Simulation of gas sweetening process using new formulated amine solutions by developed package and HYSYS

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Abstract:

Commercial packages as HYSYS consider known amine solutions such as "MDEA, DEA, MEA …" for simulation of gas sweetening processes. In the present work a software package was developed to represent equilibrium calculation of sour gases and new formulated amine solution. The software package accounts for chemical equilibria in the liquid phase and physical equilibria between the liquid and vapor phases. The Peng–Robinson– (PR) equation was used to represent the fugacity coefficient in the vapor phase. The liquid phase was treated as an electrolyte solution and activity coefficients were represented by the Deshmukh - Mather equation. In this package a suitable and perfect platform was created to enter the new formulated amine solutions required information for simulation of gas sweetening process using HYSYS. The validity of software package calculations was compared to HYSYS-Amine -Package for MDEA and reasonable agreement was achieved. The developed package as an HYSYS extension can be used for feasibility, economical and technical studies of new formulated amine solutions for gas sweetening processes.

Key words: Gas sweetening, MDEA, Extension, Equilibrium calculation, HYSYS, Software package

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Introduction:

Carbon dioxide (CO_2) has long been known as one of the important factors to global warming caused by the increase in its concentration in the atmosphere. Therefore its removal and recovery from industrial process streams and flue gas produced from burning fossil fuels have become vital and the search for efficient and economical absorbents has gained significant interests [1–3].

In gas treating plants, aqueous alkanolamines have been widely used to absorb acid gases such as CO2 and H2S, triethanolamine (TEA), a tertiary amine, being one of the first amines used for such application. Although it was alternative by methyl di ethanolamine (MDEA) and monoethanolamine (MEA)[4], its application is recommended in the removal of acid gas is.

MEA aqueous solutions are the most frequently used because of their high reactivity with CO2, low solvent cost, and ease of reclamation .It is also known, however, that MEA aqueous solutions are corrosive and require high regeneration energy. MDEA aqueous solutions are better than MEA or DEA solutions in that they have the properties of high loading capacity (mol of CO2/mol of amine) up to 1.0, less regeneration energy, and high resistance to thermal and chemical degradation. However, the slow reactivity with CO2 of MDEA solutions limits their use [4–8].

Studies have been conducted on the effect of promoters on the rate of absorption of CO2 when blended in aqueous alkanolamines solutions. It has been found out that some promoters has higher reaction rate with CO2 than monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP), and dimethylethanolamine (DMEA) and has been reported to be superior than MEA, AMP, and DMEA for CO2 absorption [9]. The addition of promoters in aqueous AMP solutions can also improve the reaction rates with CO2 [1, 9] and has significant effect on the enhancement of the CO2 absorption rate [2]. In general, blends of promoters and alkanolamine yield improvements in absorption, such as higher loading capacity, faster rate of reaction, and lower solvent regeneration energy requirements [3, 10].

Research Institute of Petroleum Industry, National Iranian Oil Company (RIPI-NIOC) carried out a wide range of experimental and modeling investigations in this area.

Commercial packages as HYSYS consider known amine solutions such as "MDEA, DEA, MEA …" for simulation of gas sweetening processes. Therefore if a formulated amine solution was made which has its own liquid reactions, HYSYS software was not responsible for equilibrium calculations. In the present work an in- house software package was developed to represent equilibrium calculation of sour gases and new formulated amine

solution. The software package accounts for chemical equilibria in the liquid phase and physical equilibria between the liquid and vapor phases.

Table1: Chemical equilibrium reactions

$R_1R_2NH + H_2O \Leftrightarrow R_1R_2NH_2^+ + OH^-$
$R_1R_2R_3N + H_2O \Leftrightarrow R_1R_2R_3NH^+ + OH^-$
$R_1R_2NH + CO_2 \Leftrightarrow R_1R_2NCOO^- + H^+$
$H_2O \Leftrightarrow H^+ + OH^-$
$H_2S \Leftrightarrow H^+ + HS^-$
$CO_2 + H_2O \Leftrightarrow H^+ + HCO_3^-$
$HS^- \Leftrightarrow H^+ + S^{2-}$
$HCO_3^- \Leftrightarrow H^+ + CO_3^{2-}$

Table2: Physical equilibrium between phases

$H_i^s(T,P)x_i\gamma_i^* \; exp\left[\frac{v_i^\infty(p-p_w^{sat})}{RT}\right] = y_iP\varphi_i \qquad (i = CO_2, H_2S)$
$P_j^{sat}\varphi_j^{sat}x_j\gamma_j \; exp\left[\frac{v_j\left(p-p_j^{sat}\right)}{RT}\right] = y_jP\varphi_j$ (j=Water,Amine)
$Ln\, K_i(or\ H_i) = C_1 + \frac{C_2}{T} + C_3 * ln\, T + C_4 * T$
$K_i = \prod_{j=1}^{c}\gamma_j^{v_{ij}}\prod_{j=1}^{c}m_j^{v_{ij}}$
$\ln\gamma_i = -\frac{AZ_i^2\sqrt{I}}{1+B\sqrt{I}} + 2\sum\beta_{i,j}m_j$
$\beta_{ij} = a_{ij} + b_{ij}T$
$I = \frac{1}{2}\sum m_jZ_j^2$
$A = 1.306548 + .1328238\times10^{-1}T - .3550803\times10^{-4}T^2 + .3381968\times10^{-7}T^3$
$\alpha = \frac{mole\ AcideGas}{mole\ A\ mine}$

The software was developed as a COMTHERMO extension beside HYSYS amine-package. It means that the entire package was developed as a COM object which its class libraries were implemented by HYSYS to perform equilibrium, thermo-physical and flash calculations (Figures1, 2).

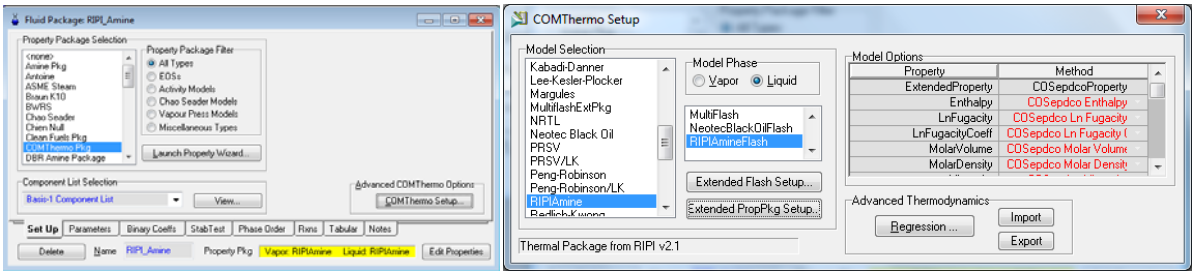

Figure.1- Procedure for linking RIPI-Amine to HYSYS

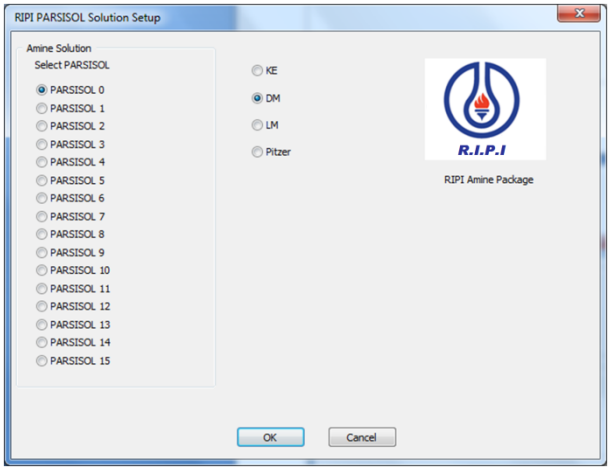

Figure.2- Menu for selecting the model and favorite amine solution

The physico-chemical correlations of MDEA solution [11-15] was implemented in developed package (RIRPI-Amine). RIRPI-Amine package is based on Deshmakh-Mather model and can be attached to HYSYS beside HYSYS amine-package and implemented in equilibrium calculations. The RIRPI-Amine results were compared to HYSYS amine-package (based on Li-Mather model) results which presented in following Tables. For testing the performance of developed package a stream with known composition, temperature and pressure was constructed and by changing the thermodynamic model the results of calculation are produced. As shown in tables 3-8 the observed differences were reasonable. The feed stream consists of a 2 molar MDEA in water solution contacted with a gas stream with a known CO2 and N2 partial pressure.

Results for 2 M & 30 °C & P_{CO2}- =1.1(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.2759	0.2759	0.114
N_2	0.001	0.00	0.00
CO_2	0.9525	0.9496	0.3946
H_2O	95.5945	95.6085	96.1442
MDEA	3.4519	3.4419	3.4612

Results for 2 M & 30 °C & P_{CO2}- =10.5(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.6394	0.6616	0.483
N_2	0.0009	0.00	0.00
CO_2	2.1797	2.2472	1.6507
H_2O	94.4104	94.3560	94.9318
MDEA	3.4091	3.3968	3.4175

Results for 2 M & 30 °C & P_{CO2}- =95.8(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.9618	0.9618	0.88
N_2	1.500e-5	0. 00	0.00
CO_2	3.2428	3.2341	2.9672
H_2O	93.3855	93.4034	93.6610
MDEA	3.3717	3.3625	3.3718

Results for 2 M & 40 °C & P_{CO2}- =1.1(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.1971	0.1971	0.103
N_2	0.0009	0.00	0.00
CO_2	0.6821	0.6802	0.3566
H_2O	95.8563	95.8685	96.1809
MDEA	3.4607	3.4513	3.4625

Results for 2 M & 40 °C & P_{CO2}-=10.0(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.5012	0.5137	0.374
N_2	0.0008	0.00	0.00
CO_2	1.7168	1.7537	1.2829
H_2O	94.8569	94.8324	95.2867
MDEA	3.4255	3.4140	3.4303

Results for 2 M & 40 °C & P_{CO2}-=94.0(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.8959	0.8959	0.805
N_2	1.947e-6	0.00	0.00
CO_2	3.0273	3.0192	2.7212
H_2O	93.5936	93.6108	93.8985
MDEA	3.3790	3.3700	3.3803

Results for 2 M & 50 °C & P_{CO2}-=1.0(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.1336	0.1336	0.079
N_2	0.0008	0.00	0.00
CO_2	0.4633	0.4621	0.2738
H_2O	96.0676	96.0791	96.2608
MDEA	3.4683	3.4588	3.4654

Results for 2 M & 50 °C & P_{CO2}-=9.7(kPa)	HYSYS Results	RIPI-Amine Results	Literature Results
Loading	0.3844	0.3807	0.298
N_2	0.0007	0.00	0.00
CO_2	1.3227	1.3055	1.0249
H_2O	95.2352	95.2650	95.5358
MDEA	3.4414	3.4295	3.4393

Conclusion:

The current study presents a software package for calculation of chemical equilibria in the liquid phase (based on Deshmakh-Mather) and physical equilibria between the liquid and vapor phases .The RIRPI-AMINE package was programmed by C++ language and attached to HYSYS as COMTHERMO extension. The RIRPI-Amine package was tested for MDEA solution and its results was compared to HYSYS package. The differences between aforementioned results were reasonable so RIRPI-Amine package can be used for equilibrium calculation of new formulated solutions. The software is easy to use and while the information of new formulated amines was entered to package correctly, the results would be reliable. The package can be used for simulation of sweetening gas plants and economical studies.

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