PERIODIC SOLUTION FOR NATURAL GAS DEHYDRATION USING SOLID DESICCANTS

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Abstract: Dehydration of natural gas is of extreme importance to avoid the formation of hydrates and other associated problems. Different dehydration methods exist; however the solid desiccant approach can dehydrate natural gas to levels of water vapor lower than other methods. This paper presents a simple formulation for simulating the dehydration of a wet methane stream flowing though a porous medium composed of hygroscopic particles. The model assumes small resistance to diffusion within particles and takes heat and mass transfer rates into account by employing constant transfer coefficients. The formulation was developed based in the traditional mass and energy conservation principles, considering a one-dimensional transient scenario. A dimensional analysis is also performed and relevant dimensionless groups are introduced. The set of dimensionless parameters are similar to effectiveness-NTU groupings, widely used in heat exchangers. The proposed formulation, despite its simplicity, represents a new contribution, since a similar analysis is apparently unavailable in the gas dehydration literature. Finally, in order to illustrate the effect of varying the dimensionless groups, the formulation is solved using a combined finite-volumes/method-of-lines approach. The results example how the dimensionless parameters can influence the dehydration process.

Keywords: Natural Gas, Methane, Adsorption, Dehydration, Desiccant, Sorbent, Gas Purification, Dimensional Analysis, Computational Simulation.

1. NOMENCLATURE

$\mathcal{A}$	area	**Subscripts**	
c_p	constant pressure specific heat	adv	advective
h_h	convective heat transfer coefficient	b	bed
h_m	convective mass transfer coefficient	δ	closed pore
i	specific enthalpy	e	effective or apparent
$\boldsymbol{j''}$	mass flux	g	natural gas
L	cylinder height	in	inlet
m	mass	i	inter-particle voids
$\dot{m}$	mass flow rate	l	adsorbed water (liquid phase)
t	time	max	maximum
T	temperature	min	minimum
v_i	inter-particles velocity	op	operation
v_b	bulk velocity	out	exit
x	distance from the cylinder entrance	p	particle
W	dry basis adsorbed water concentration	π	pore
Y	dry basis vapor concentration	s	solid phase
Greek Symbols		v	water vapor
ρ	specific mass or concentration	**Superscripts**	
ϵ	total porosity	$*$	dimensionless quantity
τ	periodical time	$\sim$	dry basis

2. INTRODUCTION

The increasing demand for oil and gas for power generation makes the oil industry continuously searching for new and larger reserves. In recent years, this goal is being achieved in places that present extra difficulties for production, e.g. in undersea fields located in deep water or ultra-deep water. Analyzing the present natural gas productive chain development scenario, one can identify a tendency to expand the employment of natural gas and associated products. For commercializing, natural gas undergoes through specific processing for dehydration and fractionation, resulting in three products: raw natural gas (methane and ethane), liquefied petroleum gas (propane and butane) and natural gasoline (pentane and heavier hydrocarbons). At this stage, the gas must already meet strict specification standards and be substantially free of contaminants, so as to avoid environmental problems and damage to equipment that will use it as fuel or raw material. From the standpoint of treatment (processing) and conditioning of natural gas, it should be brought to water levels established by rules to prevent the formation and deposition of solid hydrates that may, in the long run, reduce the useful diameter of the transmission line. These unwanted compounds can block, partly or wholly, lines, valves and equipments. To prevent hydrate formation, different techniques may be used. Among them, there are processes more widespread such as the dehydration using liquid and solid desiccant, the last being used in this study. The work of Gandhidasan, Al-Farayedhi et al. (2000) performs a study on the use of solid desiccants based on silica gel, in which the effects of changes in various parameters on the process were analyzed. Moreover, a study was developed to estimate the energy required in the regeneration process. In the study presented by Cavenati, Grande et al. (2006b), a process of removing carbon dioxide and nitrogen gas through low and moderate flows is discussed, using different goals for each type of material. This study analyzes the removal of two contaminants in natural gas in a single-cycle. Different flow directions, temperatures and adsorbent layers were analyzed as variable parameters. The work done by Kikkinides, Sikavitsas et al. (1995) presents a study of the feasibility of H_2S removal from natural gas by adsorption via pressure variation, reaching appropriate levels of concentration contaminants. The study by Cavenati, Grande et al. (2006a) uses a process of vacuum pressure swing adsorption for removal of carbon dioxide in a contaminated stream of natural gas to achieve adequate levels. The adsorbent used was zeolite 13X. A notable feature of previous works on desiccant dehydration of natural gas is that, apparently, there is little development compared to other methods of dehydration. In this context, this work presents a mathematical formulation for heat and mass transfer for desiccant dehydration of natural gas. The formulation herein presented is based on normalized dimensionless groups used in studies like those developed for heat exchangers and mass (Sphaier and Worek, 2009) and for storage of adsorbed natural gas (da Silva and Sphaier, 2010).

3. PROBLEM FORMULATION

In this section, the main formulations for the dehydration of natural gas using solid adsorbents are presented. The reservoir has only one entrance and one exit for the natural gas flow. Initially, the reservoir is empty and the pressure and temperature are equal to the surroundings. Then, as the natural gas flows into the reservoir with higher levels of water vapor the process of dehumidification begins.

3.1 Simplifying Assumptions

Earlier in the development to solve the presented problem, below are cited some assumptions used in this work such as: dilute vapor concentration in gas phase (moist gas); velocities are unaffected by variations in concentration; unidirectional flow; negligible pressure drop or loss; micro-pore diffusion is fast such that this resistance is negligible; constant specific heats; radiation effects are negligible due to the relatively low temperature differences; there is no chemical reaction nor any internal energy
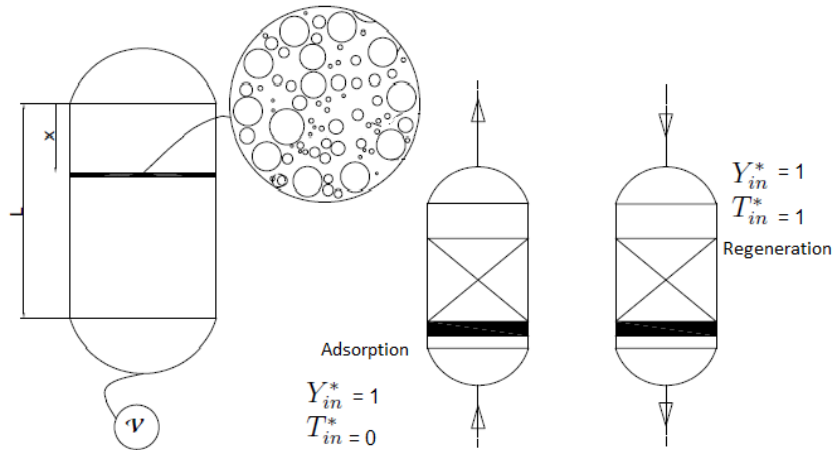
Figure 1. Volume, Porous Area View and Twin Towers Configuration.

generation of any form; the influence of body forces (such as gravity) is negligible; the pores can be modeled as cylindrical and the porosity is homogeneous; isotropic medium; the inlet fluid properties as well as the flow rate is uniform; reversible adsorption; ideal gas mixture; no phase change besides that resulting from adsorption; no heat losses to the environment and flow occurs in inter-particle voids, while diffusion may occur within particles.

3.2 Mass Balance

Since the mass of the solid portion and that of the natural gas are assumed invariable only a mass balance for water is required. Denoting $\mathcal{V}$ as a portion of the vessel (that includes all volumes) volume and $\mathcal{S}$ as its bounding surface, an integral mass balance (also termed a "weak" formulation) is written as:

$$\frac{d}{dt} \int_{x_0}^{x_1} \left(\epsilon_b \, \rho_{v,i} + (1 - \epsilon_b) \, \epsilon_p \, \rho_{v,\pi} + \rho_l \right) \mathcal{A}_x \, dx = - \left(\boldsymbol{j}''_{v,i} \cdot \hat{\boldsymbol{n}} \, \mathcal{A}_x \right)_{x=x_1} + \left(\boldsymbol{j}''_{v,i} \cdot \hat{\boldsymbol{n}} \, \mathcal{A}_x \right)_{x=x_0} \quad (1)$$

where:

$$\boldsymbol{j}''_{v,i} = \rho_{v,i} \, \boldsymbol{v}_b = \epsilon_b \, \rho_{v,i} \, \boldsymbol{v}_i = \rho_g \, Y \, \boldsymbol{v}_b \quad (2)$$

Finally, simplification yields:

$$\epsilon_b \frac{\partial Y}{\partial t} + (1 - \epsilon_b) \, \epsilon_p \frac{\partial Y_p}{\partial t} + \frac{\rho_b}{\rho_g} \frac{\partial W}{\partial t} + v_b \frac{\partial Y}{\partial x} = 0 \quad (3)$$

A general mass balance for the particles volume is given by:

$$\frac{d}{dt} \int_{x_0}^{x_1} \left(\rho_l + (1 - \epsilon_b) \, \epsilon_p \, \rho_{v,\pi} \right) \mathcal{A}_x \, dx = \int_{x_0}^{x_1} h_m \, \rho_g \, (Y - Y_p) \, S \, \mathcal{A}_x \, dx \quad (4)$$

in which:

$$S = \frac{\mathcal{A}_s}{\mathcal{V}} = \frac{1}{\mathcal{A}_x} \frac{d\mathcal{A}_s}{dx} \quad (5)$$

After simplifications, one can conclude that:

$$\frac{\rho_b}{\rho_g} \frac{\partial W}{\partial t} + (1 - \epsilon_b) \, \epsilon_p \frac{\partial Y_p}{\partial t} = h_m \, S \, (Y - Y_p) \quad (6)$$

Subtracting equation (6) from (3) yields a mass balance for the interparticle voids:

$$\epsilon_b \frac{\partial Y}{\partial t} + v_b \frac{\partial Y}{\partial x} = -h_m \, S \, (Y - Y_p) \quad (7)$$

3.3 Energy Balance

Since pressure variations are assumed negligible, the following relations apply:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{x_0}^{x_1} \left(\epsilon_b\, \rho_g \left(i_g + i_{v,i}\, Y \right) + (1 - \epsilon_b)\, \epsilon_p\, \rho_g \left(i_g + i_{v,\pi}\, Y_p \right) + i_l\, \rho_b\, W + i_s\, \rho_b \right) \mathcal{A}_x\, \mathrm{d}x =$$

$$= - \left(\rho_g \left(i_{v,i}\, Y + i_g \right) \left(\boldsymbol{v}_b \cdot \hat{\boldsymbol{n}} \right) \mathcal{A}_x \right)_{x=x_1} + \left(\rho_g \left(i_{v,i}\, Y + i_g \right) \left(\boldsymbol{v}_b \cdot \hat{\boldsymbol{n}} \right) \mathcal{A}_x \right)_{x=x_0} \quad (8)$$

Finally, simplification yields:

$$\epsilon_b\, \frac{\partial}{\partial t} \left(i_g + i_{v,i}\, Y \right) + (1 - \epsilon_b)\, \epsilon_p\, \frac{\partial}{\partial t} \left(i_g + i_{v,\pi}\, Y_p \right) + \frac{\rho_b}{\rho_g}\, \frac{\partial}{\partial t} \left(i_l\, W \right) + \frac{\rho_b}{\rho_g}\, \frac{\partial i_s}{\partial t} +$$

$$+ v_b\, \frac{\partial}{\partial x} \left(i_{v,i}\, Y + i_g \right) = 0 \quad (9)$$

The energy balance for the particles is more simple, because there is only vapor diffusion and it is given by:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{x_0}^{x_1} \left((1 - \epsilon_b)\epsilon_p \left(i_g\, \rho_g + i_{v,\pi}\, \rho_{v,\pi} \right) + i_l\, \rho_l + i_s\, \rho_b \right) \mathcal{A}_x\, \mathrm{d}x =$$

$$= \int_{x_0}^{x_1} \left(i_{v,f}\, h_m\, \rho_g \left(Y - Y_p \right) + h_h \left(T - T_p \right) \right) S\, \mathcal{A}_x\, \mathrm{d}x \quad (10)$$

Finally, simplification yields:

$$(1 - \epsilon_b)\epsilon_p\, \frac{\partial}{\partial t} \left(i_g + i_{v,\pi}\, Y_p \right) + \frac{\rho_b}{\rho_g}\, \frac{\partial}{\partial t} \left(i_l\, W \right) + \frac{\rho_b}{\rho_g}\, \frac{\partial i_s}{\partial t} =$$

$$= \left(i_{v,f}\, h_m \left(Y - Y_p \right) + \frac{h_h}{\rho_g} \left(T - T_p \right) \right) S \quad (11)$$

Subtracting equation (11) from (9) yields a energy balance for the interparticle voids:

$$\epsilon_b\, \frac{\partial}{\partial t} \left(i_g + i_{v,i}\, Y \right) + v_b\, \frac{\partial}{\partial x} \left(i_g + i_{v,i}\, Y \right) = - \left(i_{v,f}\, h_m \left(Y - Y_p \right) + \frac{h_h}{\rho_g} \left(T - T_p \right) \right) S \quad (12)$$

3.4 Simplified Energy Balances in Terms of Temperatures

Expanding equations (11) and (12), using and multiplying the mass conservation equations (6) and (7) by $i_{v,\pi}$ and $i_{v,i}$, for particles and inter particles equations, respectively, yields:

$$(1 - \epsilon_b)\epsilon_p \left(\frac{\partial i_g}{\partial t} + Y_p\, \frac{\partial i_{v,\pi}}{\partial t} \right) + \frac{\rho_b}{\rho_g} \left(W\, \frac{\partial i_l}{\partial t} + \left(i_l - i_{v,\pi} \right) \frac{\partial W}{\partial t} + \frac{\partial i_s}{\partial t} \right) =$$

$$= \left(\left(i_{v,f} - i_{v,\pi} \right) h_m \left(Y - Y_p \right) + \frac{h_h}{\rho_g} \left(T - T_p \right) \right) S \quad (13)$$

$$\epsilon_b \left(\frac{\partial i_g}{\partial t} + Y\, \frac{\partial i_{v,i}}{\partial t} \right) + v_b \left(\frac{\partial i_g}{\partial x} + Y\, \frac{\partial i_{v,i}}{\partial x} \right) =$$

$$= - \left(\left(i_{v,f} - i_{v,i} \right) h_m \left(Y - Y_p \right) + \frac{h_h}{\rho_g} \left(T - T_p \right) \right) S \quad (14)$$

Using the definitions of specific heats for perfect gases and incompressible substances:

$$(1 - \epsilon_b)\epsilon_p \left(c_{p_g} + Y_p \, c_{p_v} \right) \frac{\partial T_p}{\partial t} + \frac{\rho_b}{\rho_g} \left(W \, c_l + c_s \right) \frac{\partial T_p}{\partial t} + \frac{\rho_b}{\rho_g} \left(i_l - i_{v,\pi} \right) \frac{\partial W}{\partial t} = $$

$$= \left((i_{v,f} - i_{v,\pi}) \, h_m \, (Y - Y_p) + \frac{h_h}{\rho_g} \, (T - T_p) \right) S \quad (15)$$

$$\left(c_{p_g} + Y \, c_{p_v} \right) \left(\epsilon_b \frac{\partial T}{\partial t} + v_b \frac{\partial T}{\partial x} \right) = - \left((i_{v,f} - i_{v,i}) \, h_m \, (Y - Y_p) + \frac{h_h}{\rho_g} \, (T - T_p) \right) S \quad (16)$$

Defining dry-basis specific heats:

$$\rho_g \, \tilde{c} = \rho_g \left(c_{p_g} + Y \, c_{p_v} \right) \quad (17)$$

$$\rho_e \, \tilde{c}_e = \rho_b \left(c_s + c_l \, W \right) + \rho_g \left(c_{p_g} + Y_p \, c_{p_v} \right) (1 - \epsilon_b) \, \epsilon_p \quad (18)$$

and substituting in equations (15) and (16):

$$\frac{\rho_e}{\rho_g} \, \tilde{c}_e \frac{\partial T_p}{\partial t} + \frac{\rho_b}{\rho_g} \left(i_l - i_{v,\pi} \right) \frac{\partial W}{\partial t} = \left((i_{v,f} - i_{v,\pi}) \, h_m \, (Y - Y_p) + \frac{h_h}{\rho_g} \, (T - T_p) \right) S \quad (19)$$

$$\tilde{c} \left(\epsilon_b \frac{\partial T}{\partial t} + v_b \frac{\partial T}{\partial x} \right) = - \left((i_{v,f} - i_{v,i}) \, h_m \, (Y - Y_p) + \frac{h_h}{\rho_g} \, (T - T_p) \right) S \quad (20)$$

where ρ_e is an effective or apparent density defined as:

$$\rho_e = \rho_b + (1 + \epsilon_b) \, \epsilon_p \, \rho_g \quad (21)$$

Introducing the heats of sorption:

$$i^p_{sor} = i_{v,\pi} - i_l, \qquad i^i_{sor} = i_{v,i} - i_{v,\pi}, \qquad i_{sor} = i^p_{sor} + i^i_{sor} = i_{v,i} - i_l \quad (22)$$

and, substituting in equations (19) and (20):

$$\frac{\rho_e}{\rho_g} \, \tilde{c}_e \frac{\partial T_p}{\partial t} = \left(\varphi \, i^i_{sor} \, h_m \, (Y - Y_p) + \frac{h_h}{\rho_g} \, (T - T_p) \right) S + \frac{\rho_b}{\rho_g} \, i^p_{sor} \frac{\partial W}{\partial t} \quad (23)$$

$$\tilde{c} \left(\epsilon_b \frac{\partial T}{\partial t} + v_b \frac{\partial T}{\partial x} \right) = \left((1 - \varphi) \, i^i_{sor} \, h_m \, (Y - Y_p) - \frac{h_h}{\rho_g} \, (T - T_p) \right) S \quad (24)$$

where φ is the fraction of i^i_{sor} that contributes directly to heating (or cooling) the interparticle voids; conversely, $1 - \varphi$ is the fraction of i^i_{sor} that contributes directly to heating (or cooling) the adsorbent particles. In other words:

$$\varphi = \frac{i_{v,f} - i_{v,\pi}}{i_{v,i} - i_{v,\pi}}, \qquad 1 - \varphi = \frac{i_{v,i} - i_{v,f}}{i_{v,i} - i_{v,\pi}}. \quad (25)$$

Note that adding equations (23) and (24) gives:

$$\frac{\rho_e}{\rho_g} \, \tilde{c}_e \frac{\partial T_p}{\partial t} + \tilde{c} \left(\epsilon_b \frac{\partial T}{\partial t} + v_b \frac{\partial T}{\partial x} \right) = i^i_{sor} \, h_m \, (Y - Y_p) \, S + \frac{\rho_b}{\rho_g} \, i^p_{sor} \frac{\partial W}{\partial t} \quad (26)$$

which shows that the total heating (or cooling) effect can be subdivided into a sensible part (containing i^i_{sor}) and a latent part (containing i^p_{sor}). This analysis becomes even clearer if the mass balance for the particles (equation (6)) is used to substitute the convective mass flux

$$\frac{\rho_e}{\rho_g} \, \tilde{c}_e \frac{\partial T_p}{\partial t} + \tilde{c} \left(\epsilon_b \frac{\partial T}{\partial t} + v_b \frac{\partial T}{\partial x} \right) = i^i_{sor} \left(\frac{\rho_b}{\rho_g} \frac{\partial W}{\partial t} + (1 - \epsilon_b) \, \epsilon_p \frac{\partial Y_p}{\partial t} \right) + \frac{\rho_b}{\rho_g} \, i^p_{sor} \frac{\partial W}{\partial t} \quad (27)$$

3.5 Removed Water

There are two ways to calculate the amount of mass removed from natural gas, one by the amount of adsorbed water retained in the solid adsorbent (adsorbent on the first operation or after regeneration), and the other by using the water concentration in the natural gas at the inlet and exit of the dehydration process. Based on what was described above, the expression for the removed water amount is obtained by multiplying the difference of concentrations at the exit and inlet of the reservoir by the density of the dry gas, by the gas flow rate and integrating within the operating period:

$$m_l = \int_0^\tau \dot{m}_g \left(Y_{in} - Y_{out} \right) \mathrm{d}t \tag{28}$$

4. NORMALIZATION

4.1 Dimensionless groups

The first dimensionless groups are the dimensionless dependent and independent variables involved in the studied problem:

$$T_p^* = \frac{(T_p - T_{ref})}{(T_{min} - T_{max})}, \qquad T^* = \frac{(T - T_{ref})}{(T_{min} - T_{max})} \tag{29}$$

$$Y_p^* = \frac{(Y_p - Y_{ref})}{(Y_{min} - Y_{max})}, \qquad Y^* = \frac{(Y - Y_{ref})}{(Y_{min} - Y_{max})}, \qquad W^* = \frac{W}{W_{\max}} \tag{30}$$

$$t^* = \frac{t}{\tau}, \qquad x^* = \frac{x}{L}, \qquad m_l^* = \frac{m_l}{\rho_b \, W_{\max} \, \mathcal{V}} \tag{31}$$

The next groups are the dimensionless parameters, such as the dimensionless dwell time (residence period), volumetric and heat capacities ratios, dimensionless numbers of transfer units, dimensionless concentration of water in the adsorbent, dimensionless heat of adsorption and heat capacity ratios, expressed respectively as:

$$\tau_{res} = \frac{L}{v_b} \, \epsilon_b, \qquad \tau_{res}^* = \frac{\tau_{res}}{\tau}, \qquad \mathrm{V}_r = \frac{\mathcal{V}}{\tau}, \qquad \mathrm{V} = v_b \, \mathcal{A}_x \tag{32}$$

$$\mathrm{C}_r = \frac{c_b \, \rho_b \, L \, A_x}{\tau}, \qquad \mathrm{C} = \rho_g \, v_b \, A_x \, c_{p_g}, \qquad \mathrm{V}_r^* = \frac{\mathrm{V}_r}{\mathrm{V}}, \qquad \mathrm{C}_r^* = \frac{\mathrm{C}_r}{\mathrm{C}} \tag{33}$$

$$\mathcal{X}_i = \frac{\tilde{c}}{c_{p_g}}, \qquad \mathcal{X}_p = \frac{\rho_e \, \tilde{c}_e}{\rho_b \, c_b}, \qquad \mathrm{N}_{tu}^h = \frac{h_h \, \mathcal{A}_s}{\mathrm{C}}, \qquad \mathrm{N}_{tu}^m = \frac{h_m \, \mathcal{A}_s}{\mathrm{V}} \tag{34}$$

$$\Omega = \frac{\rho_b}{\rho_g} \frac{W_{\max}}{\Delta Y}, \qquad i_{sor}^{p*} = i_{sor}^p \frac{\rho_g \, \Delta Y}{\rho_b \, c_b \, \Delta T}, \qquad i_{sor}^{i*} = i_{sor}^i \frac{\rho_g \, \Delta Y}{\rho_b \, c_b \, \Delta T} \tag{35}$$

These dimensionless groups are similar to those recently developed in (Sphaier and Worek, 2009) for heat and mass exchangers with adsorbent materials.

4.2 Dimensionless governing equations

For the mass balance of the particles, the dimensionless equations yields:

$$\Omega \, \mathrm{V}_r^* \frac{\partial W^*}{\partial t^*} + (1 - \epsilon_b) \, \epsilon_p \, \mathrm{V}_r^* \frac{\partial Y_p^*}{\partial t^*} = \mathrm{N}_{tu}^m \left(Y^* - Y_p^* \right) \tag{36}$$

For the mass balance of the interparticle voids, the dimensionless equations yields:

$$\tau_{res}^* \frac{\partial Y^*}{\partial t^*} + \frac{\partial Y^*}{\partial x^*} = \mathrm{N}_{tu}^m (Y_p^* - Y^*) \tag{37}$$

For the energy balance for the particles, the dimensionless equations yields:

$$\chi_p \frac{\partial T_p^*}{\partial t^*} = \varphi \frac{\mathrm{N}_{tu}^m}{\mathrm{V}_r^*} i_{sor}^{i*} (Y^* - Y_p^*) + \frac{\mathrm{N}_{tu}^h}{\mathrm{C}_r^*} (T^* - T_p^*) + \Omega\, i_{sor}^{p*} \frac{\partial W^*}{\partial t^*} \tag{38}$$

For the energy balance of the interparticle voids, the dimensionless equations yields:

$$\chi_i \left(\tau_{res}^* \frac{\partial T^*}{\partial t^*} + \frac{\partial T^*}{\partial x^*} \right) = (\varphi - 1)\, \mathrm{N}_{tu}^m \frac{\mathrm{C}_r^*}{\mathrm{V}_r^*} i_{sor}^{i*} (Y_p^* - Y^*) + \mathrm{N}_{tu}^h (T_p^* - T^*) \tag{39}$$

The dimensionless removed water is the given by:

$$m_l^* = \frac{1}{\Omega\, \mathrm{V}_r^*} \int_0^1 (Y_{in}^* - Y_{out}^*)\, \mathrm{d}t^* \tag{40}$$

5. RESULTS AND DISCUSSION

To solve the problem presented, we used the Finite Volume Method (Patankar, 1980) with a uniformly spaced mesh following the methodology presented in Sphaier and Worek (2009), and the entire implementation was done in the *Mathematica* system (Wolfram, 2003). To express the relationship between the quantity adsorbed W, humidity and temperature of gas in equilibrium with this phase, we used the following adsorption isotherm:

$$\phi = \phi(T, Y) = \frac{Y}{r_M^{v,g} + Y} \frac{P_{op}}{P_{vs}\, T}, \tag{41}$$

where ϕ is the relative humidity of natural gas, presented in references (Basmadjian, 1997) and (ASHRAE, 1985).

The density of the gas was calculated assuming pure methane gas with ideal gas behavior. Table 1 presents the numerical data used in the simulations, all of which were taken from (Kohl and Riesenfeld, 1980; Çengel and Boles, 1985; Wylen, Borgnakke et al., 2003). The dimensionless inlet values, Y_{in}^* and T_{in}^*, can assume different values for each process. For the adsorption processes, the inlet condition describes that the fluid is totally saturated with water and the temperature is the minimum temperature. For the regeneration process, the absolute humidity of the gas is the same as the adsorption process inlet, however the temperature is the maximum allowed. Several cases and variable parameters were studied, however the removed water amount is of extreme importance for the petroleum and natural gas industry and for this reason it is presented in this work.

The different test-cases analyze consists of using different combinations of the dimensionless parameters. These can be summarized as:

- Case 1: $\mathrm{N}_{tu}^m = \mathrm{N}_{tu}^h = 3$, $r = 1$, $\mathrm{V}_r^* = 10^{-5}$.

- Case 2: $\mathrm{N}_{tu}^m = \mathrm{N}_{tu}^h = 3$, $r = 1/10$, $\mathrm{V}_r^* = 10^{-5}$.

- Case 3: $\mathrm{N}_{tu}^m = \mathrm{N}_{tu}^h = 3$, $r = 10$, $\mathrm{V}_r^* = 10^{-5}$.

- Case 4: $\mathrm{N}_{tu}^m = \mathrm{N}_{tu}^h = 6$, $r = 1$, $\mathrm{V}_r^* = 10^{-5}$.

- Case 5: $\mathrm{N}_{tu}^m = \mathrm{N}_{tu}^h = 12$, $r = 1$, $\mathrm{V}_r^* = 10^{-5}$.

- Case 6: $N_{tu}^m = N_{tu}^h = 3, r = 1, V_r^* = 10^{-3}$.

- Case 7: $N_{tu}^m = N_{tu}^h = 3, r = 1, V_r^* = 10^{-4}$.

Figure 2 presents the variation of the dimensionless removed water with the isotherm parameter r (the separation factor. As can be seen, the lower values of the separation factor leads to better water removal. Desiccants allowed to work with this behavior should then be better choices for the application on dehydration.
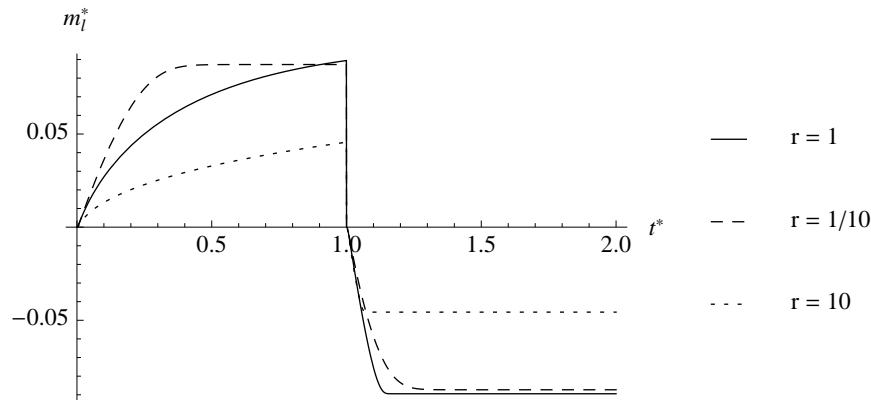

Figure 2. Study of Removed Water Amount Behavior - Separation Factor Variation r.

Table 1. Values Used in the Numerical Solution

Parameters	Symbols	Values
Maximum Temperature (K)	$T_{\max}$	400
Minimum Temperature (K)	$T_{\min}$	300
Specific Mass of Methane (kg/m^3)	ρ_g	0.5936
Specific Heat of Methane (J/kg·K)	c_{p_g}	2253.7
Specific Heat of Adsorbent (J/kg·K)	c_b, c_s	921
Specific Heat of Liquid Water (J/kg·K)	c_l	4180
Specific Heat of Water Vapor (J/kg·K)	c_{p_v}	1872.3
Maximum Concentration of Water on Adsorbent (kg H$_2$O/kg adsorbent)	$W_{\max}$	0.45
Molecular Mass of Methane (kg/kmol)	M_g	16.043
Molecular Mass of Water (kg/kmol)	M_v	18.015
Methane Gas Constant (J/kg·K)	R_g	518.35
Particle Porosity	ϵ_p	0.366
Bed Porosity	ϵ_b	0.3
Maximum Concentration of Vapor (kg vapor/kg methane)	$Y_{\max}$	32.096
Minimum Concentration of Vapor (kg vapor/kg methane)	$Y_{\min}$	10^{-6}
Adsorption Heat (J/kg H$_2$O)	i_{sor}	2.7×10^6
Heat Capacity Ratios	C_r^*	570 V_r^*
Dimensionless Period of Residence	τ_{res}^*	0.3 V_r^*
Dimensionless Concentration of Water in Adsorbent	Ω	19557
Dimensionless Heat of Adsorption	i_{sor}^{i*}	0
Inlet Initial Dimensionless Concentration (Adsorption)	Y_{in}^*	1
Inlet Initial Dimensionless Temperature (Adsorption)	T_{in}^*	0
Inlet Initial Dimensionless Concentration (Regeneration)	Y_{in}^*	1
Inlet Initial Dimensionless Temperature (Regeneration)	T_{in}^*	1

Figure 3 illustrates the variation of the removed water with the number of transfer units for $r = 1$. From this figure, one can observe that as the number of transfer units is increased, the water removal capacity also increases. This can be explained by the definition of these parameters, as shown by equaiton (34). As an example, one could increase of NTU by increasing the heat and mass transfer coefficients or transfer area, favoring the water humidity removal from the natural gas.
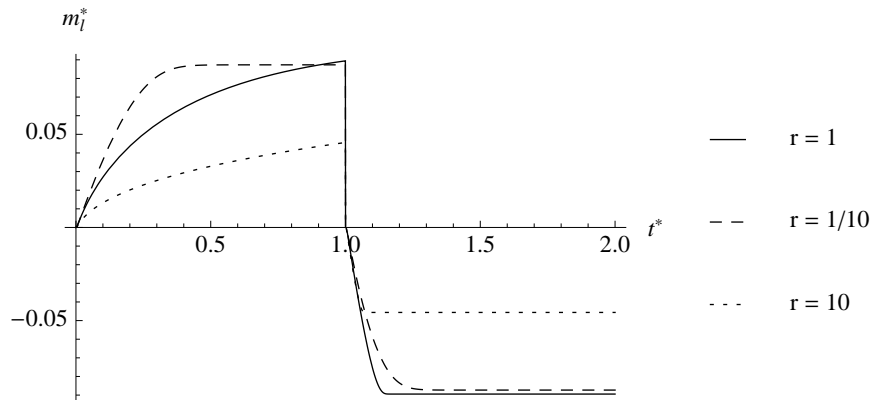

Figure 3. Study of Removed Water Amount Behavior - NTU Variation $N_{tu}^m - N_{tu}^h$.

The next results (displayed on figure 4), analyze the effect of varying the volumetric capacity ratio. As can be seen, the results shows a behavior that is quite irregular. The best response obtained was the one of an intermediate value for V_r^*.
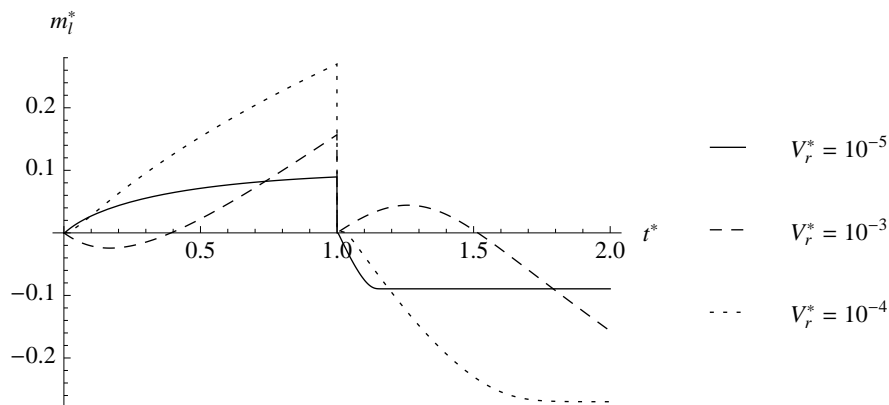

Figure 4. Study of Removed Water Amount Behavior - Volumetric Capacity Rate Variation V_r^*.

6. CONCLUSIONS

This study presented a simple mathematical model for simulating the process of natural gas dehydration using solid desiccants. A system of one-dimensional governing equations for heat and mass transfer within the adsorbent material were obtained. Dimensionless groups associated to this problem were presented and the formulation was normalized using these groups. A numerical solution of the problem was implemented using the Finite Volumes Method combined with the Method of Lines. Then, simulation results were carried-out for illustrating the effect of varying the dimensionless parameters on the amount of mass of water removed. The results showed, for the simulated conditions, that a smaller value for the separation factor yields a better water removal. In addition higher NTUs

also lead to better performance. In spite of the relevance of this study, the results are still preliminary and future research should definitely be conducted. As future works, it is interesting to study the variation of other parameters about the desiccant and with respect to the initial conditions. Others studies can be done with respect to the temperature and pressure, and joint analysis of these variations. The possibility of a 2D formulation and the use a more efficient programming language (such as Fortran or C) for the numerical solution are other aspects of future works.

7. ACKNOWLEGEMENTS

8. RESPONSIBILITY NOTICE

Benther and Sphaier are the only responsible for the printed material included in this paper.

REFERENCES

ASHRAE, 1985, ASHRAE Handbook Fundamentals, American Society of Heating, Refrigerating and Air-conditioning Engineers, Atlanta, GA.

Basmadjian, D., 1997, The Little Adsorption Book - A Pratical Guide for Engineers and Scientists, CRC Press, Florida.

Cavenati, S., Grande, C.A., and Rodrigues, A.E., 2006a, "Removal of carbon dioxide from natural gas by vacuum pressure swing adsorption", Energy & Fuels, vol. 20, no. 6, pp. 2648–2659.

Cavenati, S., Grande, C.A., and Rodrigues, A.E., 2006b, "Separation of $ch_4/co_2/n_2$ mixtures by layered pressure swing adsorption for upgrade of natural gas", Chemical Engineering Science, vol. 61, no. 12, pp. 3893–3906.

Çengel, Y.A. and Boles, M.A., 1985, Thermodynamics - An Engineering Approach, McGraw-Hill, Atlanta, GA, 3ª ed.

da Silva, M.J.M. and Sphaier, L.A., 2010, "Dimensionless lumped formulation for performance assesment of adsorbed natural gas storage", Applied Energy, vol. 87, no. 5, pp. 1572–1580.

Gandhidasan, P., Al-Farayedhi, A.A., and Al-Mubarak, A.A., 2000, "Dehydration of natural gas using solid desiccants", Energy, vol. 26, pp. 855–868.

Kikkinides, E.S., Sikavitsas, V.I., and Yang, R.T., 1995, "Natural-gas desulfurization by adsorption – feasibility and multiplicity of cyclic steady-states", Industrial and Engineering Chemistry Research, vol. 34, no. 1, pp. 255–262.

Kohl, A.L. and Riesenfeld, F.C., 1980, Gas Purification, McGraw-Hill, New York, 4ª ed.

Patankar, S.V., 1980, Numerical Heat Transfer and Fluid Flow, Routledge, New York.

Sphaier, L.A. and Worek, W.M., 2009, "Parametric analysis of heat and mass transfer regenerators using a generalized effectiveness-NTU method", International Journal of Heat and Mass Transfer, vol. 52, pp. 2265–2272.

Wolfram, S., 2003, The Mathematica Book, Wolfram Media/Cambridge University Press, New York/Champaign, IL, 5th ed.

Wylen, G.J.V., Borgnakke, C., and Sonntag, R.E., 2003, Fundamentos da Termodinâmica, Editora Edgard Blücher LTDA., São Paulo, SP, 6ª ed.