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Complete modeling dehydration unit, adsorption and regeneration

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Abstract
This paper presents the modeling and simulation of natural gas dehydration unit of Bidboland Gas Refinery. The cyclic thermal swing adsorption (TSA) technique is used in this unit and Silica gel is used as an adsorbent. The unit consists of a three-bed system with a 15-hours cycle; 5 hours of adsorption, 5 hours of heating and 5 hours of cooling. A non-isothermal one-dimensional model is used for simulation of process and the Langmuir- Freundlich model is selected for gas and solid equilibrium calculations. The simulation results are in a good agreement with the industrial data. In addition, to increase the capacity of the Bidboland dehydration unit some scenarios are investigated. The results show that the use of the four-bed system; two bad at adsorption, one bed at heating and one bed at cooling operation, can increase the capacity of the Bidboland dehydration unit up to the boundary of 9 MMSCMD.

Keywords: cyclic operation, simulation, dehydration, adsorption

Introduction
Natural gas is one of the most important sources of energy, requiring purification for distribution and consumption. Water as one of the impurities in natural gas causes problems such as corrosion and hydrate formation and blockage of transmission lines. There are various ways to remove water from the gas such as: adsorption, absorption, direct cooling, using of membrane and, etc. The adsorption process is a method widely used today for natural gas dehydration. There are many industrial adsorbents for adsorption , such as molecular sieves, silica gel and activated alumina, and etc. In this study, silica gel was used as an adsorbent to absorb water only. Although adsorption process is usually designed from laboratory data, in order to optimize and predict the behavior of packed bed adsorption, equilibrium data and balance equations can also be used to predict unit performance .Therefore, many researchers are interesting to provide an accurate mathematical model for this process.

The adsorption step of dehydrating natural gas on zeolite 5A is modeled by Gholami [1]. In the same way, Myrlla [2] has performed simulation of adsorption step of natural gas dehydration on zeolite 4A. Modeling of dehydration units and investigated heating of regeneration is also was done by Jorge [3]. Modeling of adsorption step of dehydration units are also were done by other researchers [4, 5].
In this paper the three steps of adsorption, heating and cooling are simulated for cyclic dehydration of natural gas by using the Aspen Adsorption V10. And then the results are compared with industrial data. In addition, based on the simulated model, various scenarios are investigated to increase the capacity of the dehydration unit.

Mathematical Model

The following assumptions have been used to simulate the Bidboland Refinery dehydration unit in Aspen Adsorption software [6].
a. There is no radial and axial dispersion for mass balance equation.
b. There is no radial dispersion for energy balance equation.
c. The gas flow is assumed downward in the adsorption and cooling beds and upward in the heating bed.
In the selected model, Ergun equation is used for calculating the pressure drop in the bed, Langmuir- Freundlich isotherm is used for gas-sold equilibrium calculations, and Peng Robinson equation of state for calculating the gas compressibility factor.

Mass balance

Gas phase material balance for each component in the bed:

$$\frac{\partial(v_g C_k)}{\partial z} + \varepsilon_B \frac{\partial C_k}{\partial t} + J_k = 0$$

where J_k in the above equation is the mass transfer rate of component *k* to/from adsorbent and can be calculated by:

$$J_k = \frac{\partial w_{k,j}}{\partial t} = MTC\left(w^*_{k,j} - w_{k,j}\right)$$

Where $w^*_{k,j}$ is the equilibrium concentration and is obtained from the Langmuir-Freundlich equilibrium equation for adsorption and regeneration .

$$w^*_{k,j} = \frac{IP_1 IP_2 c_i^{IP_3} e^{IP_4/T_s}}{1 + IP_5 c_i^{IP_3} e^{IP_6/T_s}}$$

Energy balance

Energy balance are considered for gas, solid and wall of the beds.
Gas phase energy balance:

$$-K_{gz}\varepsilon_i \frac{\partial^2 T_g}{\partial z^2} + c_{v_g} v_g \rho_g \frac{\partial T_g}{\partial z} + \varepsilon_B c_{v_g} \rho_g \frac{\partial T_g}{\partial t} + HTCa_p\left(T_g - T_s\right) + \frac{4H_w}{D_B}\left(T_g - T_w\right) = 0$$

Solid phase energy balance:

$$-K_{sz}\frac{\partial^2 T_s}{\partial z^2} + C_{ps}\rho_s \frac{\partial T_s}{\partial t} + \rho_s \sum_{k=1}^{n}(C_{pak}\, w_k)\, \frac{\partial T_s}{\partial t} + \rho_s \sum_{i=k}^{n}(\Delta H_k \frac{\partial w_k}{\partial t}) - HTCa_p\,(T_g - T_s) = 0$$

Wall energy balance:

$$-K_w \frac{\partial^2 T_w}{\partial z^2} + C_{pw}\rho_w \frac{\partial T_w}{\partial t} - H_w \frac{4D_B}{(D_B+w_t)^2-D_B^2}(T_g - T_w) + H_{amb}\frac{4(D_B+W_t)^2}{(D_B+W_t)^2-D_B^2}(T_w - T_{amb}) = 0$$

Boundary and initial conditions

The boundary conditions are:

$C_k(0,t) = C_{k,in}$

$T_g(0,t) = T_{gin}$ $\qquad \frac{\partial T_g}{\partial z}\Big|_{z=L} = 0$

$\frac{\partial T_s}{\partial z}\Big|_{z=0} = 0$ $\qquad \frac{\partial T_s}{\partial z}\Big|_{z=L} = 0$

$\frac{\partial T_w}{\partial z}\Big|_{z=0} = 0$ $\qquad \frac{\partial T_w}{\partial z}\Big|_{z=L} = 0$

In the cyclic simulation, the resulted profiles for each bed is used as an initial condition for the next bed. For example, the resulted profiles for the adsorption bed is used as initial condition for heating bed and so on.

The finite difference method is used for discretization of spatial derivatives; backward difference for first order and central difference for second order derivatives. Therefore, the partial differential equations (PDEs) have been transformed into 260 ordinary differential equations (ODEs). Then ordinary differential equations are solved by the Implicit Euler method whit variable step size. The maximum and minimum step size used is 30, 0.01 respectively.

Models parameters

The values of model parameters which are used in the simulation are shown in Table 1. In addition the parameters of Langmuir-Freundlich isotherm for adsorption and regeneration operations are estimated based on the empirical data and are shown in the Table 2.

Table1. Models parameters are used in the simulation

Inlet gas composition		**Bed specification**	
Components	Mole fraction	Height of bed (Ft)	25
		Interparticle voidage (m^3void/ m^3bed)	0.45
CH_4	0.88549	Inside diameter of bed (in)	102
C_2H_6	0.04162	Wall thickness of bed (in)	2.5
C_3H_8	0.00874		
i-C_4H_{10}	0.00125	**Adsorbent specification**	
n-C_4H_{10}	0.00165	Adsorbent bulk density(kg/m^3)	700
n-C_5H_{12}	0.00097	Adsorbent radius (Mm)	3.0
N_2	0.05832	Adsorbent specific heat capacity (kJ/kg.K)	1
water	0.00196	Adsorbent thermal conductivity (kW/m.K)	1.74e-4

Operation conditions inlet gas to beds

Name	Adsorption	Heating	Cooling
Temperature (^{o}F)	106	500	106
Pressure (kg/cm^2)	50.6	51	52.5
Flow rate (MMSCMD)	6.95	0.62	0.62

Others parameters

Heat of adsorption of water (kJ/kmol)	-52000
Heat capacity of adsorbed water (kJ/kmol.K)	84.00
Specific heat capacity of wall (kJ/kg.K)	0.5024
Thermal conductivity of wall (kW/m.K)	0.045
Density of wall (kg/m^3)	7800
Thermal conductivity of gas (kW/m.K)	4.75e-5
Heat transfer coefficient between wall and ambient (kW/m^2.K)	0.03
Ambient temperature (K)	308.15

Table2. Parameter of Langmuir-Freundlich isotherm for Water-silica gel system.

Adsorption		Regeneration	
Constant parameter	value	Constant parameter	value
IP_1	0.13872	IP_1	0.0016498
IP_2	1	IP_2	1
IP_3	0.56661	IP_3	0.39165
IP_4	0	IP_4	985.17
IP_5	0	IP_5	0
IP_6	0	IP_6	0

Results and discussion

Simulation results of adsorption bed

Fig. 1 shows the breakthrough curve obtained from modeling the adsorption bed compared to the industrial data. There is good agreement between the model predictions and the plant data (Based on the gas flow rate equal to 6.95MMSCMD). The outlet temperature changes of the adsorption bed are shown in Fig. 2. As can be seen, the bed temperature is almost constant during the adsorption operation.

Simulation result of heating and cooling beds

The results of heating and cooling beds in compare to plant data are shown in Fig. 3 and 4. As can be seen, the predicted bed temperatures have good agreement with plant data. It should be notice that less than 10 percent of inlet gas is used as regeneration gas and a furnace is used to increase the gas temperature to about 500 ºF.

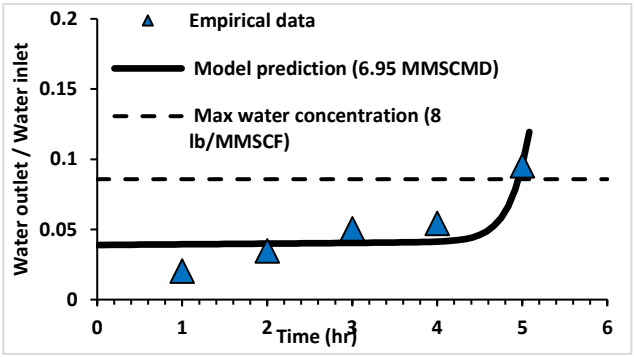

Fig1. breakthrough curve of the adsorption bed whit empirical data.

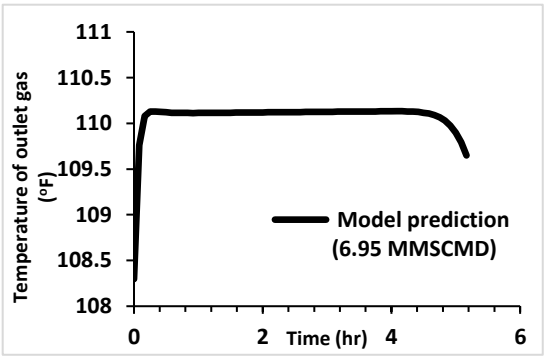

Fig2. the temperature changing of the outlet gas from adsorption bed

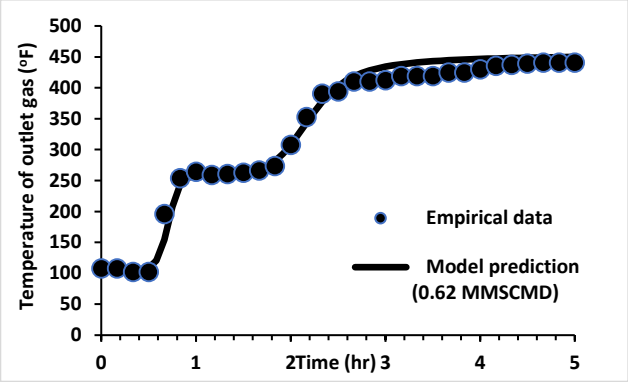

Fig3. the temperature changing of outlet gas from the heating bed.

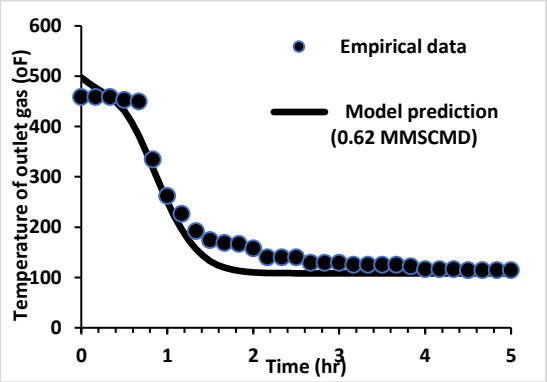

Fig4. the temperature changing of the outlet gas from the cooling bed.

In the next step, to increase the capacity of the Bidboland dehydration unit up to 9MMSCMD some scenarios are investigated .

scenario1: Using of three beds
Two beds at adsorption and one bed at regeneration (heating and cooling). What is important in this structure is the time of the regeneration (heating and cooling) which should be less than half the time required for adsorption. As can been seen in fig.3&4 requiring time for heating and cooling can be approximately 5 hours (3hours for heating and 2 hours for cooling). So, the time required for the adsorption operation should be longer than 10 hours (for each adsorption bed whit 4.5MMSCMD), in that way the first scenario to be feasible. As has been observed, the possible time for adsorption operation is less than 10 hours(7:40min). fig. 5. Accordingly, this scenario is not possible for Bidboland dehydration unit.
scenario2: Using of four beds
Two beds at adsorption and one bed at regeneration and one bed at cooling. In according fig. 5. the time requiring for adsorption operation is less than 7:40. If the 7:30 is conservatively selected for the adsorption operation time, then the time required for each heating and cooling process is 3:45. It can be seen in fig. 6 and 7. bed heating and cooling operation were completed at 3:45(for 0.7 MMSCMD flow rate). By selecting a 15-hours cycle for each bed (7:30 for adsorption,3:45 for heating and 3:45 for cooling), the capacity of each dehydration unit can be increased up to 9MMSCMD in the second scenario.

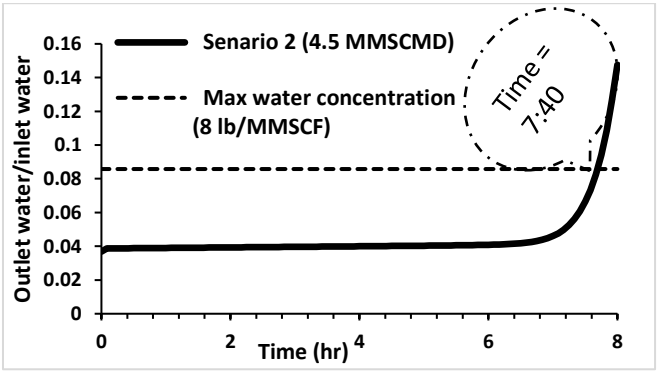

Fig5.breakthrough curve of adsorption bed
for first and scond scenario(4.5MMSCMD).

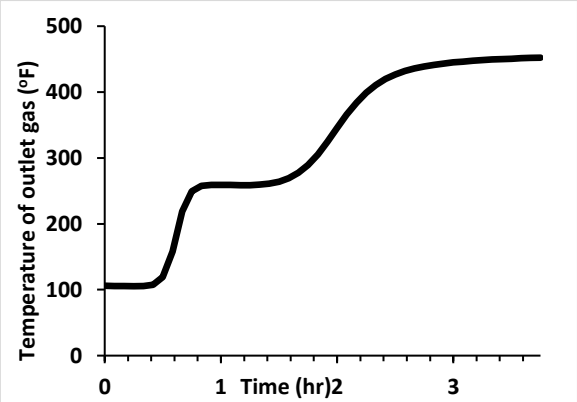

Fig6.the temperature changing of the outlet gas from the heating bed in the scond scenario
(inlet flow in the bed:0.7MMSCMD).

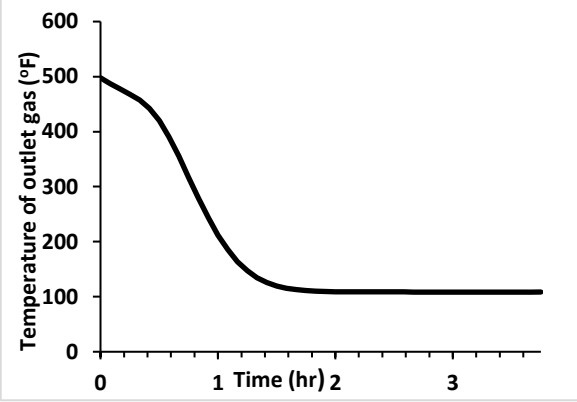

Fig7.the temperature changing of the outlet gas from the cooling bed in the scond scenario
(inlet flow in the bed:0.7 MMSCMD).

Conclusions

Dynamic simulation of Bidboland refinery dehydration process was performed in three steps of adsorption, heating and cooling by aspen adsorption. The results of the simulation showed that:

1. The time required for cooling bed is longer than 2 hours (for 0.62 MMSCMD).
2. The time required for Heating and regeneration bed is longer than 3 hours (for 0.62 MMSCMD).
3. The time required for adsorption in the 6.95MMSCMD flow rate should be less than 5 hours to meet the standard permissible humidity in the exhaust gas.

Scenarios of using three and four beds for increasing capacity of dehydration unit were investigated. According to the simulation results, the use of four beds can increase the unit capacity up to 9MMSCMD.

Acknowledgements

Thanks to Bidboland compony for providing empirical data.

Notation

C_k:Molar concentration of component k *kmol/m^3*
v_g:Gas phase superficial velocity *m/s*
MTC:Mass transfer cofficient *1/s*
$w_{k,j}$:Loading of component k *kmol/kg* j is spatial nodes in the bed
K_{gz}:Effective axial gas phase thermal conductivity *MW/m/k*
c_{v_g}: Specific gas phase heat capacity at constant volume $Mj/kmol/k$
HTC:Gas-solid heat transfer cofficient *Mj/m^2/s*
a_p:Specific particle surface per unit volume bed m^2*(particle area)/* $m^3(bed)$
K_{sz}: Effective axial solid phase thermal conductivity *MW/m/k*
C_{ps}: Specific heat capacity of adsorbent $Mj/kg/k$
C_{pak}: Specific heat capacity of adsorbed phase $Mj/kmol/k$

ΔH_k:Heat of adsorption of component k $Mj/kmol$
K_w:Thermal conductivity of column wall *MW/m/k*
C_{pw}: Specific heat capacity of column wall $Mj/kg/k$
H_w: Gas-wall heat transfer cofficient $Mj/m^2/s$
D_B:Bed diameter *m*
W_t:Whidth of column wall *m*
T_{amb}:Ambient temperature *k*
ρ_w:Wall density kg/m^3
ρ_s: Adsorbent bulk density kg/m^3
ρ_g: Gass phase molar density $kmol/m^3$
ε_i:Interparticle voidage $m^3(void)/m^3(bed)$
ε_B:Total bed viodage $m^3(void+pore)/m^3(bed)$

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