Calculation of a packed column for absorption of hydrogen sulfur from gases formed by separation of crude oil

A.B. Golovanchikov^{1*}, *V.I.Churikova*¹ and *O.A.Zalipaeva*¹

¹Volgograd State Technical University, 28 Lenin avenue, Volgograd, 400005, Russia

Abstract. According to the well-known calculating algorithm for the packed absorption column, the main technological parameters and geometric dimensions of the apparatus for hydrogen sulfide containing gases, formed during the separation of crude oil, are determined. A 2,5-n solution of monoethanolamine is selected as the absorbent. Comparative results of the calculations are showing, that the working pressure in the column should be 4 atm, since with their lower values, the flow rate of the absorbent and the size of the column are increasing. The increase in working pressure is impractical, since it will require a transition from centrifugal and compresses pumps to piston pumps. II The obtained parameters were compared for an absorption column in which the flow structure of the gas and liquid phases corresponds to ideal displacement, with the calculation results when the flow structure in the gas phase corresponds to the ideal displacement mode (as in the standard calculation algorithm) and in the liquid phase to ideal mixing. It is shown that, with the Peclet number of longitudinal diffusion $Pe < 40$ the height and volume of the column increases by 10 and more percent and should be taken into account when packed columns, intended for absorption processes, are designed. At $Pe = 30$ the height and volume of the nozzle in the column increases by 27%. Another feature of the modelling and calculation of devices is a spike in concentration, meaning, that the lower part of the working line will cross the equilibrium. Calculations in this particular case show that at ≈ 11 the working line crosses the equilibrium and theoretically column height and volume $\rightarrow \infty$.

1 Introduction

Since the 70s of the last century, in the calculations of mass transfer apparatuses starts the structure modelling of the gas (vapor) and liquid phases of the cell, diffusion and combined models, accounting local mixing, bypassing, convective and molecular diffusion zones, the

* Corresponding author: pahp@vstu.ru

formation of stagnant zones and modes, as well as other hydromechanical concentration and temperature gradient effects, leading to deviations of the gas, vapor, and liquid phases from both ideal displacement and ideal mixing [1-4]. The main emphasis in such modelling of the flow structure was made on the cell and combined models of sequential or parallel connection of ideal displacement and mixing links, described by simple differential equations for non-stationary conditions. For stationary modes, these differential equations are usually solved analytically. The situation is more complicated when the flow structure according to the diffusion model is described. Even the simplest one-parameter model of longitudinal diffusion under stationary conditions is described by a second-order non-uniform differential equation with special boundary conditions having an analytical solution of only the linear equilibrium equation [5]. An example of such analytical calculation for capturing benzene hydrocarbons is given in the monograph [6].

Goal of the work is to develop an algorithm for calculating a packed absorption column for the purification of crude oil gases from hydrogen sulfide, accounting the maximum diffusion.

2 Methods

Objectives of the research are: physical and mathematical modeling of the absorption process, taking into account the maximum mixing. Comparisons of a typical calculation of an absorption packed column with a small displacement flow structure with a developed calculation algorithm that takes into account the maximum diffusion in the annex to a specific process for the purification of crude oil gases from hydrogen sulfide.

Initial data and calculation algorithms

The initial data for the calculation of the packed column during the absorption of hydrogen sulfide from the gases, formed by separation of crude oil are presented in Table 1. Reference data related to the physical parameters of the gas and absorbent are also given in Table 1.

Table 1. Initial and reference data and calculated parameters for absorption from gases obtained after standard separation of crude oil, hydrogen sulfide.

№	Parameter Name	Dimension	Designation	Value
1	2	3	4	5
	<u>Initial data</u>			
1	Performance by initial gas	$\frac{kg}{hour}$	G_n	5000
2	Initial concentration of hydrogen sulfide (absolute. molar)	$\frac{кмольA}{кмольG}$	y_n	0.22
3	The final concentration of hydrogen sulfide (absolute. molar)	$\frac{кмольA}{кмольG}$	y_k	0.018
4	The initial concentration of hydrogen sulfide in the absorbent (aqueous solution of monoethanolamine)	$\frac{кмольA}{кмольL}$	x_n	0.01
	<u>Reference data</u>			
1	The average molecular weight of the gas	$\frac{кгG}{кмольG}$	M_g	24.5
2	The molecular weight of hydrogen sulfide	$\frac{кгA}{кмольA}$	M_a	34

№	Parameter Name	Dimension	Designation	Value
1	2	3	4	5
3	Molecular mass of absorbent (2.5 N solution of monoethanolamine in water)	$\frac{\kappa \Gamma L}{\kappa \text{моль} L}$	M_l	19
4	Henry's Law Constant	mmHg.	E	3760
5	Absorbent density	kg/m^3	ρ_l	1027
6	Absorbent viscosity	$Pa \cdot s$	μ_l	$1.43 \cdot 10^{-3}$
7	Gas viscosity	$Pa \cdot s$	μ_g	$1.56 \cdot 10^{-5}$
8	The working temperature of the gas in the packed column	$^{\circ}C$	t	25
9	Operating pressure	$atm.$	P	4
10	Specific surface area of the nozzle (Raschig rings)	m^2/m^3	σ	204
11	Porosity of the nozzle	m^3/m^3	$\mathcal{E}$	0.74
12	The outer diameter of the Raschig rings	m	d_n	0.05
	<u>Estimated parameters</u>			
1	Gas density at operating pressure and temperature	kg/m^3	ρ	3.88
2	Equivalent nozzle diameter	m	$d_{\text{э}}$	$1.45 \cdot 10^{-2}$
3	The initial relative mass concentration of H ₂ S in the absorbent after regeneration	$\frac{kgA}{kgL}$	x_n	$1.80 \cdot 10^{-2}$
4	The initial relative mass concentration H ₂ S in purified gas after regeneration	$\frac{kgA}{kgG}$	y_n	0.3914
5	Final working concentration in the absorbent	$\frac{kgA}{kgL}$	x_{κ}	0.313
6	Final working concentration in the purified gas	$\frac{kgA}{\kappa gG}$	y_{κ}	0.0254
7	Performance by absorbed hydrogen sulfide	$\frac{kgA}{\text{hour}}$	G_a	$1.315 \cdot 10^3$
8	Performance of the inert part of the cleaned gas	$\frac{kgG}{\text{hour}}$	G	$3.59 \cdot 10^3$
9	The minimum consumption of absorbent	$\frac{kgL}{\text{hour}}$	L_m	$3.71 \cdot 10^3$
10	Working consumption of absorbent	$\frac{kgL}{\text{hour}}$	L	$4.45 \cdot 10^3$
11	The equilibrium concentration in the absorbent of the extracted component. corresponding to its initial concentration in the gas	$\frac{kgA}{kgL}$	x_{κ}^*	0.375
12	The equilibrium constant for the working pressure of a given solution of monoethanolamine in water	$\frac{kgA / kgG}{kgA / kgL}$	κ	1.277
13	Performance by purified gas output from the column	$\frac{kgG}{\text{hour}}$	G_{κ}	3685
14	Coefficients of a linear equilibrium line $y = a + bx$ approximating the equilibrium dependence $y^* = y^*(x)$ by the least squares method	$\frac{kgA}{kgG}$	a b	$-2.13 \cdot 10^{-3}$ 1.038

№	Parameter Name	Dimension	Designation	Value
1	2	3	4	5
		$\frac{\text{kgA}}{\text{kgG}}$ $\frac{\text{kgA}}{\text{kgL}}$		
	<u>Parameters of a column calculated according to a standard algorithm with ideal displacement in both phases</u>			
1	Archimedes number for gas	-	Ar	$4.89 \cdot 10^8$
2	Number of gas transfer units	-	$\mathcal{Q}E\Pi_y$	12.63
3	Nozzle height equivalent to the transfer unit	m	h_l	0.523
4	Average driving force in a gas phase	$\frac{\text{kgA}}{\text{kgG}}$	Δy_c	0.029
5	The average concentration of H ₂ S in a gas	$\frac{\text{kgA}}{\text{kgG}}$	y_s	0.208
6	The average equilibrium concentration of H ₂ S in a gas	$\frac{\text{kgA}}{\text{kgG}}$	y_s^*	0.1794
7	The average working concentration of H ₂ S in the absorbent	$\frac{\text{kgA}}{\text{kgL}}$	x_s	0.476
8	Fictitious gas velocity in the column	m/s	v_y	1.02
9	Design column diameter	m	D_κ	0.623
10	The total height of the nozzle in the column	m	H_θ	6.60
11	Nozzle surface area	m ²	F_H	410.8
12	Gas mass transfer coefficient	$\frac{\text{kgA}}{\text{c} \cdot \text{m}^2 \frac{\text{kgA}}{\text{kgG}}}$	κ_y	0.0307
13	Column nozzle volume	m ³	V_κ	2.01
14	The coefficient of excess absorbent compared with its minimum consumption	-	κ_{aa}	1.2
15	Volumetric gas flow through the column at operating pressure and temperature	m ³ /s	q_v	0.311
16	Reynolds number for gas	-	Re_y	3680
17	Mass transfer coefficient for the liquid phase - absorbent	$\frac{\text{kgA}}{\text{c} \cdot \text{m}^2 \frac{\text{kgA}}{\text{kgL}}}$	κ_x	0.0392
18	The average residence time of the absorbent in the nozzle column ideal displacement	s	τ_θ	1671.7
19	The equilibrium concentration in the absorbent of the extracted component. corresponding to its initial concentration in the gas	$\frac{\text{kgA}}{\text{kgL}}$	x^*	0.0256
	<u>The parameters of the column. calculated with taking into account the diffusion structure of the flow in the liquid phase</u>			

№	Parameter Name	Dimension	Designation	Value
1	2	3	4	5
1	Fictitious speed of absorbent	m/s	v_l	$3.95 \cdot 10^{-3}$
2	Reynolds number in the liquid phase - absorbent	-	Re_l	41.19
3	Preset nozzle height in the column. taking into account longitudinal diffusion	m	H_3	10.7
4	The calculated values of the criterion Pe longitudinal diffusion in the liquid phase	-	Pe	22.14
5	Estimated nozzle height in the column. taking into account longitudinal diffusion	m	H_0	10.72
6	The input concentration of the recoverable component in the absorbent	$\frac{\text{kgA}}{\text{kgL}}$	x_0	0.02205
7	The concentration of dimensionless gradient on the input	$\frac{\text{kgA}}{\text{kgL}}$	g_0	0.0863
8	The calculated value of the initial concentration at the input	$\frac{\text{kgA}}{\text{kgL}}$	x_m	0.01815
9	The average residence time of the absorbent in the column	s	τ_d	2712.7
10	The coefficient of increase in the height of the nozzle taking into account longitudinal diffusion compared with the typical calculation of the column (excluding longitudinal diffusion. when $Pe \rightarrow \infty$.)	-	κ_H	1.62

The first part of the calculations was carried out according to the standard algorithm described in monographs and educational literature. when the flow structure of both phases corresponds to ideal displacement [3.5.7-9]. The second part of the calculations was performed taking into account longitudinal diffusion [10-12] by the numerical method according to the working line formula

$$y = y_k + (\ell / G)(x - x_n) - (\ell / G) \frac{dx}{dh} / Pe \quad (1)$$

and the mass transfer equation

$$\frac{\ell}{Pe} \frac{d^2 x}{dh^2} = \frac{dx}{dh} + \frac{k_x \sigma \tau_d}{Pe} (x^* - x) \quad (2)$$

where $Pe = \frac{v_d H_d}{D_\ell}$ и D_ℓ - longitudinal diffusion coefficient

The boundary conditions of the diffusion model:

$$x_n = x_0 - \left(\frac{dx}{dh} \right)_0 / Pe \quad ; \quad h=0. \quad (3)$$

$$h=1. \frac{dx}{dh}=0 \tag{4}$$

The Peclet number was calculated according to the formula given in the manual [6]

$$Pe=7,58\cdot10^{-3}Re_{\text{ж}}^{0,703}\frac{h_d}{d_h} \tag{5}$$

A feature of the algorithm for calculating the parameters of the packed absorption column. taking into account longitudinal diffusion according to formulas (1) - (5). is the following:

1. Set by nozzle height $H_d > h_b$
2. By the formula (3). the number Pe corresponding to this height is found.
3. When the number Pe is obtained by the numerical method according to formulas (1) and (2). taking into account the boundary conditions (3.4). gradually. increasing the average residence time in the column. $\tau_d > \tau_b$. the boundary condition (3) is fulfilled with a given accuracy (3).
4. For the found value of τ_d the height of the nozzle is determined by the formula

$$H_d=\tau_d\cdot v_l$$

5. Clarify H3 according to paragraph 2 until $H \approx H_3$ with a given accuracy.

3 Results and Discussion

The calculation results are shown in the lower part of table 1.

As can be seen from the materials in this table. for the calculated packed column. the Peclet number of longitudinal diffusion in the liquid phase $Pe=22.14$. while the height of the nozzle in the column. its volume and the average absorbent residence time should be increased by 62%. The spike in the concentration of the extracted component at its entrance to the column increases this concentration from $x_H=1.8\cdot10^{-2}kg\ A/kg\ L$ to $x_0=2.205\cdot10^{-22}kg\ A/kg\ L$

Graphs of equilibrium and working lines are shown in Figure 1.

Fig. 1. Graphs of the dependencies of the equilibrium (1) and working lines of the absorption process in the packed column ($t=25^{\circ}$. $P= 4\text{ atm.}$) for removal of H_2S from crude oil gases: line 2 - typical absorption process. an ideal liquid phase displacement ($Pe\rightarrow \infty$. $DI \rightarrow 0$) line 3 - taking into account a longitudinal mixing at $Pe=22.14$.

It can be seen from these graphs, longitudinal diffusion, firstly, reduces local driving forces (working line 3 is placed lower than working line 2 for the typical structure of the ideal displacement flow), and secondly, it is no longer straight, but concave towards the equilibrium line, this is reducing the number of transfer units and the average driving force, which resulting in the need to increase the surface of the nozzle at the expense of its height.

The concentration profiles of the extracted component by the relative height of the nozzle are shown on Figure 2.

It is necessary to pay attention to one feature related to the calculation of absorption columns according to the diffusion model, namely, for some practical number Pe^* the concentration x_e due to a spike at the input of x_n becomes equal to the equilibrium concentration x_n^* . For clarity, it is shown on Figure 3.

Fig. 2. Profiles and concentrations of the extracted component - hydrogen sulfide by dimensionless nozzle height at $Pe=22.14$: line 1 - in absorbent, line 2 - in the gas phase

Fig. 3. Dependence of the input concentration of the extracted component in the absorbent (1) and the coefficient of increase in nozzle height (2) of the Pe number of longitudinal diffusion

On the right, it is shown how the height of the nozzle in the column increases with the number Pe . Already at $Pe^*=11.7$ p the working line crosses the equilibrium line at the

entrance of the absorbent to the column. and the nozzle height. theoretically $H_d \rightarrow \infty$. In this case. it is necessary either to increase the working pressure in order to move the equilibrium concentration x_n^* to the right. or either to decrease the residual concentration x_n after desorption. before the adsorbent is entered into the column.

4 Summary

Therefore. accounting the longitudinal diffusion in the packed column with predetermined performance and initial concentrations of hydrogen sulfide in the oil gases. operating at a pressure of 4 atm. and a temperature of 25°. requires an increase in height from 6.6 m to 10.72 m with a column diameter of 623 mm and an absorbent consumption of a 2.5-n aqueous solution of monoethanolamine.

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