Expert System

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Abstract

A semi-quantitative framework employed to examine risk within chemical process industries (CPI) was initially developed over 60 years ago and then formalised as HAZOP by Kletz (1983). Nevertheless, the need for automation was soon evident as Parmer and Lees (1987) explored HAZOP automation, pioneering a rule-based, qualitative reasoning approach to identify hazards. The tool was developed to address the strong dependence on experienced personnel to conduct adequate HAZOP studies, by facilitating the passage of key risk assessment information. Nowadays the advent of big data allows us to make more rigorous quantitative models, as such, a data driven approach to HAZOP Automation was developed to make use of the technology and allow the addition of new information to the study tool to fully augment the operations of the staff. The Expert System achieves the aforementioned objectives by connecting an Object Relational Model Database to a dynamic user interface through a RESTful API, allowing the user to perform statistical analysis such as regression and classification in order to make more site-specific models, guiding the user throughout the data collection stage and safeguard selection by suggesting relevant tests, providing functions to evaluate back of the envelope design calculations and suggest best practices for powder handling and powder explosion mitigation required to meet industry standards. Nonetheless, the software provides an algorithm to estimate risk quantitatively using Fault and Event Tree Analysis, of which architecture can be fully developed by the user, who can also manually describe each leaf of the tree to also model the process qualitatively. However, the tool provides an Expert System feature to perform a more traditional HAZOP automation as the user will be provided with a complete HAZOP study table once relevant information about the process are typed into an excel file allowing for a fast implementation of the framework or a first iteration of a more robust investigation aiding the user in all the aspects of the HAZOP study.

Key words: HAZOP, API, Fault tree, Event tree

I. Introduction

The purpose of this project was to design a distillation column, associated flow system and feed heat exchanger to produce streams with target purity of 99.8 mol percent benzene in the top product stream and 99.5 mol percent toluene in the bottom product stream of the distillation column. The feed consisted of a flow of 35 tonnes/h benzene (77 mol percent), toluene (29.9999 mol percent) and hydrogen sulphide (0.0001 mol percent) mixture at an ambient temperature of 15°C. An AES shell and tube heat exchanger was used to preheat the feed before entering the distillation column with the heating medium of steam at a temperature of 162.65°C (roughly 30°C above the boiling point of toluene at the column pressure of 1.86 bara). The size of the column and size of the pump was calculated on the basis of this flow rate.

II. Storage tank Flow Systems

A. Feedstock Storage tank

Since the flash points of toluene and benzene are less than the ambient temperature, an internal float roof tank is most appropriate. The tank will be a cylinder with a conical roof to prevent build up of rain on top, while keeping material costs low. The liquid will be held entirely within the cylindrical portion of the tank, as the floating roof cannot enter the tapered section. The floating roof requires a space of 0.5m. The tank must hold feed stock for 3 days of production, which is $2873m^3$, plus an ullage of 10 percent, so a total volume of $3160m^3$.

$$V = \frac{\pi D^2 L}{4} \tag{1}$$

Using $\frac{L}{D} = 1$ as a baseline, so L=D, in the equation 1 , the required value for L and D was found to be 16.1m, including the 0.5m for the floating roof. The external roof will be conical, with a 1:5 slope. Carbon steel will be used as the tank material, as it is a very cheap material to use and the corrosion from the hydrogen sulfide at 1 part per million will be minimal, but to allow for this a slightly larger corrosion factor will be used for the wall thickness. The standard factor is 2mm, so 2.5mm will be used as at this concentration its corrosive effects will not be large. The equation used to calculate wall thickness is eqaution 2

$$e = \frac{PiDi}{2f - Pi} + C \tag{2}$$

where e, Di and C are in mm, and Pi and f are in $\frac{Ns}{mm2}$.

III. Piping decisions

The pipe diameter from the tank was calculated from two requirements. First, that the feed was 35 tonnes per hour, and second, that the ideal flow rate for liquid in a pipe is is 1-3m/s. The midpoint, 2m/s was used, and a volume calculated using a density of 873.5kg/m3 to estimate the required pipe width (8.4mm). The closest standard gauge pipe[**?**] was a 3 G/R pipe, with internal diameter 8.4926mm. By calculating the cross sectional area and dividing the volume by cross sectional area, this resulted in a flow rate of 1.97m/s. The pipes will be standard commercial steel pipes as additional corrosion resistance is not necessary at such low concentrations on hydrogen sulfide. They are beneficial as they also have a very low surface roughness, 0.046mm (Table 5.2, in [**?**]).

IV. Pumping

The pump to be used is a Chemstar centrifugal pump. A centrifugal pump is more appropriate than a positive displacement pump as it is not dealing with high pressure, high viscosity or abrasive materials, and a very continuous flow is desired.

The pump lies 5m of piping from the base of the feed storage tank. In this distance there are two 90 degree elbows and one normally open gate valve, as well as inflow effects from the tank into the pipe, and two pipe couplings have been added as an estimate. This results in a velocity head of 2.13, or a head loss of 0.42m. The frictional losses from the pipe in the same distance are 0.22m, for a total head loss of 0.64m. The pressure exerted by the floating roof on the feedstock is 1.1 bara, and the minimum liquid height is 1.5m above the outlet. The vapor pressure was calculated to be 0.77m. This results in a NSPH available of 12.9m.

The column inflow point is 16.8m above ground level, resulting in a height gain of 15.3m from the tank. The total head loss due to 6 90 degree elbows, 4 normally open gate valves, entrance effects into the pipe and 6 couplings is 1.09m, and the head loss due to friction the full 80m of pipe is 3.55m. The outflow must be at 1.86bara, or 0.76 bar above the initial pressure, resulting in a necessary head gain of 8.87m. The head loss in the heat exchanger is 2.12m. The total head requirement from the pump, when the storage tank is at its most empty, is 31m. The volume flow rate of the pump is $40\frac{m^3}{s}$. By using the Chemstar pump information graphs [?], it can be seen that an impeller diameter of 162mm is required, and a power of 5kW. The pump will operate at an efficiency of 66 percent.

V. Heat Exchanger Design

Heat exchangers can be classified by flow arrangement or by construction. The selected flow arrangement for this design is a counter current flow which provides a more consistent temperature profile across the device as such reducing the likelihood of differential expansion. the temperature profile is illustrated in Fig. 1. (b). from [?] Additionally, the heat exchanger will have a tubular construction more specifically a shell and tube since as mentioned in [?] ‘The most commonly used type of heat-transfer equipment is the ubiquitous shell and tube heat exchanger’.

A. Temperature specification

When designing the heat exchanger we start from the requirements by specifying to what temperature our feed needs to be raised. To calculate the bubble point of the stream we can use Antoine’s equation as displayed by equation 3. Assuming that the pressure of the heat exchanger is at the same pressure of the top column (1.86 bar) we obtained a bubble point temperature of 379.42K. The temperature was found using goal seek on excel, more detailed calculations can be found on the Appendix.

$$log_{10}(P^*) = A + \frac{B}{(C+T)} \tag{3}$$

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counterflowprofile.png
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Fig. 1. shows the temperature profile of a counter current flow of a shell and tube pass heat exchanger

B. Selection of Heat Exchanger

The design we have chosen is an exchanger with a split backing ring floating-head and E-type shell (AES). This is the most versatile choice in order to find a compromise between capital costs of the equipment and the maintenance costs which might be higher for cheaper alternatives such as the fixed tube sheet design that is harder to clean as such limiting its operation to the use of low fouling liquids. Nevertheless, the floating head also allows for expansions that might be problematic in cheaper designs. Selcetions of heat exchangers are categorised by the TEMA standards using letters, the chosen design will meet standard E as illustrated in Fig.2.

C. Fluid Allocation

fluid allocation is another major consideration of heat exchanger design. This is because depending on which fluid is flowing through the shell or the pass, we can lower total costs

TEMA arrangements.png

Fig. 2. shows TEMA arrangements classifications by letters

and increase heat transfer coefficient. The former can be achieved by choosing the more corrosive fluid that has the greatest tendency to foul the heat transfer surface and is higher in pressure and temperature to flow on the tube side. This will reduce the cost of expensive alloy or clad components required for corrosive substances, it will make cleaning easier and reduce capital costs as high-pressure tubes will be cheaper than a high pressure shell. In our case we opted for steam flowing through the shell side and the mixture flowing through the tube side. This is because our mixture contains hydrogen sulfide which is a corrosive compound and our heating medium is non-fouling and non-corrosive and not at very high pressure or temperature.

D. Thermal Design Procedure

1) Duty specification of the heat exchanger
: The duty of the heat exchanger can be calculated from equation 4.

$$\dot{Q} = \dot{m}C_p(t_2 - t_1) \tag{4}$$

where Q is the duty, m is the mass flowrate, C_p is the specific heat capacity normalised by mass and t_1, t_2 are the temperature of our feed mixture at the inlet and the outlet respectively. to do this we needed to compute a weighted average using the mass fraction of each species to scale their specific heat capacity contribution to the mixture's specific weighted average. Data for the physical properties was found in [**?**] and [**?**] using average temperatures for our estimate of C_p. Finally in order to compute the heat load we required to determine the terminal temperatures for the feed (t1 and t2). The full detailed calculations can be found in appendix and Table.7. summarises results from the iterations.

2) Mean temperature difference
: The log mean temperature difference T_{lm} was calculated using the equation given in [**?**]. Standard practice for shell and tube heat exchangers dictates estimating the "true temperature difference" T_{lm}, from T_{lm} by applying a correction factor F_t to allow for the true counter-current flow. For this design, as steam is condensing, $F_t = 1$ since there is no temperature difference between the inlet and outlet streams for the shell side. Hence, the value for T_{lm} for this design was equal to T_{lm}. As the correction factor is greater than 0.75 it can be deduced that an economic heat exchanger design can be achieved.

3) Estimate of the number of tubes and the diameter of the shell
: The tube dimension and arrangement choice is also crucial for our design as different arrangements will make our device easier to clean and facilitate general maintenance to be carried out and the tube diameter can affect anything from fouling to capital costs. In fact, according to [**?**] the standard dimensions suggested are 20 mm outside diameter, 16 mm inside diameter and 4.88 m long steel tubes (3/4 in x 16 ft) should be used to start design calculations. These are preferred for most duties, as they will give more compact,

and therefore cheaper, exchangers. Moreover, according to equation5 the velocity of the inner fluid is inversely proportional to the square of the pipe inner diameter. as such the smaller the inner pipe diameter the faster the fluid flowing through the tube. A fast flow is desired as the higher allowable velocity in the tubes will reduce the fouling. Furthermore, we selected a triangular pattern with a pitch 1.25 times the tube outside diameter in order to facilitate cleaning and other maintenance protocols.

$$v_i = \frac{4Q}{\pi D_i^2} \tag{5}$$

The calculated bundle diameter from iterations was 0.222m. Since we are using a split-ring floating head from [**?**] Figure 12.10, shell bundle clearance is 51mm between outermost tubes and shell internal diameter. Hence, shell diameter =324mm. This value falls in the range required to meet the TEMA standard and the British standard BS 3274 design mentioned in [**?**].

Baffles are used in the shell to direct the fluid stream across the tubes, to increase the fluid velocity and so improve the rate of transfer. The most commonly used type of baffle is the single segmental baffle from [**?**] accordingly It is recommended for this design that the single segmental baffles are used. Since we are using condensing steam for our heating medium, the baffles should be rotated through 90o to avoid restricting the condensate flow. In the same section of [**?**] is also suggested to opt for a 25 percent baffle cut, a baffle cut is the height of the segment removed to form the baffle, expressed as a percentage of the baffle disc diameter. This percentage affects both the friction factor and the heat transfer factor as shown in Fig.3., an optimum value of (20 -25) should give high heat-transfer rates, without excessive pressure drops.

4) Estimate of the tube side pressure drop

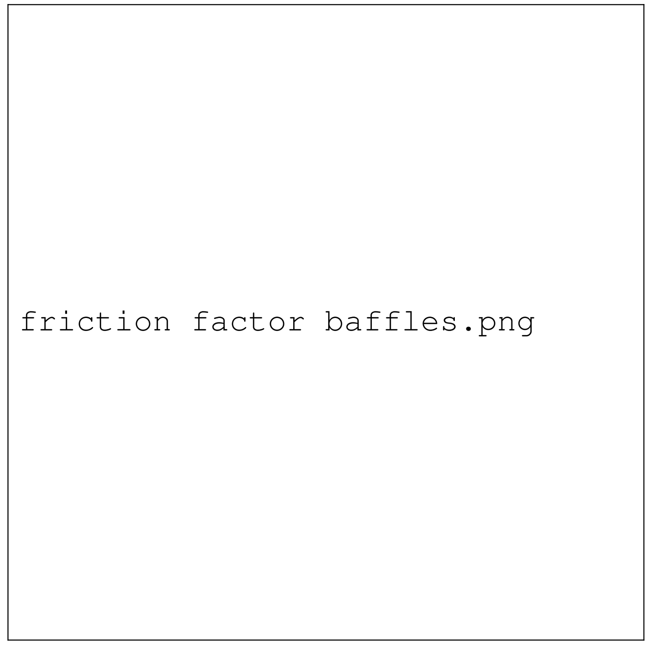

Fig. 3. shows how different baffle cuts can affect friction factors

: The tube side pressure drop can be calculated by Kern's method as explained in [**?**] This takes into account both the contribution from frictional losses and sudden changes in flow such as inlet or expansions.Frictional losses can be calculated from equation 6:

$$dP = 8J_f \frac{L'}{d_i} \rho \frac{u^2}{2} \tag{6}$$

WhereL' is the effective pipe length and J_f is the friction factor that can be calculated from the Reynolds number using the plot on Fig.4:

after observing a highly turbulent flow regime in our calculations we estimated the friction factor to be $J_f = 3.5 * 10^{-3}$.

The velocity heads contribution can be estimated using various methods, according to Kern (1950) we can add 4 velocity heads per pass, Frank (1978) suggests adding 2.5 velocity heads per pass and Butterworth (1978) even a lower 1.8 from [**?**]. Nevertheless, we can estimate which contribution is the most adequate for our frictionfactor.png

Fig. 4. shows how the friction factor is affected by the flow regime

construction and arrangement as we can approximate the contributions from sudden contractions, expansions and the pressure drop at inlet, outlet and 180 degrees bend as following from [**?**]:

type	Head loss
contraction	0.5
expansion	1.0
180* bend	1.5
inlet	1.0

We have inlet and outlet and 1 bend as displayed on the specification sheet for heat exchangers and in Fig.1. on the Heat Echanger Design section : $1{\times}1.5 + 1 \times 1.0 + 1 \times 0.5 = 3$ Therefore we can use the value suggested by Frank (1978) of 2.5 per pass

Assuming that the fluid change in viscosity with temperature is negligible since we are not using highly viscous fluids our overall pressure drop can be calculated as:

$$dp = Np[8j_f\frac{L}{d_i} + 2.5](\frac{u_t^2}{2}) \tag{7}$$

Where N_p is the number of tube passes And L is the length of one tube using equation 7 we get dp = 0.2 bar

E. Specification Sheet

see Appendix

1) Heat Exchanger Cost: When estimating the cost of the heat exchanger designed, the cost of materials of construction must be considered. Using the chart (HXCosts2005) as illustrated in Fig.6. assuming transport costs are negligible as we use a local seller). Using an AES heat exchanger (floating head) and an area of $15.41m^2$ (from iterations), when the pressure factor is 1.0 and material factor is 1.0 due to both the shell and tubes being constructed from carbon steel and steel respectively.
There is an initial cost (PCE) of £7,000 for the heat exchanger. However, this is not the total installed cost which also includes installation. The total installed cost or the physical plant cost (PPC) was found using the factorial method of cost estimation supposing that no buildings or storage were required, with f values found in table 6.1 in [**?**] as shown in Fig.5. Consequently the total cost was found using equation V-E1 where the i can take any value from 1 to 12 representing the installation factors, we found a value of PPC = £15,050. .

$$f_{tot} = \sum_{i=0}^{N}(f_i)$$

PPC = PCE(1 + f_{tot})(8)

factors.png

Fig. 5. shows the factors that can be used for our factorial model

heat_exchangercosts.png

Fig. 6. shows the costs of the equipment as the material and surface area increse

2) *Changes with Time*

: The calculated PPC cost is that for a heat exchanger designed and implemented in 2005, in order to update this value the Chemical Engineering Plant Cost Index (CEPCI) for November 2020, found in the journal 'Chemical Engineering', is used. Cost(Nov 2020) = cost(2005)* $\frac{(index(Nov2020)}{(index(2005))}$ Cost(Nov 2020) = £15,050*$\frac{600.6}{468.2}$ Cost(Nov 2020) = £19,306

Table 8. shows the summary of the iterative calculations from the heat exchanger

Property	**value**
Length (m)	4.88
Q ($\frac{j}{s}$)	1511118
Pr	6.9781
d_i (m)	0.016
$C_{p,mix}(\frac{J}{kgK})$	1703
$k_{f,mix}(\frac{W}{mK})$	0.1435
D_o (m)	0.02
$\rho_{mix}(\frac{Kg}{m^3})$(9)	873.651
$R_s(\frac{m^2K}{W})$	0.0004
$\dot{m}(\frac{Kg}{s})$	9.722
$\mu_{mix}(\frac{Ns}{m^2})$	0.000588
h_s ($\frac{W}{(m^2K)}$)	8000
$\Delta T_{lm}(K)$	94.82
j_h	0.004
$R_w(\frac{W}{K})$	0.00009091
k	0.249
n	2.207