



DESIGN OF A PACKED-BED ABSORPTION COLUMN CONSIDERING FOUR PACKING TYPES AND APPLYING MATLAB

DISEÑO DE UNA COLUMNA DE ABSORCIÓN EMPACADA CONSIDERANDO CUATRO TIPOS DE EMPAQUE Y APLICANDO MATLAB

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ABSTRACT

In the present work, a packed bed absorption column is designed to recover certain amounts of ethanol contained in a gaseous stream. Four packing types (50-mm metal *Hiflow*[®] rings, 50-mm ceramic *Pall*[®] rings, 50-mm metal *Top Pak*[®] rings and 25-mm metal *VSP*[®] rings) are considered in order to select the most appropriate one in terms of column dimensions, pressure drop and mass-transfer results. Several design parameters were determined including column diameter (D), packing height (Z), overall mass-transfer coefficient (K_m) and gas pressure drop ($\Delta P/Z$), as well as the overall number of gas-phase transfer units (N_{iOG}), overall height of a gas-phase transfer unit (H_{iOG}) and the effective surface area of packing (a_h). The most adequate packing to use for this absorption system constitutes the 25-mm metal *VSP*[®] rings, since it provided the greatest values of K_m (0.325 kmol/m³.s), and a_h (169.57 m⁻¹), as well as the lowest values of both Z (0.6 m) and H_{iOG} (0.145 m), meaning that it will supply the higher mass-transfer conditions with the lowest column dimensions. The influence of both gas mixture (Q_G) and solvent (m_L) feed flowrates on D , Z , K_m , $\Delta P/Z$, N_{iOG} and H_{iOG} was also evaluated for the four packing considered. The design methodology was solved using computing software *MATLAB*[®] version 7.8.0.347 (R2009a) (Math Works, 2009), and also Microsoft Excel[®].

Keywords: Packed absorber, design, packing, simulation, MATLAB.

RESUMEN

En el presente trabajo se diseña una columna de absorción empacada para recuperar ciertas cantidades de etanol contenido en una corriente gaseosa. Se consideran 4 tipos de empaques (anillos *Hiflow*[®] metálicos de 50 mm, anillos *Pall*[®] cerámicos de 50 mm, anillos *Top Pak*[®] metálicos de 50 mm, y anillos *VSP*[®] metálicos de 25 mm) con el fin de seleccionar el más apropiado en términos de dimensiones de la columna, caída de presión y resultados de transferencia de masa. Se determinaron varios parámetros de diseño incluyendo diámetro de la columna (D), altura del empaque (Z), coeficiente global de transferencia de masa (K_m) y caída de presión gaseosa (P/Z), así como también el número total de unidades de transferencia en fase gaseosa (N_{iOG}), altura total de unidades de transferencia en fase gaseosa (H_{iOG}) y el área superficial efectiva del empaque (a_h). El empaque más

adecuado de usar en este sistema de absorción constituye los anillos *VSP*[®] metálicos de 25 mm, ya que suministra los mayores valores de K_m (0.325 kmol/m³.s), y a_h (169.57 m⁻¹), así como también los menores valores de tanto Z (0.6 m) y H_{tOG} (0.145 m), significando que suministrará las condiciones más altas de transferencia de masa con las menores dimensiones de la columna. La influencia de los caudales de alimentación de tanto la mezcla gaseosa (Q_G) y el solvente (m_L) sobre D , Z , K_m , $\Delta P/Z$, N_{tOG} y H_{tOG} fue también evaluada para los cuatro tipos de empaques considerados. La metodología de diseño fue resuelta empleando el software *MATLAB*[®] versión 7.8.0.347 (R2009a) (Math Works, 2009), y también Microsoft Excel[®].

Palabras claves: Absorbedor empacado, diseño, empaque, simulación, MATLAB.

NOMENCLATURE

a	Mass-transfer surface area per unit volume	m ⁻¹
a_h	Effective specific surface area of packing	m ⁻¹
A	Absorption factor	Dimensionless
Ch	Hydraulic factor	Dimensionless
C_L	Mass-transfer factor	Dimensionless
C_P	Hydraulic factor	Dimensionless
C_{Sflood}	C_s coefficient at flooding conditions	m/s
C_V	Mass-transfer factor	Dimensionless
d_p	Effective particle diameter	m
D	Tower diameter	m
D_G	Gas-phase diffusion coefficient	m ² /s
D_L	Liquid-phase diffusion coefficient	m ² /s
e/k	<i>Lennard-Jones</i> parameter	K
f_{flood}	Flooding factor	%
F_p	Packing factor	ft ⁻¹
Fr	Froude number	Dimensionless
G	Mass velocity	kg/m ² .s
G_{My}	Gas molar velocity	kmol/m ² .s
G_{Mx}	Liquid molar velocity	kmol/m ² .s
h_L	Liquid holdup	Dimensionless
H	<i>Henry's</i> constant	atm
H_{tOG}	Overall height of a gas-phase transfer unit	m
k_G	Gas-phase convective mass-transfer coefficient	kmol/m ² .s
k_L	Liquid-phase convective mass-transfer coefficient	m/s
K_m	Overall volumetric mass-transfer coefficient	kmol/m ³ .s
K_v	Volumetric mass-transfer coefficient	kmol/m ³ .s
K_w	Wall factor	Dimensionless
m	Mass flowrate	kg/h
M	Molecular weight	kg/kmol
n	Factor	Dimensionless
N	Molar flowrate	kmol/h
N_{tOG}	Overall number of gas-phase transfer units	Dimensionless
$\Delta P_{limit}/Z$	Maximum pressure drop permitted	Pa/m
$\Delta P_0/Z$	Dry pressure drop	Pa/m
$\Delta P/Z$	Overall pressure drop	Pa/m
P	Pressure	atm
Q	Volumetric flowrate	m ³ /h
R	Ideal gas constant	m ³ .atm/kmol.K
%R	Removal percent	%
Re	Reynolds number	Dimensionless

Sc	Schmidt number	Dimensionless
T	Temperature	°C
T*	Factor	Dimensionless
v	Velocity	m/s
v _{flood}	Velocity at flooding conditions	m/s
V	Molar volume	cm ³ /mol
X	Flow parameter	Dimensionless
x	Mole fraction in liquid phase	Fraction
y	Mole fraction in gas phase	Fraction
y*	Mole fraction in gas phase in equilibrium with the liquid	Fraction
Z	Packing height	m

Greek Symbols

ρ	Density	kg/m ³
μ	Viscosity	Pa.s
σ	Collision diameter	Å
σ_{AB}	Average collision diameter	Å
ψ_0	Dry-packing resistance coefficient	Dimensionless
ε	Packing porosity or void fraction	Dimensionless
Ω_D	Diffusion collision integral	Dimensionless
ϕ	Distribution coefficient	Dimensionless

Subscripts

(abs)	Absorbed
CO ₂	Carbon dioxide
eth	Ethanol
G	Gas-phase / Gaseous
L	Liquid-phase / Liquid
W	Water
(1)	Bottom of column
(2)	Top of column

1. INTRODUCTION

Gas-liquid operations are used extensively in chemical and petrochemical industries for transferring mass, heat and momentum between the phases. Among the most important gas-liquid systems employed nowadays is *absorption*, defined as a mass transfer operation at which one or more soluble components contained in a gas phase mixture are dissolved into a liquid solvent whose volatility is low under process conditions. The absorption process could be classified as physical or chemical. The physical absorption occurs when the target solute is dissolved into the solvent, while the chemical absorption takes place when the target solute reacts with the solvent. The removal efficiency of any physical absorption process will depend on the physical-chemical properties (density, viscosity, diffusivity, etc.) and feed flowrates of the gaseous and liquid streams; the type of mass-transfer contact surface (packing or plate); the operating temperature and pressure (commonly, lower temperatures will favor gas absorption by the liquid solvent); gas-liquid ratio; contact time between phases; and the solute concentration at the inlet gas stream. Gas-liquid absorption operations are usually accomplished in equipment named *absorbers*.

Absorbers are used to a great extent in industrial complexes and plants to separate and purify gaseous streams, to recover valuable products and chemicals, as well as for contamination control. The most common absorber types employed in industry are plate columns, packed towers, Venturi cleaning towers and spray chambers. *Packed towers* are widely used for gas-liquid absorption operations and, to a limited extent, for distillations (Perry and Chilton, 2008). A typical packed column consists of a vertical, cylindrical shell containing a support plate for the packing material, mist eliminators, as well

as a liquid distributing device designed to provide effective irrigation to the packing (Benitez, 2009) (Figure 1). The liquid is fed at the top of the column and trickles down through the packed bed, exposing a large surface to contact the gaseous stream, which is supplied at the bottom of the tower (Ludwig, 1997) (Richardson and Harker, 2002). The tower *packing*, or *fill*, should provide a large interfacial surface between liquid and gas per unit volume of packed space, and also should have desirable hydrodynamic/hydraulic characteristics (Benitez, 2009).

Packed-bed absorbers have been widely studied, analyzed and assessed in recent years either to design or evaluate a unit for a given application (Benitez, 2009) (Brunazzi et al., 2002) (Coker, 1991) (Kleine, 1998) (Leye and Froment, 1986) (McNutly and Chohey 1994) (Mohamadbegy et al., 2005) (Siegler, 2003) (Strigle, 1987); to determine mass-transfer coefficients and determine pressure drop in packed beds (Arwika, 1981) (Bravo and Fair, 1982) (Fair and Bravo, 1987) (Lockett, 1998) (Shulman and Margolis, 2004) (Wagner et al., 1997); for modeling and optimization of absorption operations and equipment (Olutoye and Mohammed, 2006) (Rahbar and Kaghazchi, 2005); and is a frequent topic usually covered in the most important chemical engineering handbooks and mass-transfer related literature (Asano, 2006) (Ludwig, 1997) (Marcilla, 1999) (Pavlov et al., 1981) (Perry and Chilton, 2008) (Peters and Timmerhaus, 1991) (Billet and Schultes, 1995) (Richardson and Harker, 2002) (Treybal, 1980) available nowadays.

The design approach of a packed-bed absorber usually involves the determination of geometrical parameters such as *tower diameter* (D) and *packing height* (Z), as well as some other mass-transfer and operational variables such as convective mass-transfer coefficients for gas and liquid streams; dry and overall pressure drops; as well as overall mass-transfer coefficient. A well designed packed-bed tower will provide the required mass-transfer contact between gas and liquid phases, with low pressure drop, small capital and operating costs, and high removal efficiencies.

The use of simulation and modeling techniques to design, evaluate or optimize chemical processes, equipment and unit operations, either from the economic or technical point of view, have reached unprecedented levels in recent years (Boyadjiev, 2010) (Dimian and Bildea, 2008) (Finlayson, (2006). Among the most developed and common computer applications used today is the *MATLAB*[®] software (Math Works, 2009), since it provides numerical methods which permit to solve numerous mathematical, statistical, financial, trigonometric, etc. functions by using special application fields referred to as toolboxes (Karris, 2004) (Nakamura, 2002). *MATLAB*[®] software is considered a high-level software package with many built-in functions, which is very easy to use, even for people without prior programming experience, and that make the learning of numerical and mathematical methods much easier and more interesting (Karris, 2004) (Yang et al., 2005).

Several authors have used *MATLAB*[®] software to carry out the simulation of chemical processes operations and equipment, the evaluation of alternatives and base cases, as well as the optimization of existing units or plants. For example, Mušič and Matko (Mušič and Matko, 1998) used *Petri* nets and *Sequential Function Charts* (SFC) methods for modelling batch recipes on a combined discrete/continuous support, applying a simulation environment based on *MATLAB/Simulink*[®] tools. Kukurugya and Terpák (Kukurugya and Terpák, 2006) developed different approaches using *MATLAB*[®] simulation tools, for modelling of equipment installed in the raw materials processing area both at coal and limestone mines, by means of balancing elementary processes running inside of the plant and equipment. On the other hand, (González et al., 2007) proposed to incorporate the analysis of the dynamic performance of processes into the design and engineering stage of projects, by the use of base-software tools such as *MATLAB/Simulink*[®] package. These authors applied the simulation method obtained in *MATLAB*[®] in a natural gas installation in a power plant, in order to study the transients of a natural gas supply line to a steam-electric power plant. The results of the model were validated with actual data on the boiler trip obtained from the distributed control system. Finally, (Asbjörnsson, 2013) demonstrate that three different application areas of crushing/screening plants are available for dynamic, steady-state simulation using *MATLAB*[®] tools: plant performance, optimization and operator training, were each of these areas put different constraints on the modelling and simulation of these types of plants.

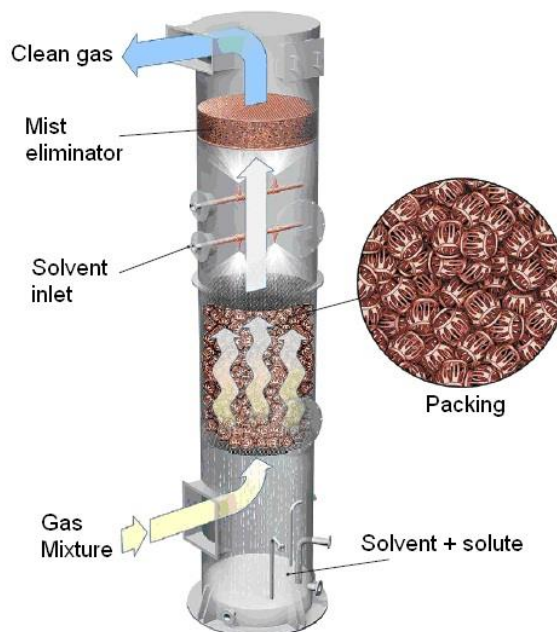


Figure 1. Typical layout of a packed-bed absorber

Source: (Benitez, 2009)

At the present work, a packed bed absorber is designed to recover certain amounts of ethanol contained in a CO₂-rich gaseous stream coming from fermentation operations. Four different packing types (*Pall*[®], *Hiflow*[®], *Top Pak*[®] and *VSP*[®]) were evaluated in order to determine which packing configuration provides the lowest column dimensions (tower diameter and packing height) as well as the highest mass-transfer coefficient for this application, without exceeding the maximum allowable pressure drop and also without affecting the requested removal efficiency. The influence of both liquid solvent and gas mixture feed flowrates on 4 important process parameters (tower diameter, packing height, gas pressure drop and overall mass-transfer coefficient) was assessed for the four packing, while the effect of this two flowrates on two design parameters (overall number of gas-phase transfer units; N_{IOG} and overall height of a gas-phase transfer unit, H_{IOG}) was also determined. The design methodology was solved using computing software *MATLAB*[®] version 7.8.0.347 (R2009a) (Math Works, 2009), and also Microsoft Excel[®] spreadsheet.

2. MATERIALS AND METHODS

2.1. Problem description

A gaseous mixture containing CO₂ and ethanol, with a molar composition of 92 % CO₂ and 8 % of the alcohol, is evolved from a fermentation process. The ethanol must be recovered by means of a countercurrent absorption process using water as the solvent (Figure 3). The gas mixture will enter the tower at a rate of 4000 m³/h, at 25 °C (298 K) and 1.1 atm, while the solvent (water) will be supplied at a flowrate of 6500 kg/h and also at 298 K. The required recovery of ethanol will be 97.0 %, while the maximum pressure drop permitted for the gas stream should not exceed 250 Pa/m of packed height. It's desired to design a suited packed-bed absorber working at 70% of flooding and operating under isothermal conditions.

For this application, four packing types will be evaluated (Figure 2):

1. 50-mm metal *Hiflow*[®] rings
2. 50-mm ceramic *Pall*[®] rings
3. 50-mm metal *Top Pak*[®] rings, and
4. 25-mm metal *VSP*[®] rings.

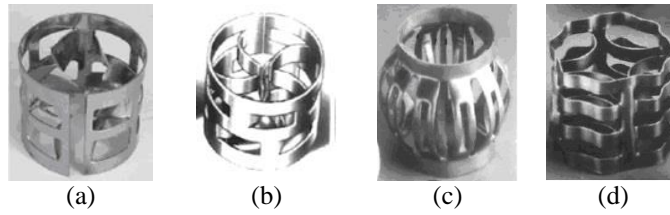


Figure 2. Configuration of the different packing types used:

- (a) Metal Hiflow® rings
 - (b) Ceramic Pall® rings
 - (c) Metal Top Pak® rings
 - (d) Metal VSP® rings
- Source: (Ludwig, 1997)

According to (Ludwig, 1997), the four packing types considered have the following performance and mass-transfer characteristics:

Table 1. Performance and mass-transfer characteristics of the different packing considered

Packing	Mass Transfer	Pressure Drop	Capacity
<i>Hiflow</i> ®	High	Low-Medium	Medium-High
<i>Pall</i> ®	Medium	Medium	Medium
<i>Top Pak</i> ®	High	Low	High
<i>VSP</i> ®	High	Medium	High

Source: (Ludwig, 1997)

Table 2. Hydraulic and mass-transfer parameters of the four packing types selected

Packing type	Hydraulic parameters					Mass-transfer parameters	
	<i>a</i>	ϵ	<i>Ch</i>	<i>C_P</i>	<i>F_p</i>	<i>C_L</i>	<i>C_V</i>
50-mm Metal <i>Hiflow</i> ® rings	92.0	0.977	0.876	0.421	52	1.168	0.408
50-mm Ceramic <i>Pall</i> ® rings	121.0	0.783	1.335	0.662	142	1.227	0.415
50-mm Metal <i>Top Pak</i> ® rings	75.0	0.98	0.881	0.604	46	1.326	0.389
25-mm Metal <i>VSP</i> ® rings	205.0	0.97	1.369	0.782	105	1.376	0.405

Source: (Benitez, 2009)

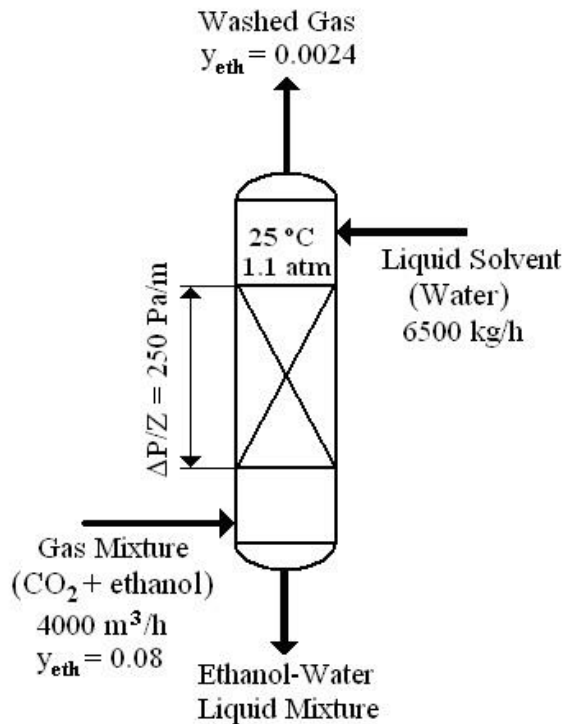


Figure. 3. Schematic drawing of the packed-bed absorber operating conditions

Since the absorption system operates at low pressure and temperature (1.1 atm and 298 K, respectively); the solute gas is very diluted in the liquid phase (that is, the liquid phase can be catalogued as a *dilute liquid solution*), the system operates under isothermal conditions and there is no reaction between the dissolved solute (ethanol) and the solvent (water), it's assumed that the system obeys the *Henry's law* (Leye and Froment, 1986) (Matos and Hing, 1990) (Perry and Chilton, 2008) (Richardson and Harker, 2002) (Treybal, 1980). According to (Perry and Chilton, 2008) (Rogers, 2007), the value of the *Henry's constant* for an ethanol-water system operating at 25 °C is $H = 0.272$ atm. Thus, the *distribution coefficient* (ϕ) for the gas-liquid system (ethanol-water system) at 25 °C and 1.1 atm is $\phi = H/P = 0.272/1.1 = 0.229$.

2.2. Packing hydraulic and mass-transfer parameters

The most important hydraulic/mass transfer characteristics of the four packing types selected are described in the Table 2 (Billet, 1989) (Perry and Chilton, 2008).

2.3. Inlet data

The inlet data necessary to carry out the design calculations are showed in Table 3:

Table 3. Inlet data of the absorption process

<i>Parameter</i>	<i>Value</i>	<i>Units</i>
<i>Inlet gas mixture</i>		
Volumetric flowrate (Q_G)	4000	m ³ /h
Mole fraction of ethanol [$y_{eth(1)}$]	0.08	
<i>Inlet solvent (water)</i>		
Mass flowrate [$m_{L(2)}$]	6500	kg/h
<i>Other data</i>		
Molecular weight of ethanol (M_{eth})	46.068	kg/kmol
Molecular weight of water (M_W)	18	kg/kmol
Molecular weight of carbon dioxide (M_{CO_2})	44.01	kg/kmol
Ethanol removal percent (%R)	97	%
Flooding factor (f_{flood})	70	%
Maximum pressure drop permitted ($\Delta P_{limit}/Z$)	200	Pa/m
Liquid density of solvent (water) at 25 °C (ρ_L)	997.047	kg/m ³
Liquid viscosity of solvent (water) at 25 °C (μ_L)	0.00089	Pa.s
Vapor viscosity of ethanol at 25 °C (μ_{eth})	0.000009	Pa.s
Vapor viscosity of carbon dioxide at 25 °C (μ_{CO_2})	0.000015	Pa.s
Molar volume of ethanol (V_{eth})	58.6	cm ³ /mol
Molar volume of carbon dioxide (V_{CO_2})	34.0	cm ³ /mol
Collision diameter of ethanol (σ_{eth})	4.530	Å
Collision diameter of carbon dioxide (σ_{CO_2})	3.941	Å
e/k parameter for ethanol (e_{eth}/k)	362.600	K
e/k parameter for carbon dioxide (e_{CO_2}/k)	195.200	K
Ideal gas constant (R)	0.0821	m ³ .atm/kmol.K
Henry constant for ethanol-water system 25 °C (H)	0.252	atm
Distribution coefficient (m)	0.229	–
System temperature (T)	25.0	°C
System pressure (P)	1.1	atm

2.4. Design methodology

The equations and correlations used to design the packed-bed absorber were taken from different sources (Billet, 1989) (Perry and Chilton, 2008) (Richardson and Harker, 2002), considering several aspects such as process operating conditions, mass transfer characteristics, and packing type.

2.4.1. Tower diameter

The *molecular weight of the gas mixture* (M_G) was determined applying the equation (1):

$$M_G = (y_{eth(1)} \cdot M_{eth}) + (y_{CO_2(1)} \cdot M_{CO_2}) \quad (1)$$

where $y_{CO_2(1)} = 1 - y_{eth(1)}$.

The *gas mixture density* (ρ_G) at 25 °C was determined using the *Kay's method* (Perry and Chilton, 2008), while the *viscosity of the gas mixture* (μ_G) was calculated using the following correlation (Pavlov, 1981):

$$\mu_G = \left[\frac{M_G}{\left(\frac{y_{eth(1)} \cdot M_{eth}}{\mu_{eth}} \right) + \left(\frac{y_{CO_2(1)} \cdot M_{CO_2}}{\mu_{CO_2}} \right)} \right] \cdot 0.001 \quad (2)$$

where μ_{eth} and μ_{CO_2} values are given in cP.

The *amount of ethanol absorbed* is;

$$m_{eth(abs)} = \left(\frac{Q_G \cdot \rho_G}{M_G} \right) \cdot y_{eth(1)} \cdot \%R \cdot M_{eth} \quad (3)$$

The *amount of solvent liquid exiting the column* is:

$$m_{L(1)} = m_{L(2)} + m_{eth(abs)} \quad (4)$$

The *flow parameter* (X), the *pressure drop parameter under flooding conditions* (Y_{flood}) and the C_S *coefficient at flooding conditions* (C_{Sflood}) were determined according to the equations (5) (6) and (7), respectively.

$$X = \frac{m_{L(1)}}{Q_G \cdot \rho_G} \cdot \left(\frac{\rho_G}{\rho_L} \right)^{0.5} \quad (5)$$

$$\ln Y_{flood} = -[3.5021 + 1.028 \cdot \ln X + 0.11093 \cdot (\ln X)^2] \quad (6)$$

$$C_{Sflood} = \left[\frac{Y_{flood}}{F_P \cdot \mu_L^{0.1}} \right]^{0.5} \quad (7)$$

The *gas velocity at flooding conditions* (v_{Gflood}), the *gas velocity* (v_G), and finally the *tower diameter* (D), were calculated by using the following correlations:

$$v_{Gflood} = \frac{C_{Sflood}}{\left[\frac{\rho_G}{\rho_L - \rho_G} \right]^{0.5}} \quad (8)$$

$$v_G = v_{Gflood} \cdot f_{flood} \quad (9)$$

$$D = \left[\frac{4 \cdot \left(\frac{Q_G}{3600} \right)}{v_G \cdot \pi} \right]^{0.5} \quad (10)$$

2.4.2. Pressure drop

Most packed-bed absorbers are designed to safely avoid flooding conditions and also to operate in the preloading region, with a gas-pressure drop limit of 200 – 400 Pa/m of packed depth [4]. In this approach, both the gas *dry* pressure drop ($\Delta P_0/Z$) and *overall* pressure drop ($\Delta P/Z$) were determined for the absorption process using well-accepted equations. The liquid holdup influence was also taken into account, that is, when the packed bed is irrigated, the liquid holdup causes an increment of the pressure drop (Benitez, 2009) (Perry and Chilton, 2008). Prior to the determination of both pressure drops, it was necessary to determine several parameters first. Among those parameters are included the *effective particle diameter* (d_p) [equation (11)]; the *wall factor* (K_w) [eq. (12)]; the *gas-phase Reynolds number* (Re_G) [eq. (13)]; the *dry-packing resistance coefficient* (ψ_0) [eq. (14)]; *liquid mass velocity* (G_L) [eq. (15)]; the *liquid velocity* (v_L) [eq.(16)]; the *liquid-phase Reynolds number* (Re_L) [eq.(17)]; *liquid-phase Froude number* (Fr_L) [eq.(18)]; the *ratio* a_h/a [eq. (19)]; the *effective specific surface area of packing* (a_h) [eq. (20)]; and, finally, the *liquid holdup* (h_L) [eq. (21)].

$$d_p = 6 \cdot \left(\frac{1 - \varepsilon}{a} \right) \quad (11)$$

$$K_w = \frac{1}{1 + \frac{2}{3} \cdot \left(\frac{1}{1 - \varepsilon} \right) \cdot \frac{d_p}{D}} \quad (12)$$

$$Re_G = \frac{v_G \cdot d_p \cdot \rho_G \cdot K_w}{(1 - \varepsilon) \cdot \mu_G} \quad (13)$$

$$\psi_0 = C_p \cdot \left(\frac{64}{Re_G} + \frac{1.8}{Re_G^{0.08}} \right) \quad (14)$$

$$G_L = \frac{4 \cdot \left(\frac{m_{L(1)}}{3600} \right)}{\pi \cdot D^2} \quad (15)$$

$$v_L = \frac{G_L}{\rho_L} \quad (16)$$

$$Re_L = \frac{v_L \cdot \rho_L}{a \cdot \mu_L} \quad (17)$$

$$Fr_L = \frac{v_L^2 \cdot a}{g} \quad (18)$$

$$\frac{a_h}{a} = C_h \cdot Re_L^{0.5} \cdot Fr_L^{0.1} \text{ for } Re_L < 5 \quad (19)$$

$$\frac{a_h}{a} = 0.85 \cdot C_h \cdot Re_L^{0.25} \cdot Fr_L^{0.1} \text{ for } Re_L \geq 5$$

$$a_h = \frac{a_h}{a} \cdot a \quad (20)$$

$$h_L = \left[12 \cdot \frac{Fr_L}{Re_L} \right]^{1/3} \cdot \left[\frac{a_h}{a} \right]^{2/3} \quad (21)$$

The gas dry pressure drop per meter of packing height ($\Delta P_0/Z$) was determined according to the following correlation:

$$\frac{\Delta P_0}{Z} = \psi_0 \cdot \frac{a}{\varepsilon^3} \cdot \frac{\rho_G \cdot v_G^2}{2} \cdot \frac{1}{K_w} \quad (22)$$

Then, the gas overall pressure drop per meter of packing height ($\Delta P/Z$) can be finally calculated:

$$\frac{\Delta P}{Z} = \frac{\Delta P_0}{Z} \cdot \left[\left(\frac{\varepsilon}{\varepsilon - h_L} \right)^{1.5} \exp\left(\frac{Re_L}{200} \right) \right] \quad (23)$$

2.4.3. Diffusion coefficients

Gas-phase diffusion coefficient: The theory describing diffusion processes in binary gas mixtures at low to moderate pressures has been studied extensively in recent years, and is well developed nowadays. Since the absorption process is a binary gas system taking place at low-pressure, the gas-phase diffusion coefficient can be estimated using the *Wilke and Lee* correlation (Benitez, 2009):

$$D_G = \frac{\left[3.03 - \left(\frac{0.98}{M_{AB}^{1/2}} \right) \right] \cdot (10^{-3}) \cdot T^{3/2}}{P \cdot M_{AB}^{1/2} \cdot \sigma_{AB}^2 \cdot \Omega_D} \cdot 0.0001 \quad (24)$$

where:

$$M_{AB} = 2 \cdot \left[\frac{1}{M_{eth}} + \frac{1}{M_{CO2}} \right]^{-1} \quad (25)$$

σ_{AB} – Collision diameter

$$\sigma_{AB} = \frac{\sigma_{eth} + \sigma_{CO2}}{2} \quad (26)$$

Ω_D – Diffusion collision integral

$$\Omega_D = \frac{1.06036}{(T^*)^{0.15610}} + \frac{0.19300}{\exp(0.47635 \cdot T^*)} + \frac{1.03587}{\exp(1.52996 \cdot T^*)} + \frac{1.76474}{\exp(3.89411 \cdot T^*)} \quad (27)$$

$$T^* = \frac{T}{\sqrt{\frac{e_{eth}}{k} \cdot \frac{e_{CO2}}{k}}} \quad (28)$$

Liquid-phase diffusion coefficient: Compared with the kinetic theory behind the gases behavior, which is well developed and available today, the theoretical basis of the internal structure of liquids and their transport characteristics are still insufficient to permit a rigorous treatment (Benitez, 2009) (Billet, 1989). Usually, liquid diffusion coefficients are several orders of magnitude smaller than gas diffusivities, and depend mostly on concentration profiles due to changes in viscosity, as well as some changes in the degree of ideality of the solution. To determine the liquid-phase diffusion coefficient in binary systems for solutes transport to aqueous solutions, the *Hayduk and Minhas* correlation was used (Benitez, 2009):

$$D_L = \frac{1.25 \times 10^{-8} (V_{eth}^{-0.19} - 0.292) \cdot T^{1.52} \cdot \mu_w^n}{10000} \quad (29)$$

where:

V_{eth} – Molar volume of ethanol [see Table (2)] [cm³/mol]

μ_w – Viscosity of water at temperature T [cP]

$$n = \frac{9.58}{V_{eth}} - 1.12 \quad (30)$$

2.4.4. Mass transfer coefficients

To determine the mass transfer coefficients for both phases, two correlations were used which were obtained from an extensive study made by *Billet* and *Schultes* (Billet, 1989), that involved measurement and correlation of mass-transfer coefficients for 31 different binary and ternary systems, equipped with 67 different types and sizes of packings, in columns of diameter ranging from 6 cm to 1.4 m.

Gas-phase convective mass-transfer coefficient (k_G):

$$k_G = 0.1304 \cdot C_V \cdot \left[\frac{D_G \cdot P}{R \cdot T} \right] \cdot \left(\frac{a}{[\varepsilon(\varepsilon - h_L)]^{0.5}} \right) \cdot \left[\frac{Re_G}{K_w} \right]^{3/4} \cdot Sc_G^{2/3} \quad (31)$$

where:

C_V – Mass transfer factor [see Table (1)]

R – Ideal gas constant

= 0.0821 m³.atm/kmol.K

ε – Packing porosity or void fraction [see Table (1)]

$$Sc_G - \text{Schmidt number for gas phase} = \frac{\mu_G}{\rho_G \cdot D_G} \quad (32)$$

Liquid-phase convective mass-transfer coefficient (k_L):

$$k_L = 0.757 \cdot C_L \cdot \left[\frac{D_L \cdot a \cdot v_L}{\varepsilon \cdot h_L} \right]^{0.5} \quad (33)$$

where:

C_L – Mass transfer factor [see Table (1)]

a – Mass transfer surface area per unit volume [see Table (1)] [m²/m³]

2.4.5. Packing Height

In those systems handling dilute solutions and when *Henry's law* applies, is very usual and convenient to work with overall mass-transfer coefficients in order to calculate the packing height (Z), which can be determined by the following expression:

$$Z = H_{tOG} \cdot N_{tOG} \quad (34)$$

where:

H_{tOG} – Overall height of a gas-phase transfer unit (HTU) [m]

N_{tOG} – Overall number of gas-phase transfer units (NTU)

Prior to determine the values of HTU and NTU, it will be necessary to calculate several parameters first, which are the *inlet gas molar velocity* [$G_{My(1)}$] [equation (38)]; the *outlet gas molar velocity* [$G_{My(2)}$] [eq. (39)]; the *average molar gas velocity* (G_{My}) [eq. (40)]; the *inlet liquid molar velocity* [$G_{Mx(2)}$] [eq. (41)]; the *outlet liquid molar velocity* [$G_{Mx(1)}$] [eq. (42)]; the *absorption factor at the bottom* [$A_{(1)}$] and *top* [$A_{(2)}$] of the column [eqs. (43) and (44)]; the *geometric average of the absorption factor* (A) [eq. (45)]; the *ethanol molar composition of outlet gas* [$y_{eth(2)}$] [eq. (46)]; the *volumetric gas-phase* (K_{vG}) and *liquid-phase* (K_{vL}) *mass-transfer coefficients* [eqs. (47) and (48), respectively]; the *overall volumetric mass-transfer coefficient* (K_m) [eq. (49)]; the *overall height of a gas-phase transfer unit* (H_{tOG}) [eq. (50)]; the *overall number of gas-phase transfer units* (N_{tOG}) [eq. (51)]; and finally the *packing height* (Z) [eq. (37)].

$$G_{My(1)} = \frac{4 \cdot N_G}{3600 \cdot \pi \cdot D^2} \quad (35)$$

where:

N_G – Gas molar flowrate

$$N_G = \left(\frac{Q_G \cdot \rho_G}{M_G} \right)$$

$$G_{My(2)} = \frac{4 \cdot (N_G - N_{eth(abs)})}{3600 \cdot \pi \cdot D^2} \quad (36)$$

where:

$N_{eth(abs)}$ – Molar flow of ethanol absorbed

$$N_{eth(abs)} = \left(\frac{Q_G \cdot \rho_G}{M_G} \right) \cdot y_{eth(1)} \cdot \%R$$

$$G_{My} = \frac{G_{My(1)} + G_{My(2)}}{2} \quad (37)$$

$$G_{Mx(2)} = \frac{4 \cdot N_{L(2)}}{3600 \cdot \pi \cdot D^2} \quad (38)$$

where:

$N_{L(2)}$ – Inlet liquid molar flowrate [kmol/h]

$$N_{L(2)} = \left(\frac{m_{L(2)}}{M_w} \right)$$

$$G_{Mx(1)} = \frac{4 \cdot (N_{L(2)} + N_{eth(abs)})}{3600 \cdot \pi \cdot D^2} \quad (39)$$

$$A_{(1)} = \frac{G_{Mx(1)}}{G_{My(1)} \cdot \phi} \quad (40)$$

$$A_{(2)} = \frac{G_{Mx(2)}}{G_{My(2)} \cdot \phi} \quad (41)$$

where:

ϕ – Distribution coefficient = 0.229

$$A = \frac{A_{(1)} + A_{(2)}}{2} \quad (42)$$

$$y_{eth(2)} = (100 - \%R) \cdot y_{eth(1)} \quad (43)$$

$$K_{vG} = k_G \cdot a_h \quad (44)$$

$$K_{vL} = k_L \cdot a_h \cdot c \quad (45)$$

where:

$$c = \frac{\rho_L}{M_w}$$

$$K_m = \frac{1}{\frac{1}{K_{vG}} + \frac{\phi}{K_{vL}}} \quad (46)$$

$$H_{tOG} = \frac{G_{My}}{K_m} \quad (47)$$

$$N_{tOG} = \frac{\ln \left\{ \left[\frac{y_{eth(1)} - (\phi \cdot x_{eth(2)})}{y_{eth(2)} - (\phi \cdot x_{eth(2)}) \right] \cdot \left(1 - \frac{1}{A} \right) \right\} + \frac{1}{A}}{1 - \frac{1}{A}} \quad (48)$$

2.4.6. Operating and equilibrium lines

The *operating line* will be elaborated using the following data:

- Mole fraction of ethanol in inlet gas mixture $[y_{eth(1)}] = 0.08$
- Mole fraction of ethanol in outlet gas mixture $[y_{eth(2)}] = 0.0024$
- Mole fraction of ethanol in inlet liquid $[x_{eth(2)}] = 0$.
- Mole fraction of ethanol in outlet liquid

$$[x_{eth(1)}] = \frac{N_{eth(abs)}}{N_{L(1)}} = \frac{N_{eth(abs)}}{N_{L(2)} + N_{eth(abs)}} = 0.038$$

While to elaborate the *equilibrium line*, the following expression will be used:

$$y^* = \phi \cdot x \quad (49)$$

3. RESULTS AND DISCUSSION

The main physical parameters calculated for the gas mixture (that is, molecular weight, density and viscosity) are showed in Table 4, while the calculated *tower diameter* (D) and *overall gas pressure drop* ($\Delta P/Z$) values for each packing type, among other important design variables, are showed in Table 5.

Table 6 shows the calculated values of the diffusion and convective mass-transfer coefficients for both fluids (gas and liquid), whereas the values obtained of *packing height* (Z) and other significant flow and mass-transfer parameters are listed in Table 7, all of them for the four packing types selected.

Finally, Table 8 presents a summary of the most important geometrical and mass-transfer parameters calculated for the four packing types.

Figure 4 shows a graphical comparison between Z and D for each packing type; while the values obtained of *gas pressure drop* and *overall mass-transfer coefficient* for each packing are given in Figure 5 and Figure 6, respectively.

The resulting values of *tower diameter*; *gas pressure drop*; *overall mass-transfer coefficient* and *packing height* for each packing as a function of *gas mixture feed flowrate* (Q_G) and *liquid solvent feed flowrate* (m_L) are reported in Figure 7 and Figure 8, respectively. The behavior of the variables N_{iOG} and H_{iOG} with respect to Q_G and m_L are showed in Figure 9 and Figure 10, respectively. Finally, both the operating and equilibrium lines are illustrated in Figure 11.

Table 4. Calculated physical parameters

Parameter	Units	Equation No.	Value
Gas mixture molecular weight [M_G]	kg/kmol	(1)	44.17
Gas mixture density [ρ_G]	kg/m ³		2.006
Gas mixture viscosity [μ_G]	Pa.s	(2)	0.0000142

Table 5. Tower diameter and pressure drop results for each packing type

Parameter / Packing	Units	Eq.	Hiflow [®]	Pall [®]	Top Pak [®]	VSP [®]
$m_{eth(abs)}$	kg/h	(3)	649.35	649.35	649.35	649.35
$m_{L(1)}$	kg/h	(4)	7149.35	7149.35	7149.35	7149.35
X	–	(5)	0.0400	0.0400	0.0400	0.0400
Y_{flood}		(6)	0.261	0.261	0.261	0.261
C_{Sflood}		(7)	0.101	0.061	0.107	0.071
v_{GF}	m/s	(8)	2.243	1.357	2.385	1.578
v_G	m/s	(9)	1.570	0.950	1.669	1.105
D	m	(10)	0.949	1.221	0.921	1.132
d_p	m	(11)	0.0015	0.0108	0.0016	0.0006
K_w		(12)	0.956	0.974	0.945	0.983
Re_G		(13)	13822.75	6475.80	17821.18	4466.63
ψ_0		(14)	0.355	0.597	0.499	0.730
G_L	kg/m ² .s	(15)	2.806	1.698	2.984	1.975
v_L	m/s	(16)	0.0028	0.0017	0.0030	0.0020
Re_L		(17)	34.27	15.77	44.70	10.77
Fr_L		(18)	0.000074	0.000036	0.000068	0.00082
Ratio a_h/a		(19)	0.696	0.812	0.742	0.823
a_h	m ⁻¹	(20)	64.05	98.29	55.66	169.57
h_L		(21)	0.0233	0.0262	0.0216	0.0396
$\Delta P_0/Z$	Pa/m	(22)	91	140	118	199
$\Delta P/Z$	Pa/m	(23)	112	159	152	223

Table 6. Diffusion and mass-transfer coefficients for each packing type

Parameter / Packing	Units	Eq.	Hiflow [®]	Pall [®]	Top Pak [®]	VSP [®]
M_{AB}		(25)	45.02	45.02	45.02	45.02
σ_{AB}	Å	(26)	4.236	4.236	4.236	4.236
Ω_D		(27)	1.364	1.364	1.364	1.364
T^*		(28)	1.120	1.120	1.120	1.120
D_G	cm ² /s	(24)	0.0821	0.0821	0.0821	0.0821
D_L	cm ² /s	(29)	0.0000136	0.0000136	0.0000136	0.0000136
k_G	kmol/m ² .s	(31)	0.00221	0.002061	0.00209	0.002056
Sc_G		(32)	0.862	0.862	0.862	0.862
k_L	m/s	(33)	0.000110	0.000109	0.000121	0.000125

Table 7. Packing height determination for each packing type

<i>Parameter / Packing</i>	<i>Units</i>	<i>Eq. No.</i>	<i>Hiflow</i> [®]	<i>Pall</i> [®]	<i>Top Pak</i> [®]	<i>VSP</i> [®]
$G_{My(1)}$	kmol/m ² .s	(35)	0.071	0.043	0.076	0.050
$G_{My(2)}$	kmol/m ² .s	(36)	0.066	0.040	0.070	0.046
G_{My}	kmol/m ² .s	(37)	0.069	0.041	0.073	0.048
$G_{Mx(2)}$	kmol/m ² .s	(38)	0.142	0.086	0.151	0.100
$G_{Mx(1)}$	kmol/m ² .s	(39)	0.147	0.089	0.157	0.104
A_1		(40)	9.017	9.017	9.017	9.017
A_2		(41)	9.408	9.408	9.408	9.408
A		(42)	9.212	9.212	9.212	9.212
$y_{eth(2)}$		(43)	0.0024	0.0024	0.0024	0.0024
K_{vG}	kmol/m ³ .s	(44)	0.142	0.203	0.116	0.349
K_{vL}	kmol/m ³ .s	(45)	0.391	0.592	0.372	1.172
K_m	kmol/m ³ .s	(46)	0.131	0.188	0.109	0.326
H_{tOG}	m	(47)	0.524	0.221	0.671	0.148
N_{tOG}		(48)	3.809	3.809	3.809	3.809
Z	m	(34)	2.0	0.8	2.6	0.6

Table 8. Summary of the most important packed column design parameters for the four packing considered

<i>Parameter</i>	<i>Hiflow</i> [®]	<i>Pall</i> [®]	<i>Top Pak</i> [®]	<i>VSP</i> [®]
D [m]	0.949	1.221	0.921	1.132
Z [m]	2.00	0.80	2.60	0.60
$\Delta P/Z$ [Pa/m]	112	159	152	223
K_{vG} [kmol/m ³ .s]	0.142	0.203	0.116	0.349
K_{vL} [kmol/m ³ .s]	0.391	0.592	0.372	1.172
K_m [kmol/m ³ .s]	0.131	0.188	0.109	0.326
H_{tOG} [m]	0.524	0.221	0.671	0.148
a_h [m ⁻¹]	64.05	98.29	55.66	169.57

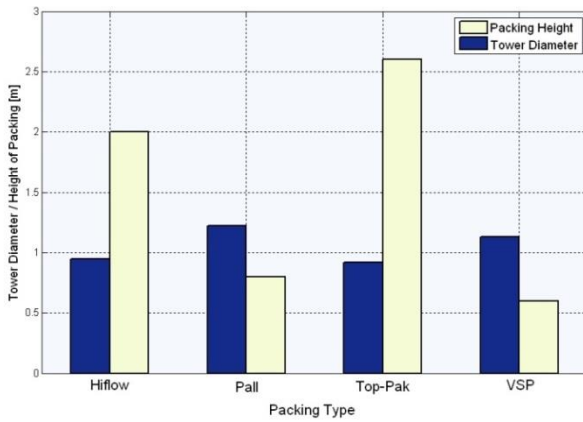


Figure 4. Comparison between Tower Diameter and Packing Height as a function of packing

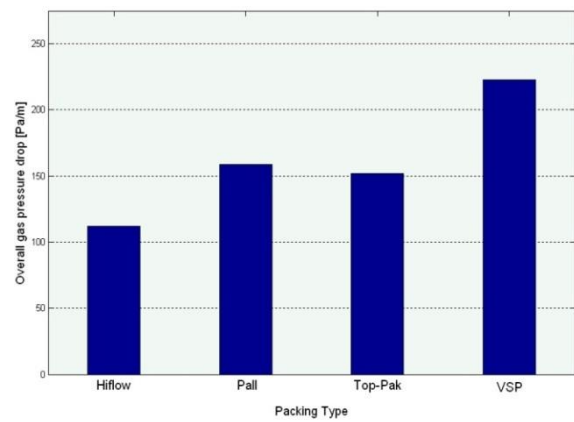


Figure 5. Overall gas pressure drop values determined for each packing

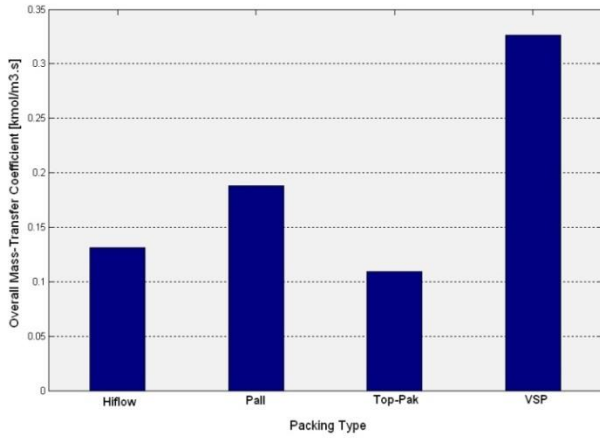


Figure 6. Overall Mass-Transfer Coefficients calculated for each packing

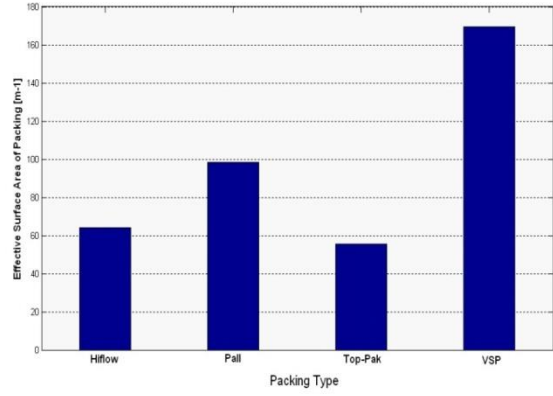


Figure 7. Effective surface area determined for each packing

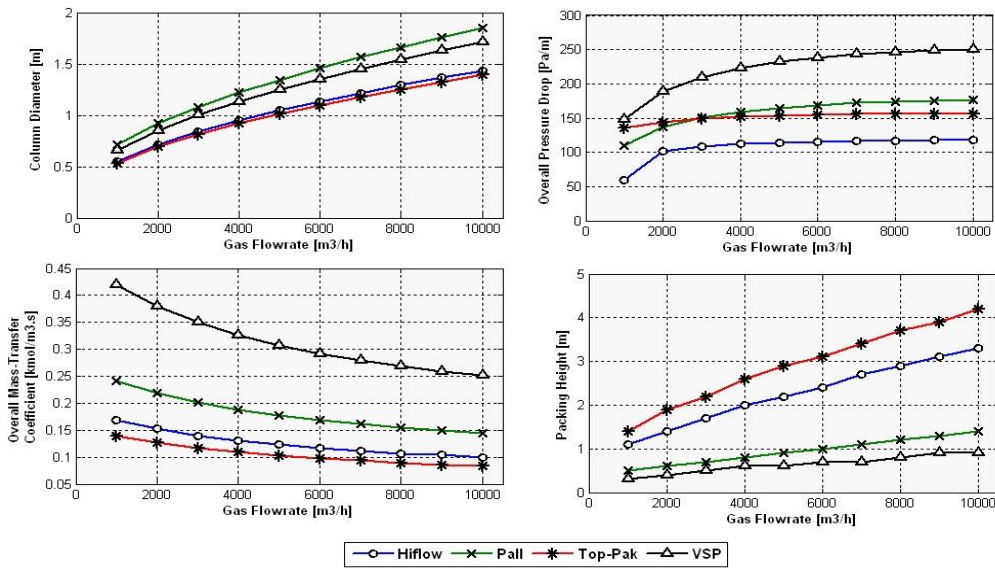


Figure 8. Calculated Tower Diameter; Gas Pressure-Drop; Overall Mass-Transfer Coefficients and Packing Height values for the different packing types as a function of Gas Mixture Feed Flowrate.

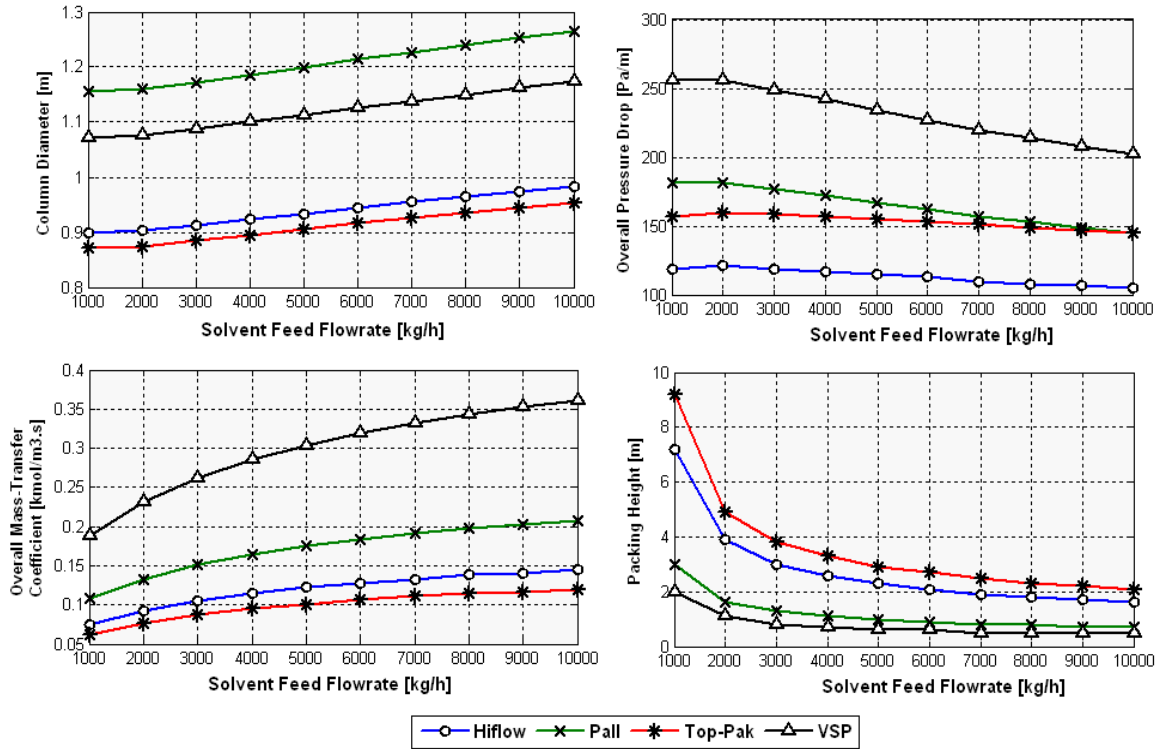


Figure 9. Calculated Tower Diameter; Gas Pressure-Drop; Overall Mass-Transfer Coefficients and Packing Height values for the different packing types as a function of Solvent (Water) Feed Flowrate.

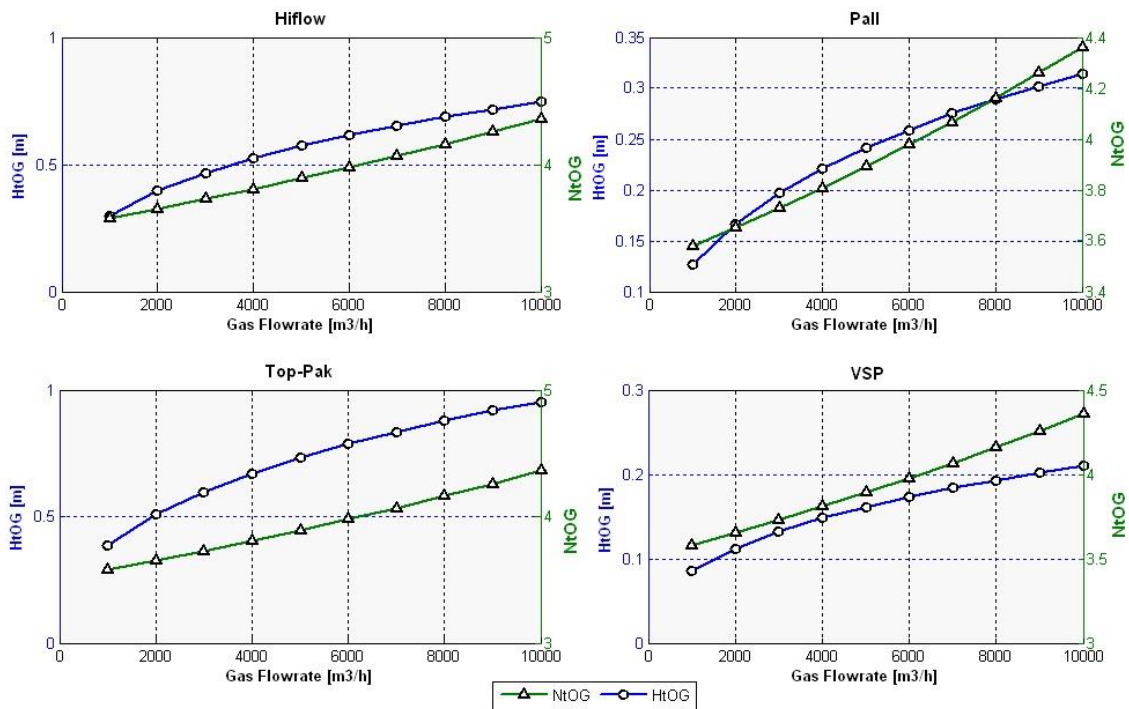


Figure 10. Calculated HtOG and NtOG values for each packing type as a function of Gas Mixture Feed Flowrate.

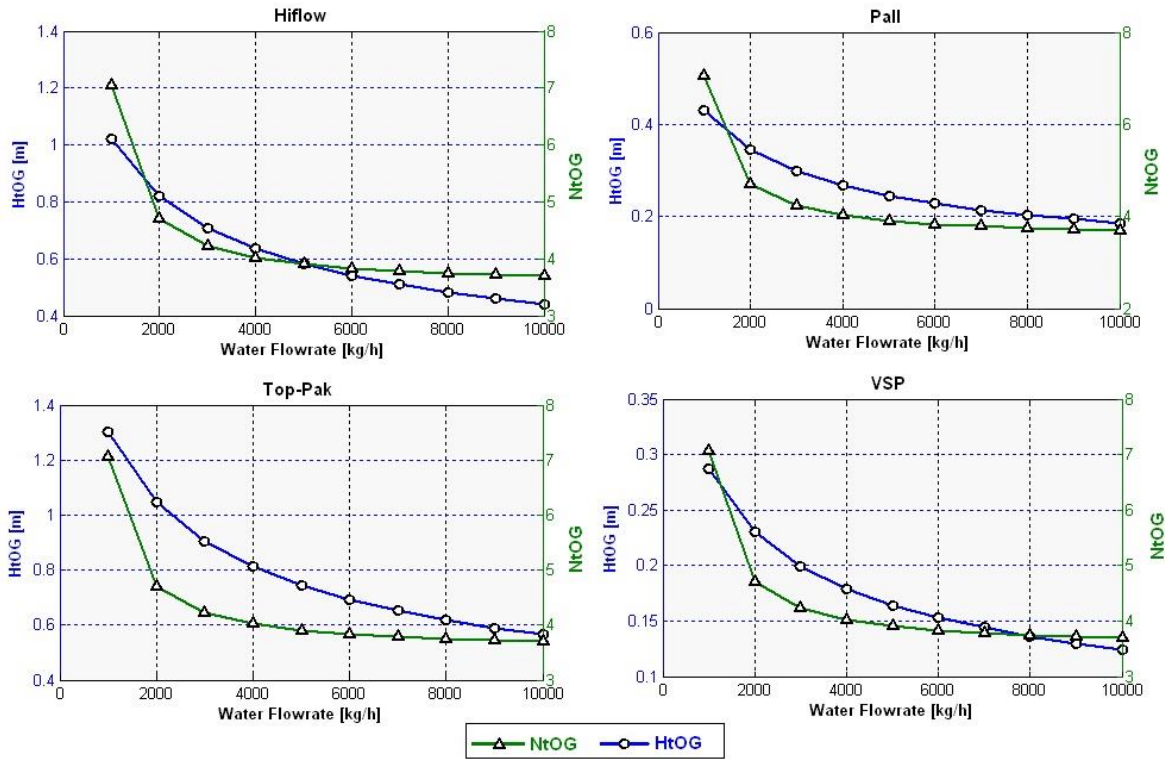


Figure 11. Calculated HtOG and NtOG values for each packing type as a function of Liquid Solvent (Water) Feed Flowrate.

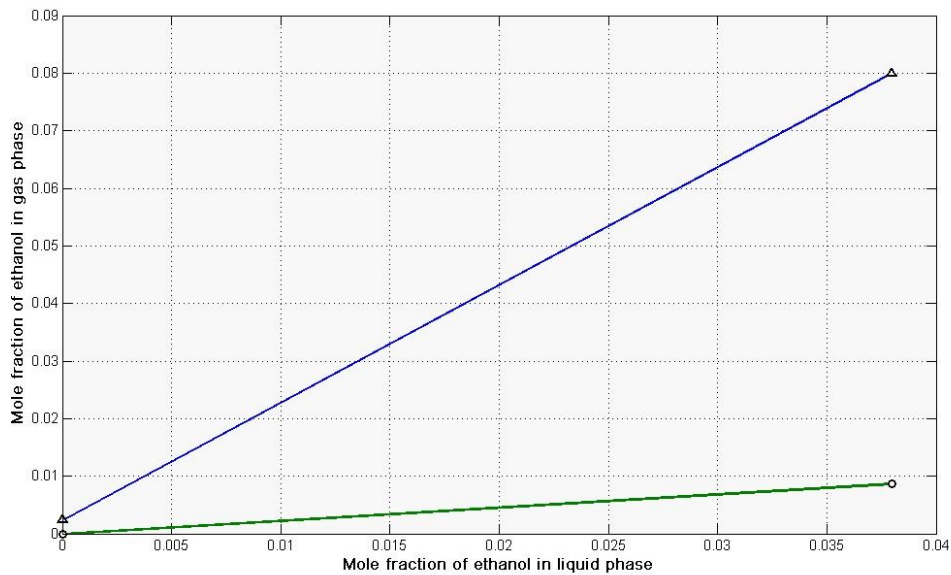


Figure 12. Operating and equilibrium lines for the absorption system

Figure 4 shows that the maximum result of *packing height* (Z) is obtained if *Top Pak*[®] rings are employed (2.60 m), whereas the lowest value of Z corresponded to *VSP*[®] rings (0.90 m). Regarding *tower diameter* (D), *Top Pak*[®] rings supplied the lowest value of D (0.921 m), while the *Pall*[®] rings had the highest value of D , with 1.221 m. According to the correlations used during this work, the value to obtain of D is

directly related with the *packing factor* (F_p) value of each packing type, that is, if F_p increases so will increase the value of D .

As for the calculated values of *gas pressure drop* ($\Delta P/Z$) (Figure 5), the *VSP*[®] rings exhibited the highest value of this parameter (223 Pa/m), while the lowest value of this parameter corresponded to *Hiflow*[®] rings, with 112 Pa/m. This variable depends on several factors, being the most important to consider (without taking into account the influence of the physical-chemical parameters of the fluids being handled) the *gas mixture* (Q_G) and *solvent* (m_L) *feed flowrates*, *mass-transfer surface area per unit volume of packing* (a); *packing porosity* (ε), F_p and D . In general, $\Delta P/Z$ will increase if a , m_L and D decreases and if ε , Q_G or F_p increases.

Finally, *VSP*[®] rings supplied the greater value of the *overall volumetric mass-transfer coefficient* (K_m) (Figure 6) corresponding to 0.326 kmol/m³.s, while the lowest value of this parameter belonged to *Top Pak*[®] rings (0.068 kmol/m³.s). The most influential variables on K_m are the hydraulic factor Ch and the mass-transfer factor C_v ; as well as Q_G , m_L , F_p , a , D and ε . In that case, the value of K_m will increase with an increment of Ch , C_v and a , as well as with a reduction of F_p , D and ε . On the other hand, an increment of Q_G and a reduction of m_L will decrease the value of K_m for the four packing types evaluated, according to the results showed in Figure 8 and Figure 9.

Regarding to the results showed in Figure 8, an increment of the Q_G (maintaining constant the value of m_L) will increase the value of D , $\Delta P/Z$ and Z , while K_m will decrease. On the other hand, an increment of the m_L (keeping constant the value of Q_G) will increase the values of D and K_m , while both $\Delta P/Z$ and Z decrease for the four packing types.

As for the results displayed in Figure 10, an increment of Q_G will increase both the *overall height of a gas-phase transfer unit* (H_{IOG}) and the *overall number of gas-phase transfer units* (N_{IOG}) for all the four packing types evaluated. In contrast, the Figure 11 showed the opposite pattern, that is, both the H_{IOG} and N_{IOG} decrease with an increment of the water feed flowrate. The results obtained in both figures mean that both the height of the apparatus required to accomplish the requested separation and the number of theoretical stages required to carry out the same separation in a plate-type apparatus will increase if Q_G increases (m_L constant), and will decrease if m_L increases (Q_G constant).

Analyzing and summarizing the results showed in Table 9, the *Pall* rings supplied the highest value of D (1.221 m), while *Hiflow*[®] rings provided the lowest value of $\Delta P/Z$ (112 Pa/m). On the other hand, *Top Pak*[®] rings presented the highest values of both H_{IOG} (0.671 m) and Z (2.60 m), as well as the lowest values of D (0.921 m), K_m (0.109 kmol/m³.s) and a_h (55.66 m⁻¹). Finally, *VSP*[®] rings had the highest values of $\Delta P/Z$ (223 Pa/m), K_m (0.326 kmol/m³.s) and a_h (169.57 m⁻¹), and the lowest values of both H_{IOG} (0.148 m) and Z (0.60 m). It should be noted that the value of D obtained for *VSP*[®] rings, which is the second highest value of D of all the packing types considered, is only 18.6 % higher than the lowest value of D obtained, corresponding to *Top Pak*[®] rings (0.921 m).

Considering the results obtained for the four packing types evaluated, it can be concluded that the most appropriate packing to use for this service or application is the *VSP*[®] rings, since it supply the most economic geometrical results and the highest mass-transfer conditions.

4. CONCLUSIONS

The *Pall*[®] rings provided the greatest value of tower diameter (D) [1.221 m]. The *Hiflow*[®] rings supplied the lowest value of the overall pressure drop ($\Delta P/Z$) [112 Pa/m].

The *Top Pak*[®] rings presented the lowest values of D [0.921 m], the volumetric gas-phase mass-transfer coefficient (K_{vG}) [0.116 kmol/m³.s], the volumetric liquid-phase mass-transfer coefficient (K_{vL}) [0.372 kmol/m³.s], the overall convective mass-transfer coefficient (K_m) [0.109 kmol/m³.s], and the effective specific surface area of packing (a_h) [55.66 m⁻¹]; as well as the greatest values of the overall height of a gas-phase transfer unit (H_{IOG}) [0.671 m] and packing height (Z) [2.60 m].

The VSP° rings presented the highest values of $\Delta P/Z$ [223 Pa/m], K_{vL} [1.172 kmol/m³.s], K_{vG} [0.349 kmol/m³.s], K_m [0.326 kmol/m³.s] and a_h [169.57 m⁻¹], as well as the lowest values of H_{iOG} [0.148 m] and Z [0.6 m].

An increment of the *gas mixture feed flowrate* (Q_G) (keeping constant m_L) increases the values of D , $\Delta P/Z$ and Z , while K_m decreases for the four packing types considered. An increment of the *solvent feed flowrate* (m_L) (maintaining constant Q_G) will increase the values of D and K_m , while both $\Delta P/Z$ and Z decreases for the four packing types evaluated. An increment of Q_G will increase the values of both the H_{iOG} and the *overall number of gas-phase transfer units* (N_{iOG}) for the four packing types.

Both the H_{iOG} and N_{iOG} decrease with an increment of m_L . The most adequate packing to use on this absorption system is the VSP° rings since it provided the highest mass-transfer conditions with the lowest column dimensions.

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