution. Liquid dispersion coefficients required for bed height influence simulations or for distributors/packed bed interaction have been determined for previous-generation packings (Bemer and Zuiderweg, 1978; Hoek *et al.*, 1986) and

some values exist for recent structured packings (Fourati *et al.*, 2012) but data are still lacking for recent random packings.

There are thus still important developments needed for the gas/liquid/solid interaction closure terms, in particular if one wants to develop new technologies (packings, gas and liquid distributors). However, it is shown here that, for existing equipment and with existing tools with appropriate modeling, it is already possible to perform two-way coupling simulations that enable column design optimization and consequently make CO₂ cost reduction possible.

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