PILOT SCALE RECTIFICATION COLUMN MODELING AND DESIGN FOR THE SEPARATION OF FATTY ACID MIXTURE

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ABSTRACT

Rectification is one of the distillation techniques which is widely used in the chemical industry to separate the miscible liquids mixture. Heat acts as the separating agent in this operation. The main objective of this research is to model, simulate and optimise a pilot scale rectification process in separating a mixture of fatty acids by Aspen Plus simulator. The input specifications for the simulation are based on the design specifications of the rectification column. A base case model is developed by the rigorous simulation model in Aspen Plus (RadFrac), with suitable thermodynamic model chosen. Shortcut simulation and manual calculation are carried out to estimate some parameters for rigorous simulation. Next, sensitivity analysis is carried out for the base case model, in which will help us to determine the parameters to be optimised and its range for optimisation. Finally, parametric optimisation is performed to obtain the optimum operating conditions of the rectification column.

Keywords: Simulation; Optimisation; Rectification; Sensitivity Analysis; Aspen Plus; Fatty Acids.

1.0 INTRODUCTION

1.1 Rectification

Rectification is one of the distillation techniques which is widely used in industry. It is a thermal liquid separation process and generally named as distillation in industry. Other distillation techniques are flash distillation, steam distillation, azeotropic distillation and extractive distillation (Larian, 1958). Rectification is known as fractionation in petroleum refinery (Larian, 1958).

Rectification is a separation technique that based on the difference of the physical properties, specifically, relative volatilities of the components in liquid. Rectification can be applied to separate a binary mixture and multi-component mixture. Billet (1979) reported that rectification gives better separation with higher product purity compared to simple distillation. In rectification process, vapor mixture and condensate flow in counter-current direction. This enhances optimum exchange of material between two streams (i.e. vapor mixture and condensate). As a result, an effective separation occurs. In this research, the rectification column is packed with structured packing (MellapakPlus). Olaño *et. al.* (1994) had reported that packed column posses greater flexibility with lower design cost and lower energy requirements since packings are designed to provide higher surface area per unit volume, efficient flow of contacting fluids, and lower pressure drop. The objective of the rectification process is to produce stearic acid with 98% purity, which is primarily used in the manufacturing of foods, pharmaceuticals, flavours and cosmetics.

1.2 Simulation and optimisation

Process modeling, simulation and optimisation are practiced to reduce production cost, shorten research and development period, increasing the process effectiveness, improving product quality, handle the sophisticated problem in industry (Turton *et. al*, 1998). Process simulator, such as Aspen Plus simulator, plays an important role to accomplish these objectives. Simulator can also be used to design and scale up

a new plant, or optimise an existing plant. The general steps for running a process simulation are illustrated by Fig. 1 (Turton *et al.*, 1998)

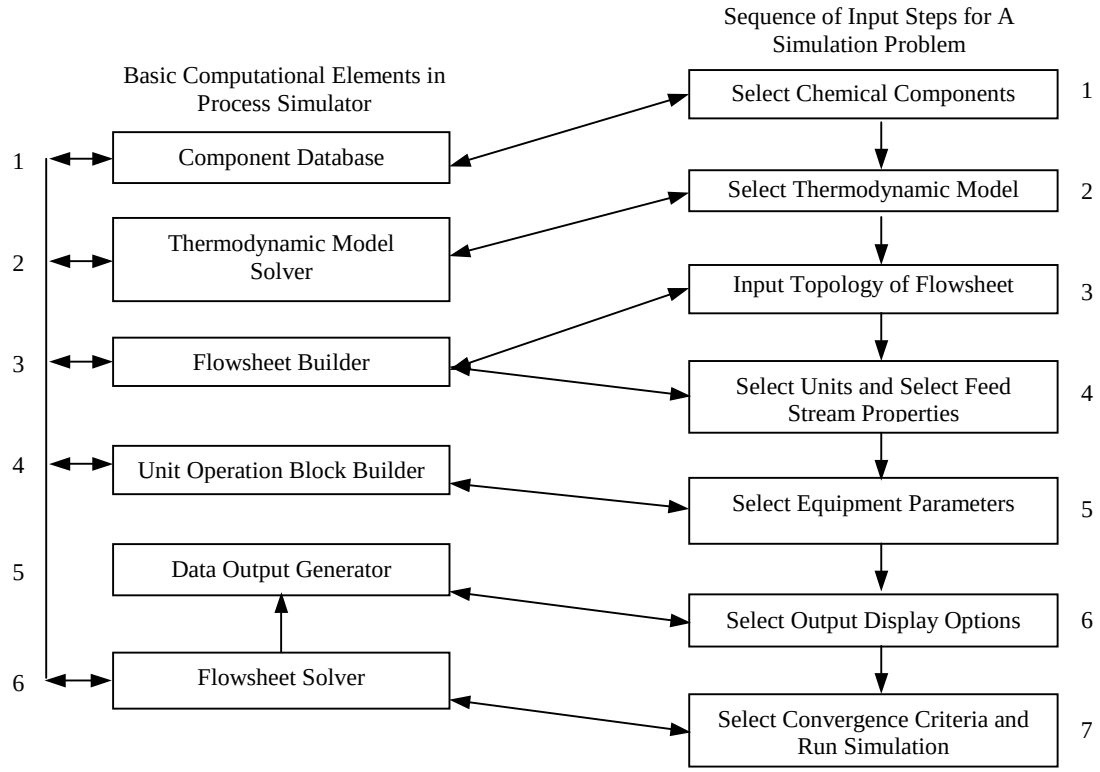

Fig.1. Relationship between basic computational elements and required input to solve a process simulation problem

2.0 METHODOLOGY

A shortcut model (DSTWU) in Aspen Plus simulator and manual calculation (i.e. Fenske and Underwood equations, and Gilliland correlation) are used to predict the initial column pressure and reflux ratio for RadFrac model. The rectification process is modelled and simulated by using RadFrac model in Aspen Plus simulator according to the steps in Fig. 1. The column specifications and the feed conditions are tabulated in Table 1.0 and Table 2.0, respectively. The column is shown in Fig. 2. According to Aly and Ashour (1992), the column is operated under vacuum to minimise the risk for chemical decomposition of the fatty acids. The thermodynamic model called UNIQ-NTH is used for simulation in this research. The Nothnagel (NTH) model takes account of the effect of dimerisation, solvation and association of fatty acids in vapour phase at low pressure (Aspen, 2000). These phenomena should be taken into account because the association will drastically affect the volatility of the acids (Aly and Ashour, 1992). For determining the column pressure drop, a commercialise software called Sulpak 3.0 (Fig. 5) is used. Besides the column pressure drop, capacity, flow parameter and liquid load of the column can also be predicted by Sulpak. Steps in determining the column pressure drop which subject to the operating condition is shown in Fig. 3. The rectification column model is shown as Fig. 4.

Table 1.0 Specifications of the column

Parameters	Specifications
Packing height (m)	6
Column diameter (m)	0.22
Column packings	Structured packings of Sulzer (MellapakPlus)
Number of theoretical stages equivalent to packings height	30
Feed stage	17
Column Top Pressure (mbar)	4

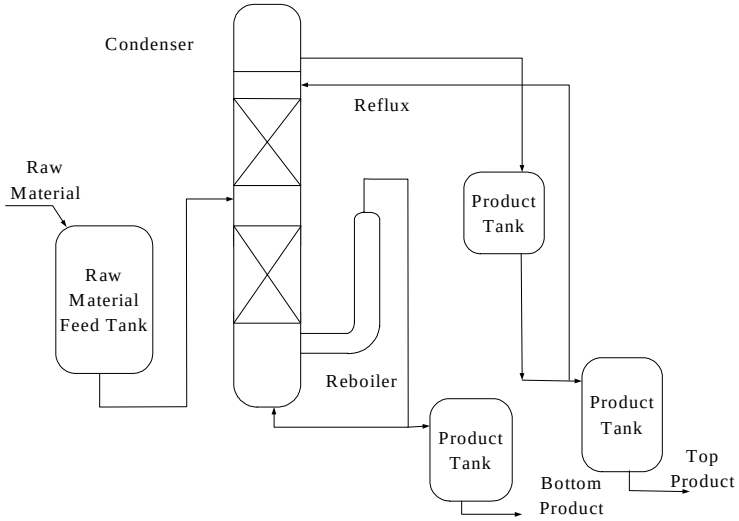

Fig. 2. The pilot scale rectification column

Table 2.0 Column feed condition

Components	Composition (w/w)
Lauric Acid	0.005
Myristic Acid	0.011
Palmytic Acid	0.614
Stearic Acid	0.370
Feed flow rate	30 kg/hr
Liquid fraction	1
Feed temperature	200ºC
Feed pressure	20 mbar

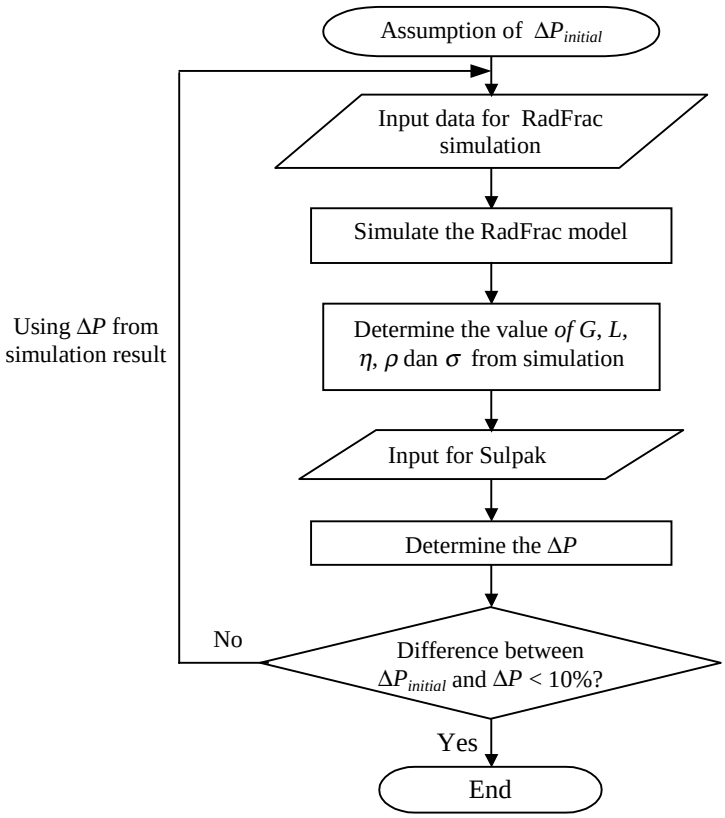

Fig.3. Steps to determine the column pressure drop

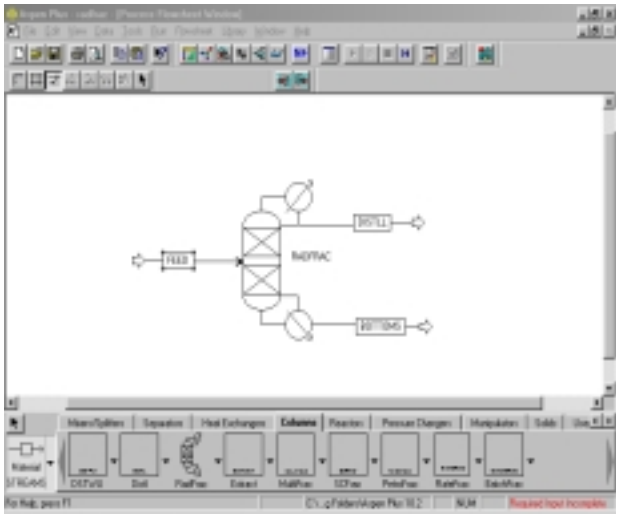

Fig.4. RadFrac model in Aspen Plus simulator

Fig.5. Interface of Sulpak 3.0

3.0 RESULTS

By using Aspen Plus simulator and Sulpak 3.0, the column pressure drop is 11.48 mbar with the top pressure 4 mbar. The results of simulation using Aspen Plus simulator are shown by figure 6, 7, 8 and 9.

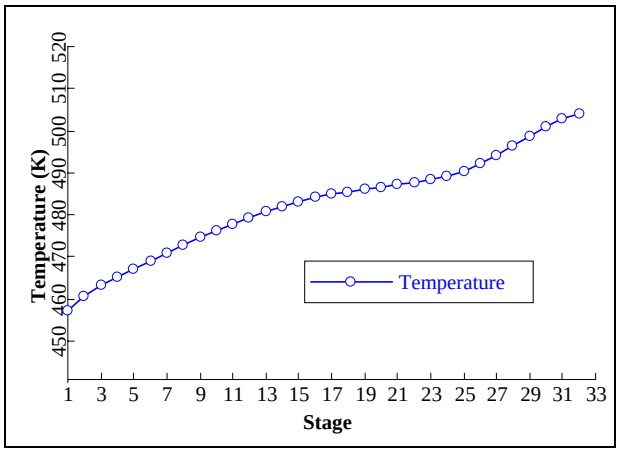

Fig. 6. Temperature (K) versus stage number

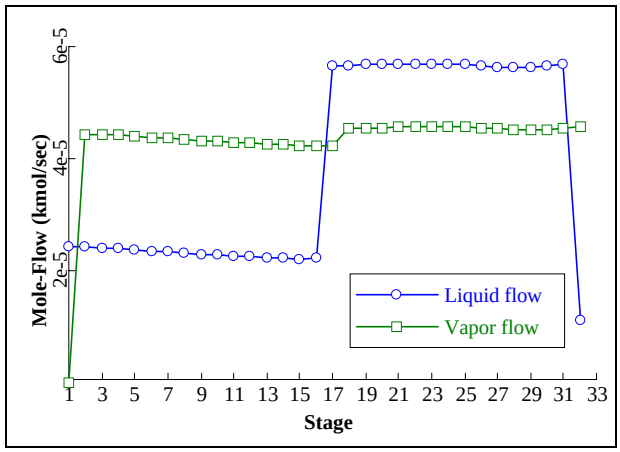

Fig. 7. Mole-flow versus stage number

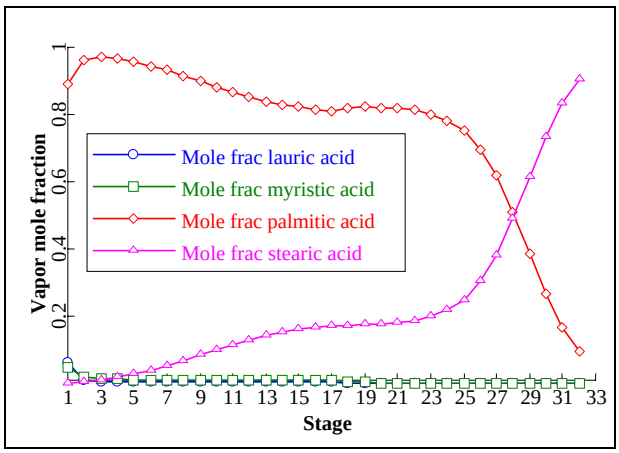

Fig.8. Vapor mole fraction versus stage

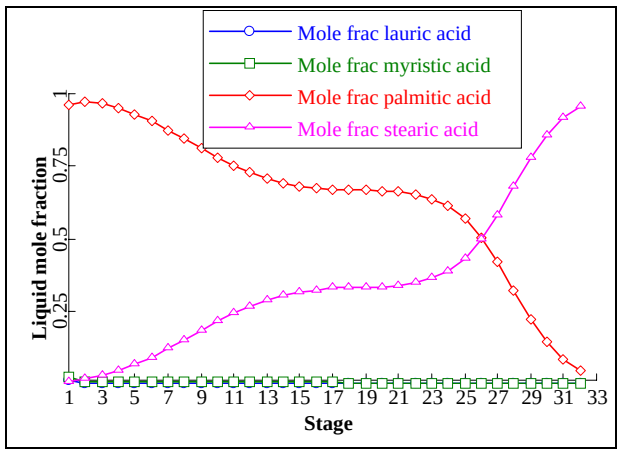

Fig. 9. Liquid mole fraction versus stage

The results of simulation depend on the availability and precision of input data such as material composition, geometric design targets and heat requirements (Gaiser *et. al.*, 2001). Therefore, sensitivity analysis has been carried out. Zeck (1993) has defined the sensitivity analysis as an investigation of the effects exerted by changes in the degree of sensitivity on the output variables characterizing the behaviour of the system, e.g., chemical engineering system. In this research, sensitivity analysis is done to identify the critical variables or parameters, and the range of parameter for optimisation. The results of this analysis are illustrated in Figure 10 to 15.

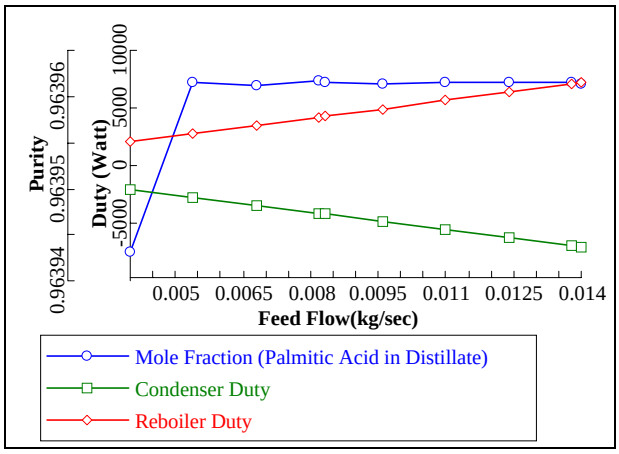

Fig.10. Purity and duty versus feed flow

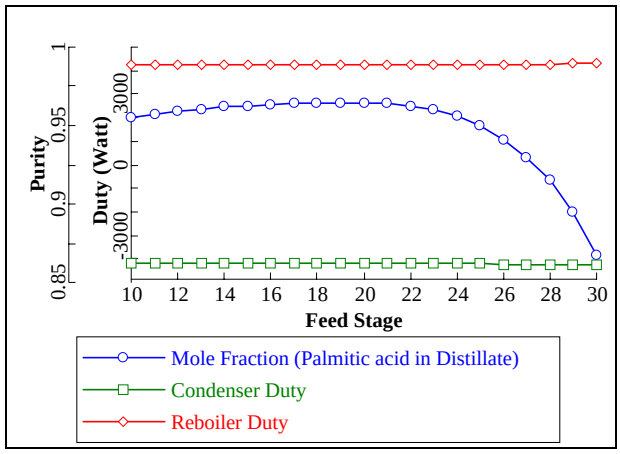

Fig.11. Purity and duty versus feed stage

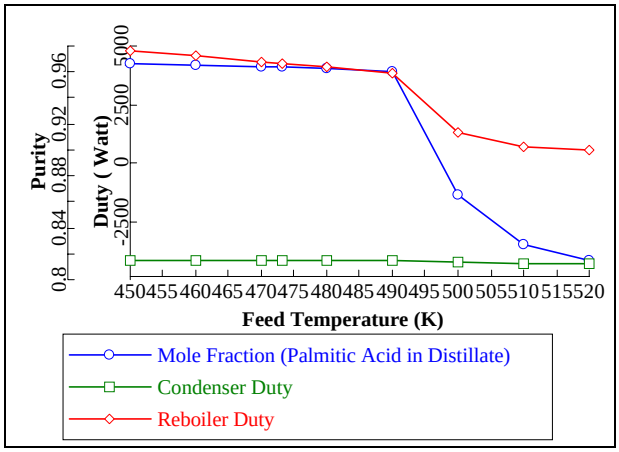

Fig.12. Purity and duty versus feed temperature

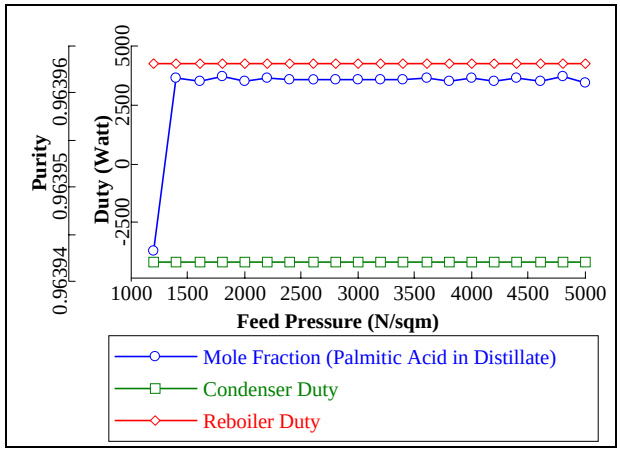

Fig.13. Purity and duty versus feed pressure

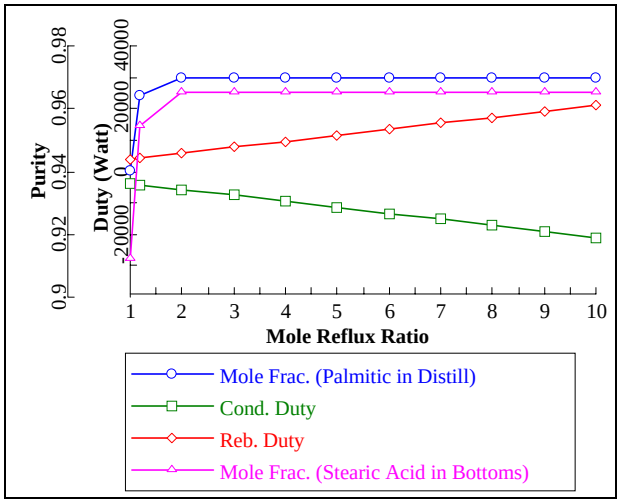

Fig.14. Purity and duty versus mole reflux ratio

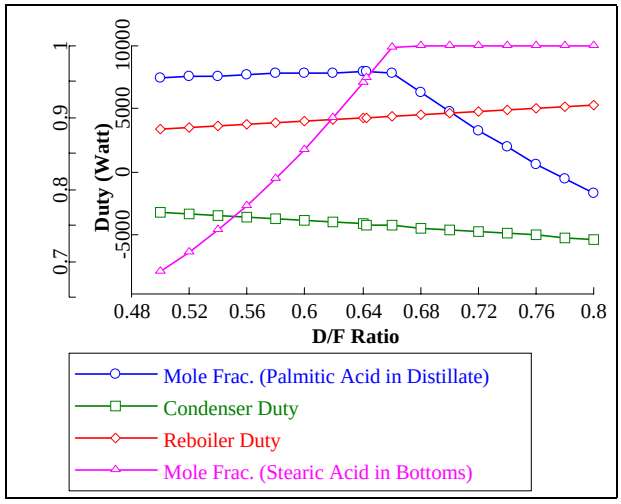

Fig.15. Purity and duty versus distillate/feed ratio

Fig. 11 and 13 show that heat duty of reboiler and condenser are less sensitive to the feed location and feed pressure (within certain range). The duty increase with mole reflux ratio, distillate/feed ratio and feed flow rate (as shown by Fig. 10, 14 and 15). Meanwhile the reboiler duty is reduced when the feed temperature is rising. Palmitic acid in distillate and stearic acid in bottom product increase to certain purity and then constant with increasing the mole reflux ratio (Fig. 14). The purity of stearic acid in bottom product is also changing in the same trend when distillate/feed ratio is increased. Therefore, the purity of stearic acid in bottom product is set as the objective function for optimisation, and the variable is reflux ratio. The objective is to increase the purity of stearic acid with minimum reboiler duty. According to Skogestad (1997), the separation (factor) can be increased by either increasing the number of stages in the column or the energy usage (i.e. the reflux).

Parametric optimisation of the column is done by the optimisation function in Aspen Plus simulator. The model is then resimulated in Aspen Plus and Sulpak (follow the same steps in Fig.3) to ensure the feasibility of the optimum condition. The results after optimisation is that the purity of product and the reflux ratio are increased. Meanwhile, the condenser and reboiler duty are reduced (Table 3.0). However, the feed flow rate in this case is also decreased to avoid flooding or overflow in the column.

Table 3.0 Comparison of results (before and after optimisation)

	Before optimisation	After optimisation
Purity (Palmitic acid in distillate) (%)	96.4	96.7
Purity (Stearic acid in bottom product) (%)	95.5	98.0
Condenser duty (kW)	– 4.2050	– 3.9776
Reboiler duty (kW)	4.2616	4.0072
Reflux ratio	1.20	2.44
Feed flow-rate (kmol/hr)	0.1130	0.0677

4.0 CONCLUSION

A rectification model for separating a mixture of fatty acids has been developed in Aspen Plus simulator. The selected thermodynamic model is UNIQ-NTH. Sensitivity analysis has also been carried out to identify the critical parameters/variables the effect of variables (manipulated) on certain parameters. In this research, optimisation results in lower condenser and reboiler duty, but higher product purity.

5.0 ACKNOWLEDGEMENTS

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