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Research Article

## Simulation and Evaluation of Effective Solutions in Reducing Mercaptan and Sulfur in Liquid Gas Exit in Sulforex Unit

Mahdi Hamed Siam<sup>1</sup>, Farhad Shahraki<sup>2</sup>, Mohammad Reza Sardashti Birjandi<sup>3\*</sup>, Bahareh Bidar<sup>4</sup>, Mohammad Esmail Dorostkar<sup>5</sup>

<sup>1</sup> M.Sc Student, Department of Chemical Engineering, Shahid Nikbakht Faculty of Engineering, University of Sistan and Baluchestan, Zahedan, Iran

<sup>2</sup> Professor, Department of Chemical Engineering, Shahid Nikbakht Faculty of Engineering, University of Sistan and Baluchestan, Zahedan, Iran

<sup>3</sup> Assistant Professor, Department of Chemical Engineering, Shahid Nikbakht Faculty of Engineering, University of Sistan and Baluchestan, Zahedan, Iran

<sup>4</sup> Assistant Professor, Department of Chemical Engineering, Shahid Nikbakht Faculty of Engineering, University of Sistan and Baluchestan, Zahedan, Iran

<sup>5</sup> Refining Engineering Officer of Fluid Catalytic Cracking (FCC), Abadan Oil Refining Company, Barim, Abadan, Iran

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### 1. ABSTRACT

Liquefied petroleum gas (LPG) refers to the hydrocarbon gases propane, butane or their combination. Liquid gas is often used for heating purposes and vehicle fuel. In refineries, the hydrocarbon flow of propane, butane and pentane contains impurities such as methyl mercaptan, ethyl mercaptan and other mercaptans. In this research, the simulation of mercaptanization unit of Abadan refinery has been done. First, the unit was simulated in the ProMax software and after the validation of the simulation, the effect of process variables such as the caustic flow rate, caustic concentration, sour feed flow rate and washing column pressure on the concentration of mercaptan in product has been investigated. The concentration of mercaptans in the output product has been discussed. The results of the simulation show that the total calculation error is less than 10%, which indicates the accuracy of the simulation in steady state. Based on the simulation results, with the increase of caustic flow rate, concentration of caustic solvent and washing column pressure, the amount of produced product (ethyl mercaptan and methyl mercaptan) decreases. Only by increasing the flow rate of sour feed, the amount of produced product will increase.

**Keywords:** Caustic, Solvent, Mercaptan, Simulation, Washing Column, Oxidizer.

### 1. INTRODUCTION

Liquefied petroleum gas or LPG is one of the best products of gas refineries and is composed of a mixture of hydrocarbon compounds with common sulfur compounds as elemental sulfur, hydrogen sulfide, mercaptans (RSH) and so on. The increasing use of heavy crude oil with high sulfur and the popularity of processing heavier wastes in refineries along with stricter environmental norms (up to 20 ppm mercaptan in light hydrocarbon products) is a growing challenge for process designers and refineries [1]. Sulfur compounds in fuels such as LPG cause problems in two ways: they release toxic gases during the combustion process and damage metals and catalysts in engines and fuel cells. These compounds are usually removed using a liquid treatment that absorbs the LPG's sulfur compounds, but this process is somewhat difficult and requires cooling and reheating of the hydrocarbon, which makes the fuel less energy efficient. To solve these problems, researchers have turned to solid metal oxide adsorbents, but these adsorbents have their own challenges. While they operate at high temperatures and eliminate the need to cool and reheat the fuel, their performance is limited by stability issues. Caustic is the primary reagent for extracting mercaptans from hydrocarbon streams, because it is economical and more importantly, it is environmentally acceptable [2].

\* m.r\_sardashti@eng.usb.ac.ir

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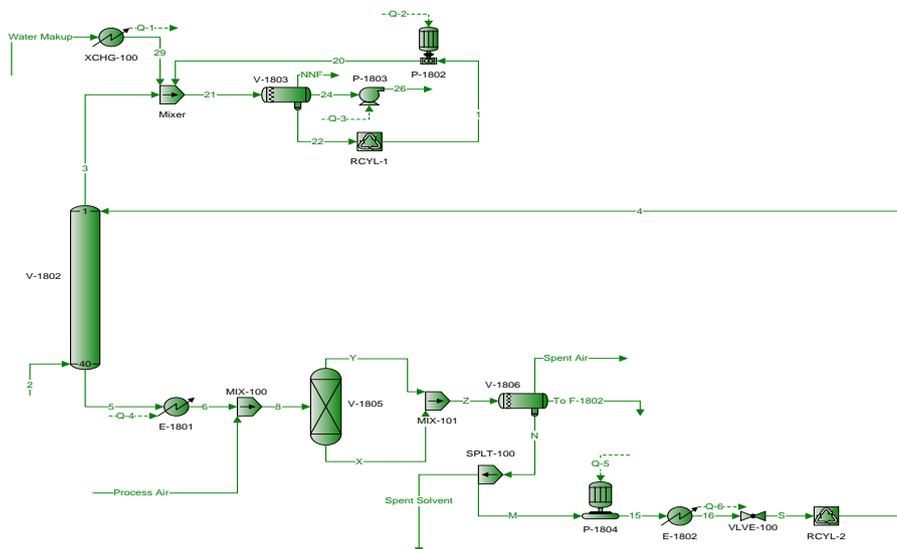
## 2. SIMULATION

### 2.1. Thermodynamic model

According to the recommendation of ProMax, for modeling a chemical system containing caustic, the caustic treatment properties package should be used to obtain valid results. In this property package, the ELR electrolyte model is used to obtain accurate viscosity values for caustic solution. In addition, the Promax manufacturing company recommends that the COSTALD relationship be used for the molar volume model when simulating the system containing caustic [3].

### 2.2. Model validation

Figure 1 shows the simulation schematic of LPG feed sweetening process and removal of mercaptans from it by caustic solvent flow in Abadan refinery using ProMax software.



**Figure 1.** Schematic simulation of the current LPG flow purification process in Abadan refinery with ProMax software

## 3. EFFECT OF PROCESS PARAMETERS

### 3.1. Assessment of caustic flow rate

According to Figure 2, as well as the amount of methyl mercaptan and ethyl mercaptan in the input feed, the content of ethyl and methyl mercaptans in the product has been reduced by increasing the caustic flow rate. The reason for this is the increase in the amount of caustic along with the increase in the flow rate of the solvent and the increase in the reaction between caustic and sulfur.

### 3.2. Evaluation of caustic concentration

According to Figure 3, caustic soda concentration has a strong effect on reducing the sulfur content of the output product. With the increase in soda concentration, the reaction between caustic and sulfur increases, as a result, the solvent can perform sweetening operations more easily and better.

### 3.3. Evaluation of sour feed flow rate

According to Figure 4, the increase in sour feed flow rate has a greater effect on ethyl mercaptan, and the upward trend has become more noticeable for this sulfur compound. Of course, according to this figure, there is an upward trend in the concentration at the output, but with the difference that the reactivity of methyl mercaptan is much higher than that of ethyl mercaptan, and for this reason, the values are slightly higher for ethyl mercaptan.

### 3.4. Pressure analysis of washing column

According to Figure 5, the sulfur content (ethyl mercaptan and methyl mercaptan) of the product was gradually reduced by increasing the pressure of the washing Column. In the process of washing mercaptans, increasing the pressure increases the absorption of mercaptans, and as shown in Figure 5, the sulfur content in the output product is high at low pressures, and these values will cause the product to go out of production specifications; therefore, it is better to perform caustic washing at high pressure.

## 4. CONCLUSION

In this article, the process of caustic washing of sour hydrocarbon flow with high sulfur content is simulated by ProMax software (case study of Abadan oil refinery). At first, the simulation validation determined. Then the effect of process variables such as the caustic flow rate, caustic concentration, sour feed flow rate and washing column pressure on the concentration of mercaptan in product has been investigated. According to the parameter evaluation, with the increase of caustic flow rate, concentration of caustic solvent and washing tower pressure, the amount of produced product (ethyl mercaptan and methyl mercaptan) decreases. Only by increasing the flow rate of sour feed, the amount of produced product will increase.

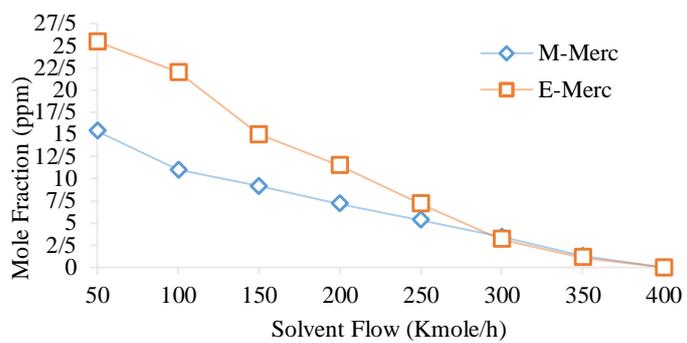


Figure 2. The effect of caustic solvent flow rate changes on the content of mercaptans in the product

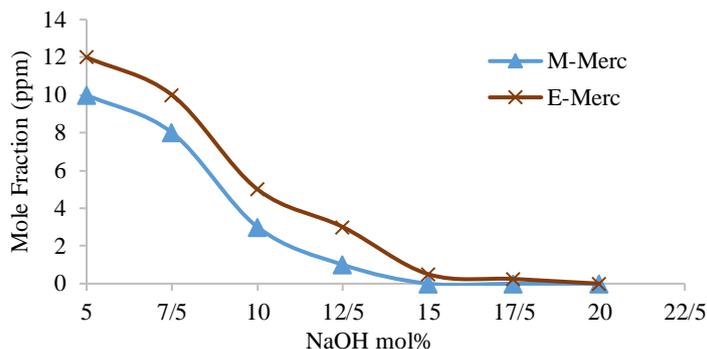


Figure 3. The effect of caustic concentration changes on the content of mercaptans in the product

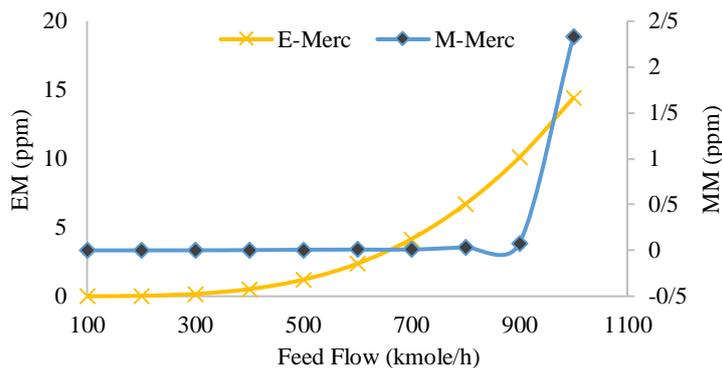


Figure 4. The effect of sour feed flow rate changes on the content of mercaptans in the product

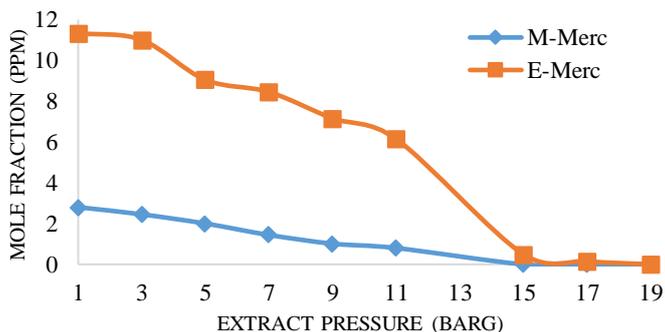


Figure 5. The effect of pressure changes in the washing column on the content of mercaptans in the product



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