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Dedicated to Professor Luminița Silaghi-Dumitrescu on the occasion of her 65th anniversary

DEVELOPMENT OF THE SOUR WATER PLANT DYNAMIC SIMULATOR FOR IMPROVING DESIGN AND OPERATION

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ABSTRACT. Sour water system (SWS), as vital part of refineries, is aimed to process wastewater produced during different refining processes. Sour water contains contaminated water with H_2S and NH_3 and/or alkali metals or hydrocarbon traces. The main objective of SWS is to reduce the concentration of these contaminants below undesirable level and to make possible water reuse in the refinery. H_2S is generally stripped from the sour water and sent to the Claus Unit. The paper reviews two possible designs for SWS. The first one corresponds to the traditional design of the SWS unit, while the second design uses an internal stream to heat up the feed flow. For analyzing the two different design configurations, dynamic simulators were developed in Aspen-Hysys using industrial and literature data. Different operating scenarios were tested, also involving the SWS control loops. Dynamic simulation results reveal incentives for the second analyzed design from the energy cost reduction perspective, as external need of heat utilities is diminished and this is associated to an improved separation of the contaminants.

Keywords: *sour water system, dynamic model, design, pollution, energy consumption*

INTRODUCTION

Oil and gas production use a significant amount of water. The source of water may have different origin: surface, rain, ground water, water in crude or recycled water. Figure 1 reveals the raw balance of the water in a refinery

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[1]. Sour water is produced by different plants, such as: crude, vacuum, catalytic cracker, delayer coker, visbreaker, hydrotreater, hydrocracker and sulphur plant units, or in the isomerization, Claus and alkylation processes [1, 2]. Sour water contains water contaminated with hydrogen sulfide (H_2S), ammonia (NH_3), traces of CO_2, salts, phenols, caustic. Non-phenolic sour water contains exclusively H_2S and NH_3. It is produced exclusively by hydro-treating processes and it is usually recycled in the upstream process. Phenolic sour water is generally not recycled for reuse because it contains contaminants which can undesirably affect the upstream process [3].

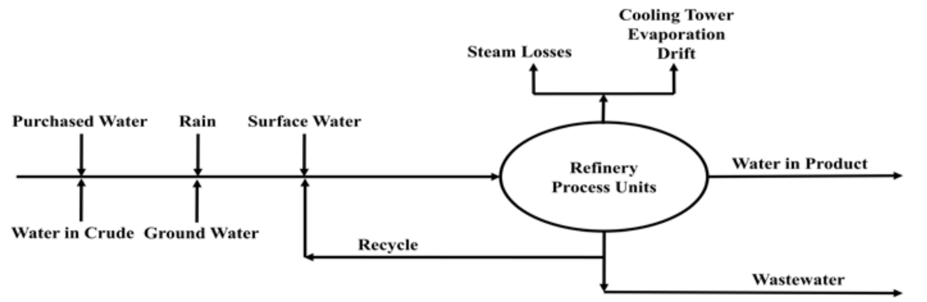

Figure 1. Water balance in a refinery [1].

The main concern with sour water is the H_2S content. Commonly, the concentration of the H_2S has to be kept below 1ppm [2, 3]. Presence of ammonia is also undesired. The treated water has to contain limited amount of NH_3 as its concentration must lie between 30-80 ppm [2-4].

The process of treating sour wastewater contains two main steps. In the first step H_2S is eliminated in a Sour Water (SW) Stripper. In the second stage the water is introduced in an absorption column where the remained NH_3 is separated. The vapor streams separated at the top of the SWS columns are sent to the Claus Unit, where the H_2S is broken down to its elemental molecules H_2 and S, for later use in other industrial processes.

Nowadays, SWS gets more attention in industrial plants [5]. The process is important because of the increasing emphasis on regulating the quality of the effluent water and saving energy [6-10].

RESULTS AND DISCUSSIONS

The paper presents two dynamic models for differently designed SWSs. The models represent the first step of the wastewater purification, which is performed in the SW Stripper. Figure 2 shows a traditional SWS design and its schematic representation. The contaminated water from the refinery enters the Flash Drum where the gases are separated from the liquid part (water and oil). The gas is sent directly to the top of the SW Stripper. The liquid is directed by the Feed Pump to the Feed Heat Exchanger where the inlet stream is heated up to the desired temperature, using hot water as heating agent. The heated sour water is sent to the SW Stripper. During the distillation (stripping) process the dissolved H_2S and NH_3 leave at the top of the SW Stripper and the purified water at the bottom. The heat for the distillation is provided by live steam injection at the bottom of the column. High efficiency of the SW Stripper is provided by a pump around consisting in a controlled recycled flow which leaves one tray of the column, it is cooled down by an air cooler and sent back to an upper tray. The stripped water bottom product is driven by the Striper Water Pump to a cooler and sent downstream to the absorption column for separation. This first design and model will be further referred as Model A.

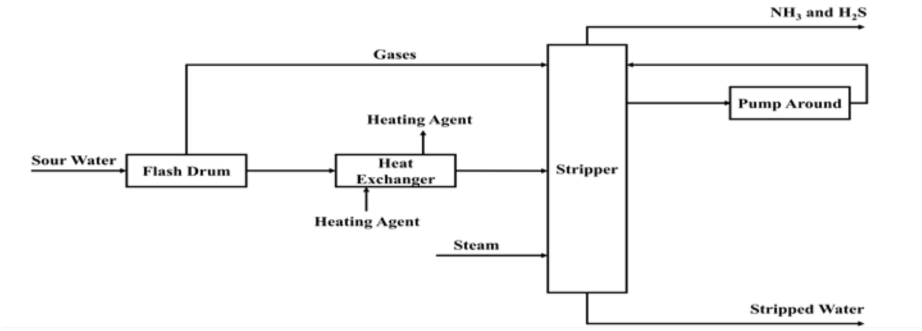

Figure 2. SWS flow sheet for Model A.

Table 1 lists the equipment of the SWS simulator.

Table 1. SWS equipment description [11].

Equipment Name	Description
SWS - V - 001	Flash Drum
SWS – P - 001A	Feed Pump
SWS - HX - 001	Feed Heat Exchanger
SWS - C - 001_TOP SWS - C - 001_MIDDLE SWS - C - 001 SWS - C - 001_BOTTOM	SW Stripper
SWS – P - 003A	Pump-Around Pump
SWS - EA - 001	Pump-Around Air Cooler
SWS – P - 002A	Stripper Water Pump
SWS - EA - 002	Stripped Water Air Cooler

Figure 3 represents the second investigated design for the SWS, in which the heating agent for the Feed Heat Exchanger of Model A was replaced by the stripped water from the bottom of the SW Stripper. This new design recovers heat and is intended to spare costs with the heating agent. This second design and model will be further referred as Model B. Figure 4 presents the SWS simulator implemented in Aspen Hysys for the SWS setup described in Figure 3.

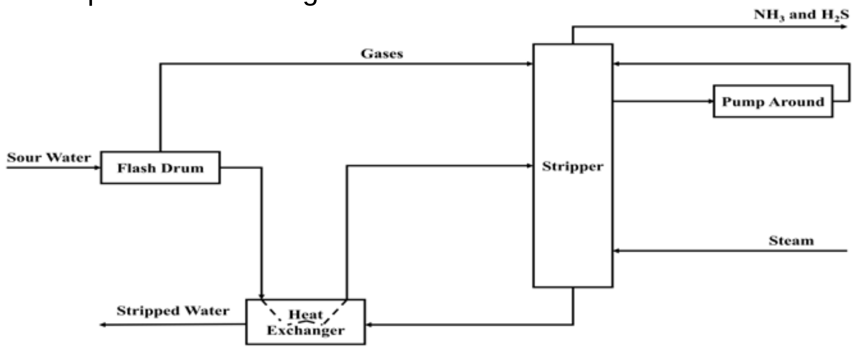

Figure 3. SWS flow sheet for Model B.

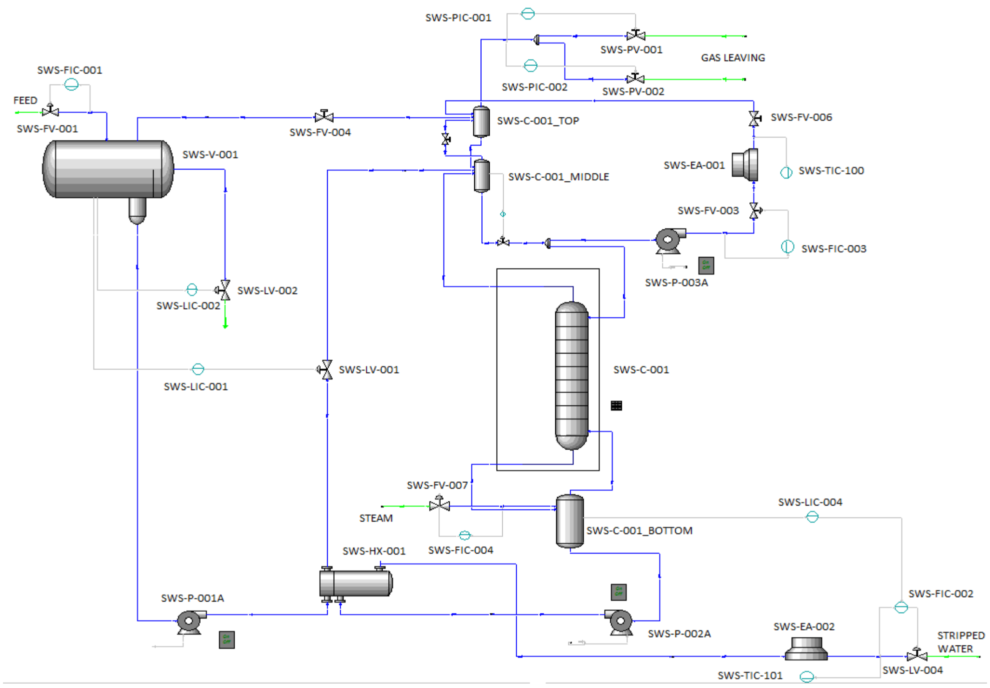

Figure 4. Model B implemented in Aspen Hysys.

Table 2 presents the feed stream composition [12-18]. The main parameters of the feed stream are: inlet feed pressure of 300 kPa, inlet feed temperature of 62.3 °C and mass flowrate of 19860 kg/h.

The most important and complex equipment of a SWS is the SW Stripper. Generally, the SWS stripper is modeled as a series of equilibrium stages [2, 3, 6, 7, 16]. The SW Stripper in both Model A and Model B, contains 50 equilibrium trays. Sieve trays were used for modeling the internal part of the column. The feed stream enters the column at tray 5. Tray 5 is critical because the pump around flow also leaves at this level and it is important to maintain the tray level. The pump around flow reenters the column in tray 1, where the vapors coming from the Flash Drum also enter the column.

Table 2. SWS feed stream composition.

Components	Mass Fraction
Hydrogen	0.0002064
i-Butane	0.0000107
n-Butane	0.0000251
Propane	0.0000352
Ethane	0.0000402
Methane	0.0000956
H_2O	0.9459771
H_2S	0.0344657
Ammonia	0.0191440

Model A and Model B designs contain the controllers listed in Table 3.

Table 3. Controllers used in Models A and B.

Controller Name	Description
SWS - FIC - 001	Inlet flow controller in the Flash Drum
SWS - LIC - 001	Water level controller in the Flash Drum
SWS - LIC - 002	Oil level controller in the Flash Drum
SWS - PIC - 001 SWS - PIC - 002	Top pressure controllers for the SW Stripper
SWS - FIC - 003	Flow controller for the pump around flow of the SW Stripper (SWS-EA-001)
SWS - TIC - 100	Temperature controller for the pump around of the SW Stripper
SWS - LIC - 004	Master loop of the bottom level controller for the SW Stripper which has as slave loop SWS – FIC - 002
SWS - TIC - 101	Temperature controller for the stripper water after EA-002
SWS - FIC - 002	Flow controller for the stripper water (slave loop of the bottom level controller, is in cascade with SWS – LIC - 004)
SWS - FIC - 004	Flow controller for the live steam injected at the bottom of the SW Stripper

Controllers are important because they affect the dynamics of the process [18, 19]. Most of them are PID controllers. Two types of control systems were used: feed-back control and cascade control. Cascade control was used for controlling the level in the SW Stripper.

Comparison of the two dynamic models

Model B design uses the hot water stream from the bottom of the SW Stripper to heat the Feed stream, instead of the external hot water utility of Model A. This new design shows energy saving incentives. The Models have been undertaken to several analyses in order to determine the design most appropriate for industrial implementation. Table 4 shows the main temperature, pressure and flow variables of the inlet and outlet streams, revealing also the overall mass balance of the plant.

Table 4. Main variables and mass balance of the plant for both Models A and B.

	INLET			OUTLET	
Model A	**FEED**	**Live steam Injected**	**Feed Heat Exchanger External Agent**	**Gas Leaving**	**Stripped Water**
Temperature [°C]	62.3	150	122	73.83	89.94
Pressure [kPa]	300	290	1800	225	600
Molar Flow [kmol/h]	1087	120.3	498.6	32.52	1175
TOTAL Flow	1207.3			1207.52	
Model B	**FEED**	**Live steam Injected**	**Feed Heat Exchanger External Agent**	**Gas Leaving**	**Stripped Water**
Temperature [°C]	62.3	150	-	78.58	60.21
Pressure [kPa]	300	290	-	225	400
Molar Flow [kmol/h]	1087	119.1	-	35.1	1171
TOTAL Flow	1206.1			1206.1	

As expected, Model A presents higher bottom temperature and higher pressure, compared to Model B. Model A shows lower temperature at the top of the SW Stripper. The Feed stream temperature to the SW Stripper is controlled with the Stripped Water flow, as the latter is already used for the bottom level cascade control (in the slave loop). Consequently, the temperature of the inlet stream in the SW Stripper of Model B is about 4 °C higher than in Model A. Table 5 presents the outlet streams composition.

Table 5. Mass fraction composition of the outlet streams from the SW Stripper.

	Model A		Model B	
Components	***Gas Leaving***	***Stripped Water***	***Gas Leaving***	***Stripped Water***
Hydrogen	0.0627	0	0.0579	0
i-Butane	0.0001	0	0.0001	0
n-Butane	0.0003	0	0.0002	0
Propane	0.0005	0	0.0005	0
Ethane	0.0008	0	0.0008	0
Methane	0.0036	0	0.00034	0
H_2O	0.1572	0.9843	0.1919	0.9861
H_2S	0.619	0	0.5722	0
Ammonia	0.1558	**0.0157**	0.1731	**0.0139**

Table 5 shows that all light hydrocarbons are found in the gas phase leaving the top of the SW Stripper. H_2S separation is very efficient as the whole H_2S amount can be found in the gas phase that is sent to further operations. The stripped water is free of H_2S but there is a small amount of NH_3 (1.39%). It is worthy to notice that NH_3 concentration is lower in the case of Model B design, favouring the separation. Figure 5 shows temperature and the pressure profiles of the SW Stripper along the column height.

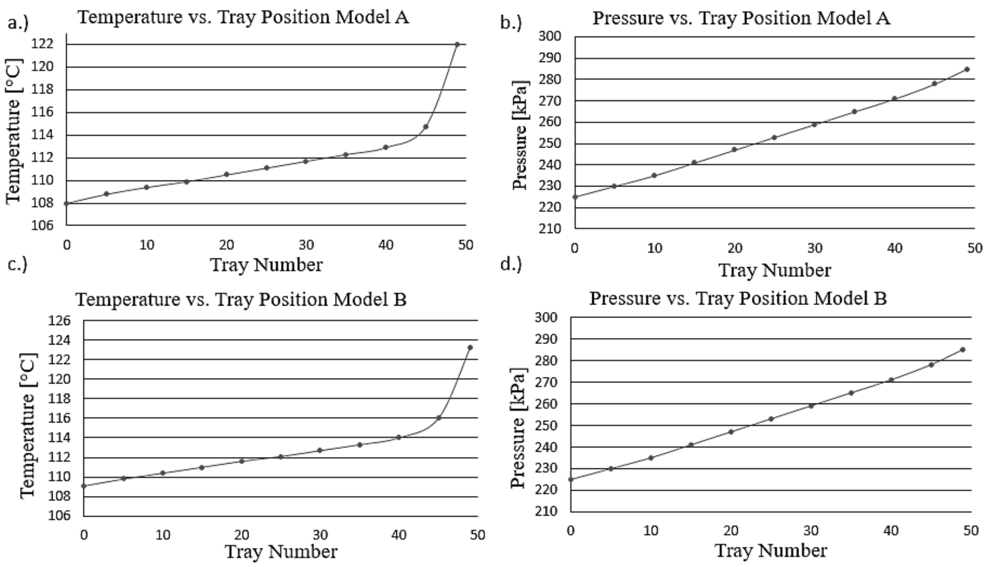

Figure 5. Temperature and pressure profiles of the SW column in function of the tray position (0 is the top of the column and 50 is the bottom of the column).

As expected, both the temperature and the pressure decrease from the bottom to the top of the column. The overall temperature profile is higher in the case of Model B. The main difference between the two models consists in their energy efficiency perspective. Model A uses utility water with the temperature of 122 °C, pressure of 1800 kPa and flow of 8984 kg/h in order to warm up the feed stream for the SW Stripper. Model B uses the bottom stripped water to warm up the feed stream to the SW stripper. The stripped water leaves the column at temperature of 127 °C and pressure of 1743 kPa. This makes possible to replace the warm water utility with a process stream leading to a significant energy saving of about 59 GJ/day.

Based on the above results it is relevant to conclude that Model B is more efficient than Model A and demonstrates incentives for industrial application. As a result, further analysis will be made on Model B.

Effects of changing the feed temperature

In order to show the SWS simulator behavior several operating scenarios were investigated. Two of them are presented in the following.

The operating scenario presented in Figure 6, shows effects of an increasing step change in the inlet feed temperature, from 63 °C to 80 °C. As the stripping temperature increases, more of the heavier components, such as H_2O and NH_3, leave at the top of the column, Figure 6.c. and Figure 6.d. The quantity of the H_2S removed remains the same at the top of the column, although Figure 6.b shows a decreasing profile. The latter is due to the fact that mass of the other top column components are increasing and consequently, the H_2S concentration is decreased.

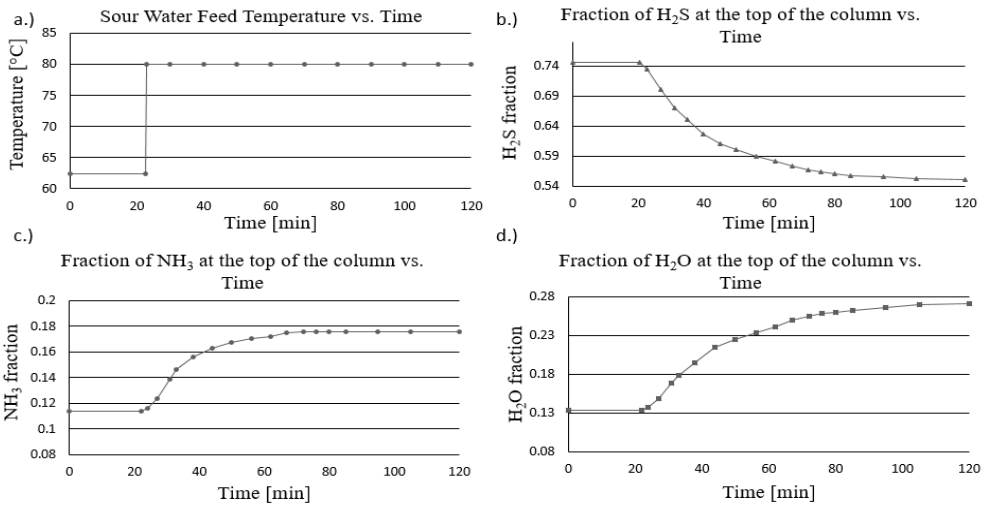

Figure 6. Effects of changing the SWS inlet temperature on the mass fraction of the components at the top of the column.

Effects of changing the pump around flow rate on the top column gas composition

In normal operating conditions, part of liquid leaves tray 5 of the column and after it is cooled down from the temperature of 100°C to the temperature of 60 °C it enters again the top of the column. This pump around increases the efficiency of the column. The operating scenario reveals the effects of decreasing followed by increasing of the pump around flow. Due to the pump around flow decrease from the value of 7800 kg/h to the value of 2000 kg/h, Figure 7.a, the top temperature of the column increases and higher amount of NH_3 component leaves at the column top.

During the reverse action, when at 77 minutes the pump around flow is increased from the value of 2000 kg/h to the value of 12000 kg/h, the temperature at the top of the column decreases and consequently, higher amount of the heavier components is condensing. Figure 7.b reveals an increase of the H_2S mass fraction due to the fact that both NH_3 and H_2O condensate and the vapor phase which leaves at the top of the column contains more H_2S compared to the other components.

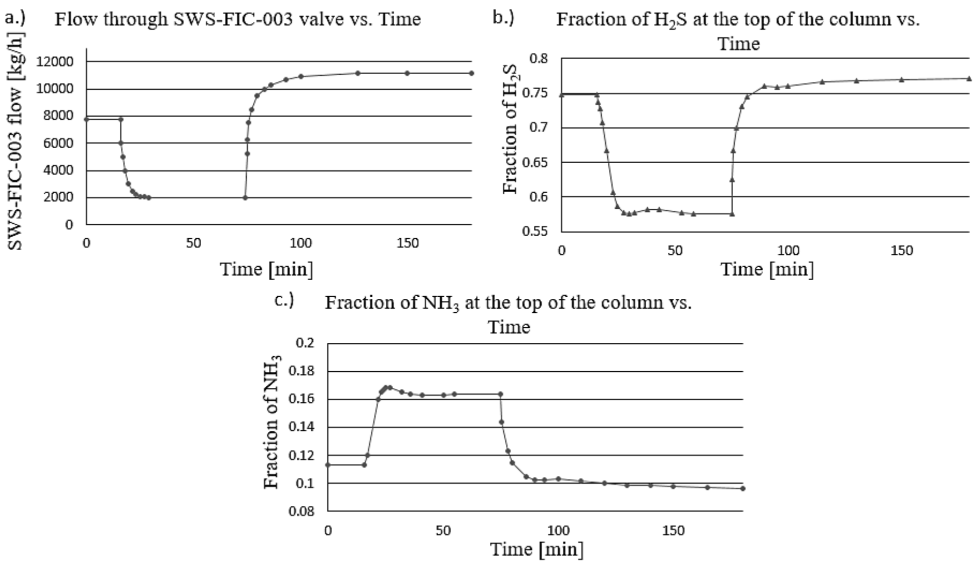

Figure 7. Effects of decreasing followed by increasing the pump around flow of the SW Stripper on the H_2S and NH_3 mass fractions at the top of the column.

Efficiency of the SWS-LIC-004 cascade loop

The bottom level in the SW Stripper is controlled by a cascade level control system. Cascade control loops have two measurement signals to control the primary level variable. The output (OP) of the primary controller (level master loop) determines the set-point (SP) for the secondary flow loop (level slave loop). The master loop of the controller is the SWS-LIC-004 and the slave loop of the system is the SWS-FIC-002.

In order to check the operation of the cascade level control system the set-point of the level in the bottom of the SW Stripper was changed from the value of 3 m to the value of 2.5 m. Figure 8 shows the result of this last operating scenario.

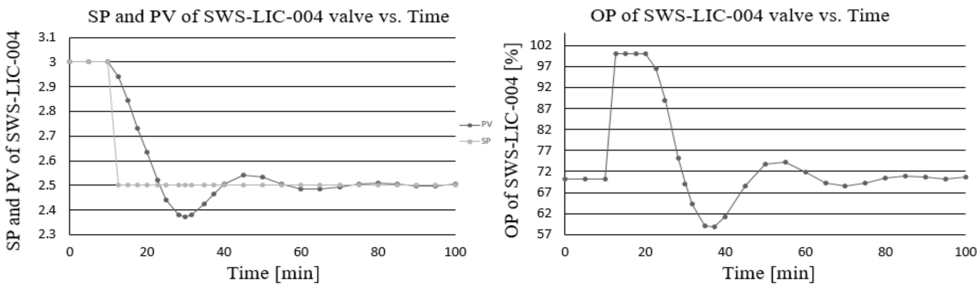

Figure 8. Effect of the level set-point change for the cascade control SWS-LIC-004; a. Changes of the level set-point variable SP and level process variable PV; b. Change of the master controller output (OP).

As a result of the level set-point SP change, Figure 8.a, the output of the level master controller opening percentage OP increases, Figure 8.b. Following a damped oscilation, the level PV is brought to the new set-point with zero offset and reduced overshoot, Figure 8.a.

CONCLUSIONS

Design and operation of the sour water stripping plant were investigated. Two dynamic models and their associated dynamic simulators were developed and implemented in Aspen Hysys simulation software. The results of the dynamic simulations are consistent with the data from the literature and with the measured data from the real plant.

Two dynamic models were investigated. Model A corresponds to the traditional design of the SWP unit, while Model B design uses an internal stream to heat up the feed flow. Investigated operating scenarios revealed that Model B is more efficient than Model A, as the former shows incentives from energetic perspective for reducing heat utilities and sparing costs. Better separation of the hazardous components is also achieved by the proposed Model B design. The same amount of H_2S is sent to the top of the column in both models but the NH_3 mass fraction concentration of 0.0157 remains in the stripped water stream for the case of Model A, while a diminished NH_3 concentration of 0.0137 is obtained for the Model B design.

Different control loops were proposed and implemented in the simulators for controlling pressure, level, flow and temperature, in either feedback of cascade configuration. Tests were run and results showed their effectiveness.

The developed simulators may be further exploited for the design of advanced control systems, elaboration of operator training software, operational optimization and investigation of new design improvements.

EXPERIMENTAL SECTION

The SWS models have been implemented in Aspen Hysys version V8.0 flowsheet simulation software. Model A and B parameters were calibrated on the basis of the literature data and data measured from the real plant [6, 12, 14-16].

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