Modelling and Simulation of Glycol Dehydration Unit of a Natural Gas Plant

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ABSTRACT

Mathematical models for the prediction of water content, gas and solvent temperatures of the absorber of a natural gas glycol dehydration facility were developed. The models developed contain contributions from bulk and diffusion flows, however only the effect of diffusion on the process occurring in the absorber was studied. The developed models were second order partial differential equations. The Laplace transform technique was applied to obtain analytical solutions of the model equations. The models were validated using the plant data from an SPDC TEG unit in Gbaran Ubie, Bayelsa State. The results showed a reasonable agreement between the model predictions and industrial plant data. The model predicted the amount of water in the gas stream at the end of the absorption process very accurately with a deviation of 0%, the gas and solvent temperatures with deviations of 1.584% and 2.844% respectively. These results show that diffusion alone can be used to accurately model the absorption process. The effects of certain process variables such as residence time, gas inlet water content, mass and thermal Diffusivities of the gas on the performance of the absorber was studied.

Keywords: modeling, simulation, absorption unit, dehydration, natural gas, water content, Triethylene glycol.

NOMENCLATURE

- \( C_{Ag} \): Concentration of water vapour in the gas stream, mol/m³
- \( D_A \): Mass diffusivity of water vapour, m²/s
- \( K_G \): Thermal diffusivity of TEG, m²/s
- \( K_L \): Thermal conductivity of TEG, KW/m²K
- \( K_T \): Thermal diffusivity of water vapour, m²/s
- \( M_i \): Molar mass of component i, kg/kmol
- \( s \): Laplace transforms variable
- \( t \): Residence time, s.
- \( T_g \): Gas temperature, °C
- \( T_L \): Liquid (TEG) temperature, °C
- \( V_1 \): Molar volume of water vapour, m³/kmol
- \( V_g \): Gas velocity, m/s
- \( \chi_2 \): Solvent association parameter for TEG
- \( x_A \): Water content, weight %
- \( y_A \): Water content, mole %, mole fraction or lb H₂O/MMscf
- \( y_A' \): Water content in the Laplace domain
- \( z \): Packing height, m
- \( \mu_2 \): Viscosity of TEG, Pa.sec
- \( \pi \): Pi
- \( \rho_i \): Density of component i, kg/m³
1. INTRODUCTION

Raw natural gas can be obtained from oil wells, gas wells and condensate wells (Ikoku, 1992). It is “associated gas” when it is obtained from oil wells and can exist separate from the crude oil (as free gas) or dissolved in the oil (as dissolved gas); it is “non-associated gas” when obtained from gas or condensate wells; in this form it is found with little or no crude oil (Guo and Ghalambork, 2005). Natural gas is composed almost entirely of methane. However, whatever its source, natural gas commonly exists in a mixture with other hydrocarbons, principally ethane, propane, butane, and pentanes. In addition, raw natural gas also contains water vapor, hydrogen sulphide, carbon dioxide, helium, nitrogen and other trace compounds (Spieght, 2007).

Natural gas from the well has to be transported via pipelines to where it is processed and to end users or buyers. Natural gas to be transported by pipelines or processed, must meet certain specifications. Such specifications include delivery pressure, rate, temperature, allowable concentrations of contaminants such as carbon dioxide (CO₂) and hydrogen sulfide (H₂S), cleanliness (allowable solid content), minimum heating value and maximum water content (water dew point) (Kazemi and Hamidi, 2011).

Water vapour is the most common undesirable impurity found in natural gas and is usually present in concentrations in the range of 400-600 lbH₂O/MMSCF of gas (Ikoku, 1992). In the course of transmission and processing, change in temperature and pressure of the natural gas occur. These changes in temperature and pressure condense the natural gas vapor altering its physical state from gas to liquid and or liquid to solid. These changes in state result in diverse problems for the physical state from gas to liquid and or liquid to solid. These problems can be solved by cooling or pressure condense the natural gas vapor altering its physical state from gas to liquid and or liquid to solid. These changes in state result in diverse problems for the physical state from gas to liquid and or liquid to solid. These changes in state result in diverse problems for the natural gas to levels required for safe gas transmission by pipelines and that do not cause any damage to equipment.

To achieve this, the dehydration unit or plant has to be properly designed. Modeling and simulation of the absorber gives insight into the performance of the absorber at varying operating conditions and provides sufficient data required for proper design. Modeling of the absorber could be performed via a thermodynamic or fundamental model.

Thermodynamic models involve the selection of a suitable thermodynamic model and software simulator while fundamental models involve the use of conservation principles to develop mathematical equations of the process. Works on thermodynamic models abound (Kazemi and Hamidi, 2011), Peyghambazardeh and Jafarpour (2006)); where the thermodynamic behavior of the system (TEG-Water) were represented by means of the Peng and Robinson equation of state or the cubic equation of state while software simulators commonly used includes Aspen-Hysys, Chemcad and Pro II. Thermodynamic modelling of the TEG-water system is still being reported (Kazemi and Hamidi, 2011) to be rather inaccurate.

Fundamental models are derived from mass, energy and momentum balances of the process, these abound for similar systems with very complexities; Gomez et al., (2003) modeled only bulk flow contribution while Ahmed et al., (2007) and John, (2009) modeled bulk and diffusion contributions. The contribution of the diffusion term to the absorption process and the efficiency of the absorber have not been investigated. The effects of diffusion on the mathematical models for gas absorption are therefore investigated in this work.

2. PROCESS DESCRIPTION

Methods for water treating of natural gas includes: adsorption (Kohl and Riesenfeld, 1974), absorption (Campbell et al., 1982), membrane process (Shell, 1982.), methanol process (Minkkinen, 1992.) and refrigeration (Kindnay and Parish, 2006). Amongst these methods absorption using liquid solvent (triethylene glycol TEG) as absorbent remains the most popular (Kindnay and Parish, 2006), Manning and Thomson, (1991), Gas Processors Suppliers Association, (2004)). The treatment method used is expected to reduce the amount of water in the natural gas to levels required for safe gas transmission by pipelines and that do not cause any damage to equipment.

To achieve this, the dehydration unit or plant has to be properly designed. Modeling and simulation of the absorber gives insight into the performance of the absorber at varying operating conditions and provides sufficient data required for proper design. Modeling of the absorber could be performed via a thermodynamic or fundamental model.

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2. PROCESS DESCRIPTION

Figure 1(a) shows a simplified TEG absorber with the inflow and outflow streams, while in Figure 1(b), an elemental packed height is shown, with its associated inflow and outflow streams.
In Figure 1(a), G is the molar flow rate of the gas stream, \( y_0 \) its initial water content, \( C_{AOG} \) the inlet water vapor concentration, G, y and \( C_{AG} \) are respectively the dry gas parameters. For the TEG stream, L, \( x_0 \) and \( C_{A0L} \) represent the inlet flow rate, initial water content and water concentration respectively, similarly, L, x and \( C_{AL} \) are their respective rich TEG parameters. Fig. 1(b) shows a material balance on the elemental packing height (\( \Delta Z \)). The component balance for component A (water vapor) is taken across the elemental packing height (\( \Delta Z \)).

2.1 TEG-Dehydration Process

A typical TEG-dehydration process can be divided into two major parts, gas dehydration and solvent (triethylene glycol, TEG) regeneration. In the dehydration, water is removed from the gas using TEG and in the regeneration, water is removed from the solvent (TEG). Natural gas enters the unit at the bottom of the absorber tower and rises through the tower where it intimately contacts the TEG solution flowing from the top of the absorber downward across the trays or structured packing. Through this contact, the gas gives up its water vapor to the TEG. The water laden TEG is circulated in a closed system, where the water is boiled from the TEG. The regenerated TEG is then re-circulated to the contacting tower.

3. METHODOLOGY

3.1 MODEL DEVELOPMENT

Mathematical models that could predict the performance of the absorber were developed using the principle of conservation of mass and energy. The models would predict the amount of water vapor removed from the gas stream and the temperature progression along the packing height of the absorber for the gas and liquid (TEG) phases.

3.2 Model Assumptions

The following assumptions were made in the development of the model equations:

Packed column is used, the absorber is well-lagged, hence secondary heat effects (heat losses and heat of mixing) are negligible, there is no reaction occurring, hence the reaction term is not considered, the effect of change in total flow rate in the column is ignored, and an average constant value is assumed (McCabe et al., 2005). Since the water vapour is the only diffusing component, the diffusion term was not considered for the liquid phase. The diffusion term is accounted for using the Flicks’ law. The glycol loses some amount of heat (Q) to the gas phase by conduction which will be accounted for by Fourier’s law. Plug flow conditions prevail.

MATERIAL BALANCE

With these assumptions water vapor component mole balance and energy balance (for the gas and liquid phases) for a differential element of the absorber as shown in Figure 1b results in the following equations:

\[
\frac{\partial y_A}{\partial t} = -V_g \frac{\partial y_A}{\partial z} + D_A \frac{\partial^2 y_A}{\partial z^2}
\]

(1)

Where \( V_g \) is the gas velocity in m/s

Energy Balance for Gas Phase

\[
\frac{\partial T_g}{\partial t} = -\frac{G}{A_{AG}} \frac{\partial T_g}{\partial z} + K_T \frac{\partial^2 T_g}{\partial z^2} + \frac{L C_{pl}}{A_{AG} C_{pg}} \frac{\partial T_L}{\partial z}
\]

(2)

Equation (2) is simplified to give:

\[
\frac{\partial T_g}{\partial t} = -\frac{G}{A_{AG}} \frac{\partial T_g}{\partial z} + K_T \frac{\partial^2 T_g}{\partial z^2} + \beta
\]

(3)

Energy Balance for Liquid Phase

\[
\frac{\partial T_L}{\partial t} = -\frac{L}{A_{AL}} \frac{\partial T_L}{\partial z} + K_G \frac{\partial^2 T_L}{\partial z^2}
\]

(4)

Where \( K_G, K_T \) are the thermal diffusivity of the liquid and water vapor, \( C_{pg} \) and \( C_{pl} \) are the specific heat of the water vapor in the gas stream and liquid stream, \( T_{og} \) and \( T_g \) are the inlet and outlet temperatures of the gas stream, A is the cross-sectional area of the packed section, \( T_L \) is the temperature of the liquid stream, \( C_{Ag} \) is the concentration of water vapor in the gas stream.

Neglecting the contribution from bulk flow, the model equations for adsorption by diffusion only with the appropriate boundary conditions are as follows:

Gas water content:

\[
\frac{\partial y_A}{\partial t} = D_A \frac{\partial^2 y_A}{\partial z^2}
\]

(5)
Gas Temperature progression:
\[
\frac{dT_G}{dt} = K_T \frac{\partial^2 T_G}{\partial z^2} + \beta
\]  
(8)

TEG Temperature progression:
\[
\frac{dT_L}{dt} = K_G \frac{\partial^2 T_L}{\partial z^2}
\]  
(11)

4. SOLUTION TECHNIQUE OF MODEL EQUATION

The model equations developed were 2nd order partial differential equations. The transform method which reduces a given partial differential equation and its boundary conditions to an ordinary differential equation by applying the integral transform with respect to one of the independent variables (Stephenson, 1986), in this case time (t) was adapted for the solution of the model equations. The Laplace transform was used to transform the differential term with respect to the independent variable (t) in the model equations, thus converting the equations to 2nd order ordinary differential equations in the independent variable, z. The resultant 2nd order differential equations were then solved analytically; the results being in the s domain were inverted back to the t domain using inverse Laplace transform and finally given in a suitable form using appropriate mathematical manipulations.

Applying this procedure to equation (5); the Laplace transform of eqn. (5) with respect to time gives:
\[
\mathcal{L}\{T_G(z,0)\} = 0, \quad \text{for } Z > 0
\]  
(9)
\[
\mathcal{L}\{T_G(0,t)\} = T_{og}, \quad \text{for } t > 0
\]  
(10)

Substituting the boundary condition, equation (6) into equation (14) gives:
\[
S\mathcal{L}\{T_G(z,s)\} - Y_A(z,0) = D_A \frac{\partial^2 \mathcal{L}\{T_G(z,s)\}}{\partial z^2}
\]  
(14)

Substituting the boundary condition, equation (6) into equation (14) gives:
\[
S\mathcal{L}\{T_G(z,s)\} - D_A \frac{\partial^2 \mathcal{L}\{T_G(z,s)\}}{\partial z^2} = 0
\]  
(15)

The solution of equation (15) is:
\[
\mathcal{L}\{T_G(z,s)\} = A e^{\lambda_1 z} + B e^{-\lambda_2 z}
\]  
(16)

5. OPERATING PARAMETERS

To use the final model equations of the absorber (eqns. (21), (22) and (23)) require the determination of certain constants, physical properties and compositions of natural gas, water vapor and triethylene glycol. These properties were determined as follows:

5.1 Mass Diffusivity (DA)

The mass diffusivity of water vapour in triethylene glycol (TEG) was obtained using equation given by Perry et al (1999):
\[
D_A = D_{12} = 1.1728 \times 10^{-16} \frac{r(X_G M_G)^{1/2}}{\mu_2 \nu_i^{0.6}}
\]  
(24)

where \(\mu_2\) is the solvent viscosity at temperature T in Pa sec, \(\nu_i\) is the solute molar volume at the normal boiling
point in m³/kmole, x₂ is the solvent association parameter and M₂ the solvent molecular weight.

5.2 Thermal Diffusivity (Kₜ)
The thermal diffusivity of water vapor was obtained online from [http://en.wikipedia.org/wiki/thermal_diffusivity](http://en.wikipedia.org/wiki/thermal_diffusivity).

**Physical Properties of Gas and Glycol (TEG)**
The physical properties of the wet gas and glycol were obtained from Perry et al (1999) and tabulated as shown in Table 1.

<table>
<thead>
<tr>
<th>Property</th>
<th>TEG</th>
<th>H₂O</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar mass</td>
<td>150.17</td>
<td>18.02</td>
<td>19.83</td>
</tr>
<tr>
<td>Molar volume, m³/kmol</td>
<td>0.01813</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass diffusivity, m²/s</td>
<td>3.80x10⁻¹⁰</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal diffusivity, m²/s</td>
<td>2.338x10⁻⁵</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density, kg/m³</td>
<td>1125</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>Solvent Viscosity (Pa sec.)</td>
<td>0.01355515</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Data from a Shell Petroleum Development Company gas dehydrating unit at Gbaran Ubie in Bayelsa State are given in Table 2 (SPDC Plant data, 2007).

<table>
<thead>
<tr>
<th>COMPONENT</th>
<th>GAS STREAM (Weight %) INPUT</th>
<th>OUTPUT</th>
<th>GLYCOL STREAM (Weight %) INPUT</th>
<th>OUTPUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEG</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂O</td>
<td>0.17</td>
<td>0.01</td>
<td>0.49</td>
<td>4.64</td>
</tr>
<tr>
<td>GAS</td>
<td>99.83</td>
<td>99.99</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOTAL</td>
<td>100.00</td>
<td>100.00</td>
<td>100.00</td>
<td>100.00</td>
</tr>
<tr>
<td>TEMP</td>
<td>50.00</td>
<td>51.30</td>
<td>55.00</td>
<td>51</td>
</tr>
<tr>
<td>Absorber height</td>
<td>0.004m</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

6. DISCUSSION OF RESULTS

6.1 Model Validation

The input data in Table 2 were used in equations (21), (22) and (23) to obtain the amount of water in the gas stream and temperature of the gas and solvent streams as predicted by the models developed. The results obtained were tabulated in Table 3 with the outlet values of these parameters from the SPDC gas absorption unit in Gbaran Ubie for comparison.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Plant data</th>
<th>Model result</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas water content, mole</td>
<td>0.00011</td>
<td>1.0717x10⁻¹⁴</td>
<td>0</td>
</tr>
<tr>
<td>Gas temperature, °C</td>
<td>51.3</td>
<td>50.4874</td>
<td>1.584</td>
</tr>
<tr>
<td>TEG temperature, °C</td>
<td>51</td>
<td>49.5497</td>
<td>2.844</td>
</tr>
</tbody>
</table>

The results showed a reasonable agreement between the model predictions and industrial plant data. The model predicted the amount of water in the gas stream at the end of the absorption process very accurately with a deviation of 0%. The results also showed that the models accurately predicted the gas and solvent temperatures with deviations of 1.584% and 2.844% respectively. These trends are shown in Figures 2 and 3 respectively.
The temperature of the gas stream increased gradually and very slightly as the gas flows up the column while that of the solvent decreased as it flows down the column. From the ideal gas law, as temperature increases, the volume of a gas also increases; therefore, at higher temperatures, less gas is absorbed due its larger volume. This trend is seen in Figure 2 from the very slow rate of absorption after the initial high rate as the gas temperature increased slightly.

6.2 Model Simulation

The effects of residence time, gas inlet water content, mass and thermal Diffusivities of the gas on the models developed were investigated. The effects of varying each of these parameters on performance of the absorber are presented.

Effects of Natural Gas Residence Time on the Absorber Performance (Outlet Water Content of Natural Gas)

The effects of residence time on the water content of the gas along the column height are shown in Figure 4 below.
There was a reduction in the water content of gas stream as the gas flows along the column height from bottom to top for all residence time considered. However, the lower the residence time of the gas in the column the lower the amount of water in the gas stream at the exit of the column, that is the lower the residence time the higher the rate of absorption of water vapor, the more efficient the absorber and vice versa.

Effects of Gas and Solvent Residence Time on the Gas and Solvent Temperature

The effects of the gas and solvent residence time on the gas and solvent outlet temperatures are shown in Figures 5 and 6 respectively.
These Figures showed that the temperature of the gas stream increased as the gas flows up the column while that of the solvent decreased as the solvent flows down the column for all residence time considered. The Figures also showed that the outlet temperature of the gas stream decreased while that of the solvent increased with increase in gas and solvent residence time.

The residence time is the duration a component (gas or solvent) spends in the absorber. Higher residence times can be achieved by a reduction of the component flow rate and vice versa. Reduction of the component flow rate results in a reduction in the pressure of the column. From the ideal gas law, the reduction in column pressure will result in a decreased gas temperature. Hence the higher the gas residence time the lower the outlet gas temperature. At higher residence time less gas and solvent flows into the absorber. The quantity of water from the gas stream is less hence the amount of water absorbed by the solvent is also reduced (smaller). This reduced quantity of water absorbed by the solvent results in higher temperatures of the solvent.

Temperature has also been found to affect solubility (Gomez and Schbib, 2003), as temperature increases the amount of gas that can be absorbed by a liquid decreases. That is, solubility decreases with temperature. This trend the model predicts accurately in Figure 4 as the outlet water quantity in the gas stream increased at higher residence times indicating a reduction in absorption rate hence, a reduction of the gas solubility in the solvent as the gas temperature (Figure 3) increase and in Figure 6 where this reduction in gas solubility results in higher outlet temperatures of the solvent.

**Effect of Mass Diffusivity on Absorber Performance (Outlet Gas Water Content)**

The mass diffusivity was varied with respect to the value calculated for water vapor. The mass diffusivity of water vapor was calculated using equation (24). The effects of the mass diffusivity of water vapor on the absorber performance indicated by the outlet gas water content are shown in Figure 8.
The mass diffusivity of a material determines the rate at which a given component is transferred across a concentration gradient. Water vapor is transferred from the gas stream to the liquid solvent stream. The observed effect of mass diffusivity on the rate of water vapor transfer from the gas stream to the solvent liquid stream is shown in Figure 8.

Figure 8 showed that the rate of absorption of water vapor (the rate of transfer of water vapor to the triethylene glycol stream) decreases as the gas flows up the column for all values of mass diffusivity investigated. Figure 8 also showed that the water content in the gas stream at the outlet of the absorber reduced as the mass diffusivity was reduced (lower values of mass diffusivity). That is, the rate of absorption of water vapor increases as the mass diffusivity decreases. At lower values of mass diffusivity the rate of absorption was higher.

The higher the diffusivity (of one substance with respect to another), the faster they diffuse into each other (http://en.wikipedia.org/wiki/thermal_diffusivity). That is, if the mass diffusivity of the water vapor is decreased keeping that of TEG constant, the higher the diffusivity of TEG with respect to that of water vapor, then the faster the water vapor diffuses into the TEG solvent. This trend the developed model predicted accurately as shown in Figure 8 where the rate of absorption of water vapor increases as the mass diffusivity decreases (higher diffusivity of TEG relative to that of water vapor). Mass diffusivity increases with increasing temperature and decreases as pressure increases. The pressure of the column can be increased by increasing the component flow rate and vice versa, hence increasing flow rate decreases the mass diffusivity and vice versa.

**Effect of Thermal Diffusivity on Absorber Performance (Solvent (TEG) Temperature)**

The effects of the thermal diffusivity of water vapor on the absorber performance indicated by the outlet temperature of solvent (Tri ethylene glycol) are shown in Figure 9.

![Fig. 9: Variation of temperature of TEG at different thermal diffusivities at t= 20 seconds](image)

Figure 9 showed that the temperature of the solvent (triethylene glycol) decreases down the column at a given thermal diffusivity. This decrease is faster as the thermal diffusivity decreases. Figure 9 also showed that the outlet temperature of the solvent decreases as the thermal diffusivity decreases. Thermal diffusivity is the property of a material which describes the rate of heat flow through the material. A high thermal diffusivity means a higher conductivity compared to heat capacity. This means that the material conducts more heat rather than stores it. Therefore the higher the thermal diffusivity of the gas, the more heat it conducts out which is absorbed by the triethylene glycol stream. Hence an increase in the thermal diffusivity increases the temperature of the triethylene glycol stream as predicted by the model in Figure 9.

**7. CONCLUSION**

Mathematical models of the absorber of a glycol dehydration facility was developed using the principles of conservation of mass and energy. The model predicted the water content of natural gas (in mole fraction) across an absorber column. Similar models were developed for the variation of the gas and liquid (TEG) temperatures across the packing height of the absorber. The models developed contain contributions from bulk and diffusion flows. The effect of diffusion on the process occurring in the
absorber was studied in this work. The models were validated using the plant data from an SPDC TEG unit in Gbaran Ubie, Bayelsa State. The results showed a reasonable agreement between the model predictions and industrial plant data. The model predicted the amount of water in the gas stream at the end of the absorption process very accurately with a deviation of 0%. The results also showed that the models accurately predicted the gas and solvent temperatures with deviations of 1.584% and 2.844% respectively. Results showed that diffusion alone can be used to model the absorption process. The effects of certain process variables such as residence time, gas inlet water content, mass and thermal Diffusivities of the gas on the performance of the absorber was studied, thus provides new range of operating conditions to meet stringent industry and environmental concerns.

REFERENCES


