A NEW STRATEGY FOR SELECTING AND EVALUATING PHYSICAL SOLVENTS FOR GAS ABSORPTION

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SUMMARY

This work describes how the physical properties of a solvent affect the design variables of a physical gas absorption process. The role of every property in determining the capital and the running cost of a process has been specified. Direct mathematical relationships have been formulated between every item of capital or running cost and the properties which are related to that item. The accuracy of the equations formulated has been checked by comparing their outcome with some actual design data. A good agreement has been found. The equations formulated may be used to evaluate on the basis of economics any suggested new solvents.

A group of solvents were selected for evaluation. Their physical properties were estimated or collected as experimental data. The selected ones include three important solvents, the first is polyethylene glycol dimethyl ether (Selexol) which represents the currently most successful one. The other two solvents are acetonyl acetone (B2) and n-formyl morpholine which have been suggested previously as potential credible alternatives to the current ones. The important characteristics of acetonyl acetone are its high solubility and its low viscosity, while the n-formyl morpholine is characterised by its low vapour pressure and its high selectivity. It was found that acetonyl acetone (B2) is the most attractive solvent for commercial applications particularly for process configurations that include heat exchangers and strippers.

The effect of the process configuration on the selected solvent was investigated in detail and it was found that there is no universal solvent which is the best for any process configuration, but that there is a best solvent for a given process configuration.

In previous work, acetonyl acetone was suggested as a commercially promising physical solvent. That suggestion was not fully based on experimental measurement of all the physical properties. The viscosity of acetonyl acetone and its solubility at 1 atm were measured but the vapour pressure and the solubility of CO_2 and CH_4 at high pressure were predicted. In this work, the solubilities of CO_2, CH_4 and C_3H_8 in acetonyl acetone were measured for a partial pressure range of (2 - 22) bar at 25°C. The vapour pressure of this solvent was also measured, and the Antoine equation was formulated from the experimental data.

The experimental data were found to be not in agreement with the predicted ones, so acetonyl acetone was re-evaluated according to the experimental data. It was found that this solvent can be recommended for further trials in a pilot plant study or for small scale commercial units.

Key words:- (1) Acetonyl acetone (B2); (2) Solvent evaluation; (3) Physical properties; (4) Carbon dioxide

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Introduction

The removal of acidic gases from gas mixtures by certain solvents is a widely practised industrial gas absorption process. For example, in the manufacture of ammonia, the carbon dioxide which forms from the reaction of hydrocarbons or coal with steam, must be removed from the hydrogen before this can be sent to the ammonia synthesis reaction stage.

In several applications a mixture of gases is already at high pressure, and this has led to the development of processes based on physical absorption rather than chemical absorption. Physical solvents lend themselves to a more economic removal of acid gases from streams of high pressure and high acid gas contents, because of the considerably lower energy requirement for solvent regeneration compared with chemical absorption. This has encouraged the development and application of a number of physical solvent processes which reduce the capital and operating costs of the plants.

The efficiency and the cost of any physical absorption process depend directly on the physical properties of the solvent utilised. By using a solvent with more appropriate physical properties, the cost of the process will be less. The physical properties of any solvent are related to the type and the number of the groups which make up the molecular structure of that solvent. Normally the physical properties can be measured experimentally for any existing solvent but if a new solvent is to be designed, the physical properties for the suggested molecular structure have to be predicted by using some reliable estimation methods. Techniques are available for the prediction of most physical properties with sufficient accuracy for engineering applications. Most of these techniques are based on the concept that a certain physical property of a component can be considered to be made up of the contributions from the constituent atoms, groups, and bonds, the contributions being determined from experimental data, which provides engineers with simple and convenient methods for physical property prediction. This approach requires only the knowledge of the structural formula of the compound.

The solubility, selectivity, viscosity and vapour pressure of the solvent are the most important properties which have to be considered in evaluating an existing solvent or in designing a new molecular formula due to their significant effect on the size of the equipment and on the operating cost. Sitthiosoth (44) has described the molecular design of a solvent for removing CO_2 and H_2S from gas mixtures after predicting the above mentioned properties using the group contribution technique. Accordingly, he suggested a new commercially promising solvent (acetonyl acetone) for further study. Acetonyl acetone was proposed due to its high solubility and low viscosity and also it has acceptable vapour pressures and selectivity.

Macchietto (29) has presented a systematic procedure to select or to design a new solvent for gas absorption processes, also utilising the group contribution method to predict the effective physical properties. Then he showed that the optimum solvent is the one that has maximum ratio of the solubility to the viscosity.

From the above two researches (Sitthosoth's and Macchietto's) it can be seen that evaluating an existing solvent or designing a new one requires two main steps. The first is to obtain (by measurement or from the literature) or to predict the effective physical properties by using some reliable estimation method and the second is to set an objective function which will be minimised or maximised according to the required criteria. With respect to the first step, both Sitthiosoth and Macchietto (29) have predicted the required physical properties by using the group contribution technique and this is the only appropriate way to achieve the first step if a new solvent is to be designed. But with respect to the second step, Sitthiosoth did not formulate an objective function, but depended on intuition and logical assessment when he suggested his new solvent, while Macchietto assumed that the objective function which has to be maximised is the ratio of the solubility to the viscosity. Both approaches leave the question, which method is the more appropriate that could be used to select the best solvent from some alternatives? Is it possible to develop a new straight-forward technique to evaluate a physical solvent? Answering these questions is one of the objectives of this work.

The configuration of any physical separation process depends mainly on the process objective and also it depends, to some extent, on the characteristics of the utilised solvent. For example, it is likely for the process which requires reduction of a dissolved acid gas component (usually H_2S) to a very low level that stripping at high temperature will be required to produce a lean enough solvent. For this type of process, heat exchangers are required to heat the solvent up to the stripping temperature and to cool it down to the absorption temperature. In another example, where bulk removal of carbon dioxide from methane is required, there is no need to use a stripper or heat exchangers. These two examples raise the important questions, is there an universal objective function which could be used to minimise the cost of any possible configuration and is the same solvent the best for any configuration? Allowing for these complications is another objective of this work.

It was mentioned that Sitthiosoth (44) thought that acetonyl acetone is potentially competitive to the most successful commercial physical solvents. He measured the solubility of CO_2 in this solvent at 1 atm pressure and also its viscosity at different temperatures. The rest of the properties had been predicted by him. This solvent can not be recommended for a pilot plant study or for small scale commercial applications without measuring the effective physical properties. Accordingly, this work concludes by presenting the results of experimental measurement of the solubilities of CO_2, CH_4 and C_3H_8 in the new solvent at high pressure in addition to the experimental relationship between the vapour pressure of the solvent with temperature.

A new procedure to evaluate physical solvents is expected from this work. This procedure together with the experimental measurement of the required properties then can be used to re-evaluate acetonyl acetone and to decide whether to recommend its use or not.

CHAPTER ONE

Literature Review

1-1 Introduction

The term absorption refers to a transfer of one or more components of a gas phase to a liquid phase, while stripping is exactly the reverse. The absorption could be chemical or physical. For several years absorption processes were dominated by chemical solvents, until the discovery of natural gas at high pressure containing very high concentrations of CO_2 and H_2S, this resulted in a shift to the use of physical solvents. In physical absorption, there are no new chemical species formed, so the heats of absorption and desorption are much smaller than with chemical solvents. This offers a cost advantages because of savings in the heat to regenerate the solvent. These savings are offset by higher capital investment for physical solvent processes, because absorbers are generally tall and costly or, if shorter, the liquid circulation rate increases for the same purification duty. A detailed comparision between the use of physical solvents and chemical ones, when the acid gas loading is at high pressure, has been set out by Strelzof (49), while Sweny and Valentine (48) have shown a comparision of the capital and running cost of a physical process (Selexol) with that of two chemical processes (MEA and hot potassium carbonate). Their conclusion was that physical solvents are more economical than chemical ones when the partial pressure of the component to be removed is high, usually 50 psi or above. However the disadvantage of the physical solvents is their tendency to co-absorption of fuel gases, particularly methane, carbon monoxide and hydrogen, which reduces the energy content of the purified gases and increases the need for interstage flash recycling.

The main items of equipment which could be used for physical gas absorption are absorbers, strippers, flash tanks, compressors and heat exchangers. In every physical absorption process, an absorber and flash tank have to be used, but it is not necessary to use strippers, compressors or heat exchangers for every individual physical gas absorption process. The need for one or more of these items depends mainly upon the required objective. For example, if a high purity of a gas product from H_2S is required, in this case, a stripper and heat exchangers must be used to achieve highly lean solvent. Another example is if the utilised solvent absorbs significant amounts of the gas product. Here, it is neccessary to use a compressor to recycle some of the gas product to the absorber. This discussion suggests that physical absorption processes could have different configurations and which is determined mainly by the nature of the duty of the process. Figures (1-1), (1-2) and (1-3) show different process configurations which are used for different purposes.

Treybal (52) has explained the role of some physical properties and he set out the following properties as guidelines for selection of a suitable solvent for any absorption process.

1- Solubility:- The gas solubility in a solvent is usually the first property which has to be assessed in determining the suitability of a solvent for a specific absorption system, because the higher the solubility, the higher the rate of absorption which results in a decrease in the required solvent circulation. The flow rate of the re-circulated solvent sets the size of most of the equipment in use, in addition to the heating, cooling and pumping energies required.

2- Viscosity:- High viscosity reduces mass transfer rates and tray efficiency and increases packing or tray requirements. This effect becomes significantly noticeable at reduced temperatures, since it is usually desirable to reduce the temperature to increase the solubility. The other advantages of low viscosity are good heat transfer characteristics and low pressure drop for pumping.

3-Volatility:- The vapour pressure of the solvent used should be as low as possible, because usually the gas leaving the absorption/desorption towers would be saturated with the solvent vapour, resulting in a considerable loss of the solvent or considerable cost in a solvent recovery system.

4- Miscellaneous considerations:- Another factor of importance is the usual inevitable presence of water vapour in the gas stream. The ideal solvent should be one in which water is substantially insoluble or it is easy to control the water content. Finally the solvent should be cheap, nontoxic, nonflammable, noncorrosive and chemically stable.

Some other important properties have not been mentioned by Treybal (52) namely, the selectivity, the specific heat and the thermal conductivity. The selectivity determines the relative compression horsepower required to recycle the flash gases from the intermediate flash tank to the high pressure contactor. The specific heat is related proportionally to the rate of the required heating steam and cooling water, while high thermal conductivity means a low heat transfer resistance which results in high heat transfer coefficients. The heat transfer coefficient is one of the important factors which determine the size of the heat exchangers.

1-2 Solubility Prediction

Over the years, developments have been made in the theories of estimating the solubility of different gases in certain solvents. Fredenslund et al. (11) proposed the most frequently used method, called the UNIFAC group contribution method. This theory is not widely used in industry for gas solubility prediction due to certain limitations, such as the non-availability of group contribution parameters for the unit structural of some gas structural units, the restricted temperature and pressure covered and the inability to predict the effect of the interaction between the neighbouring functional groups upon gas solubility. Sander et al. (61) have overcome some of these limitations by accommodating structural groups representing acid gases, such as CO_2, COS and H_2S so as to calculate their solubilities at low to moderate pressures and low solubilities (up to 0.1 mole fraction) for both polar and non-polar solvents. For a wide range of temperatures and pressures a new group contribution equation of state (GCEOS) has been developed by Skjold-Jorgensen (42).

Sitthiosoth (44) has summarised the historical development of solubility prediction from 1928 to 1987 and he reviewed in detail the UNIFAC theory, the developments that have been made by Sander (61) (which provided him with an excellent tool for searching for a new solvent), the GCEOS theory and some other less widely used theories.

After 1987, Sweeney et al. (47) have assessed the solubility parameter theory (SPT) . The original solubility-parameter theory, which applies only to non-polar solvents, had been developed by Hildebrand (47). The new version of SPT theory (by Sweeney) is applied to the estimation of gas solubility in both polar and non-polar solvents to yield suitable data for engineering purposes. The theory involves a combination of thermodynamic principles with simple solution models. The parameters required for the application of the equations can usually be estimated directly, but in some cases indirectly, by using group contribution methods, a summary of this theory is given in the following section.

1-2-1 Solubility Parameter Theory

In SPT, the mole fraction solubility of a gas in a physical solvent, X_1 is given by,

$$-\ln X_1 = \ln(\frac{f_1^L}{f_1}) + (\frac{v_1}{RT})(\delta_1^2 + \delta_2^2 - 2\delta_1\delta_1) \qquad (1\text{-}1)$$

δ = Solubility parameter
f = Fugacity, atm
f^L = Saturation fugacity, atm
R = Gas constant, 82.067 atm-cm^3-mol/K
T = Temperature, K
v = Molar volume, cm^3/mol
X = Mole fraction
1,2 = Refer to the gas and the solvent respectively

The above equation is valid when the difference in the molar volumes of the components is not very large. But if so, the Flory-Huggins (47) entropy of mixing term is more reliable.

$$-\ln X_1 = \ln(\frac{f_1^L}{f_1}) + (\frac{v_1}{RT})(\delta_1^2 + \delta_2^2 - 2\delta_1\delta_1) + \ln(\frac{v_1}{v_2}) + (1 - \frac{v_1}{v_2}) \qquad (1\text{-}2)$$

For ideal gases, the fugacity f_1, may be replaced by the partial pressure (p_1). The first term of the right hand side represents the ideal solubility. The saturation fugacity $f_1{}^L$ is hypothetical for supercritical gases and could be calculated from Prausnitz-Shair equation (47).

$$\frac{f_1^L}{P_C} = \exp(5.8763 - 6.8119\frac{T}{T_C} + 0.50607(\frac{T}{T_C})^2 + 10.79\ln(\frac{T}{T_C})) \qquad (1\text{-}3)$$

P_c = Critical pressure, atm
T_c = Critical temperature, K
Equation (1-3) is valid for $0.6 < T/T_C < 3$

The solubility parameter is the square root of the cohesive energy density.

$$\delta = \left(\frac{\Delta U_v}{V}\right)^{1/2} \approx \left(\Delta H_v - \frac{RT}{V}\right)^{1/2} \qquad (1\text{-}4)$$

ΔH_v = Enthalpy of vaporisation, J/mol
Δu_v = Energy of vaporisation, J/mol

The calculated solubilities of CO_2, H_2S and COS in some gas-purification solvents are compared with the experimental values in table (1-1), which demonstrates that equation (1-2) failed badly for the polar components. Several formulae extended the SPT to solutions containing polar components. The simplest uses a new parameter L_{12};

$$-\ln X_1 = \ln\left(\frac{f_1^L}{f_1}\right) + \left(\frac{v_1}{RT}\right)\left(\delta_1^2 + \delta_2^2 - 2L_{12}\delta_1\delta_{\cdot}\right) + \ln\left(\frac{v_1}{v_2}\right) + \left(1 - \frac{v_1}{v_2}\right) \qquad (1\text{-}5)$$

The term L_{12} is a binary parameter, close to unity, that characterizes the solute-solvent interaction. Many researchers have failed to estimate its value theoretically, nonetheless, if L_{12} is treated as a purely empirical correction factor, equation (1-5) can be used sufficiently for engineering purposes. A more sophisticated approach is to divide the solubility parameter into nonpolar, polar and hydrogen-bonding components.

$$\delta^2 = (\delta^{np})^2 + (\delta^{n})^2 + (\delta^{h})^2 \qquad (1\text{-}6)$$

So equation (1-5) becomes

$$-\ln X_1 = \ln\left(\frac{f_1^L}{f_1}\right) + \left(\frac{v_1}{RT}\right)\left(\delta_1^2 + \delta_2^2 - 2L_{np}\delta_1\delta_2^{np} - 2L_p\delta_1\delta_2^p - 2L_h\delta_1\delta_2^h\right) + \ln\left(\frac{v_1}{v_2}\right) + \left(1 - \frac{v_1}{v_2}\right) \qquad (1\text{-}7)$$

A comparision between the calculated and the experimental solubilities of CO_2 and H_2S in some commercial solvents is shown in table (1-2). Although there is a considerable improvement over equation (1-2), the results for H_2S are still poor, which means that the binary parameters (L_{np}, L_n and L_h) are too crude to be used for practical purposes. The solution to this uncertainity is to introduce an additional binary parameter, L_{12}, so equation (1-7) becomes,

$$-\ln X_1 = \ln(\frac{f_1^L}{f_1}) + (\frac{v_1}{RT})\,(\delta_1^2 + \delta_2^2 - 2L_{np}\delta_1\delta_2^{np} - 2L_{12}L_p\delta_1\delta_2^p - 2L_{12}L_h\delta_1\delta_2^h) + \ln(\frac{v_1}{v_2}) + (1 - \frac{v_1}{v_2}) \quad (1\text{-}8)$$

This parameter can be regarded as a fine correction factor for specific classes of solvents. Equations (1-7) and (1-8) require considerably more binary and pure component data than are required for equation (1-5). Fortunately, equations (1-7) and (1-8) need to be used only for strongly hydrogen-bonded solutions, such as alcohols. For other polar solvents, such as ketones, equation (1-8) offers no significant advantages over equation (1-5).

1-2-1-1 Solubility Parameter Estimation

The solubility parameter is a physical constant used to describe the relationship between the physical properties of the solvent and its effectiveness in dissolving specific solutes. The procedure of solubility parameter estimation includes two steps, the estimation of the total solubility parameter and the component solubility parameters. The first can be calculated from equation (1-4). If experimental data for calculating ΔH_v are unavailable, the group contribution method suggested by Feddors (47) can be used. Table (1-3) shows the contribution of differant groups to the total enthalpy of vaporization and the total molar volume. The energy of vaporization and the molar volume are the sum of the individual groups given in table (1-3) as shown in equations (1-9) and (1-10), however, it is advisable to use experimental data for the molar volume whenever possible.

$$\Delta H_v = \Sigma \Delta H_i \qquad (1\text{-}9)$$

$$V_m = \Sigma V_i \qquad (1\text{-}10)$$

Some other simple methods, suggested by Hildebrand (47), could be used to predict the total solubility parameter, these require only the boiling point of the solvent.

$$\Delta H_v = -12340 + 99.2T_b + 0.084T^2_b \qquad (1\text{-}11)$$

For hydrogen-bonded liquids a correction should be made to the calculated values: alcohols 1.4; esters 0.6 and ketones ($T_b \leq 100°$ C) 0.5

The component solubility parameters are calculated as follows.

1- Non-polar component:- This parameter can be found from the refractive index of the solvent which is usually known.

$$\delta^{np} = -2.24 + 53X - 58X^2 + 22X^3 \quad (X>0.28) \qquad (1\text{-}12)$$

$$\delta^{np} = 30.7X \quad (X<0.28) \qquad (1\text{-}12A)$$

$$\text{where: } X = \frac{\{(n_D^{20})^2 - 1\}}{\{(n_D^{20})^2 + 2\}} \qquad (1\text{-}12B)$$

n_D^{20} =Refractive index at 20° C

Alternatively, the equation of Wingerfors and Liljenzin (47) may be used for the same purpose.

$$(\delta^{np})^2 = \frac{\{a(T_r) - b(T_r)^{v_m}\}^{.124687}}{4.184} \qquad (1\text{-}13)$$

$$\text{with: } a(T_r) = 1022.31 - 1586.36T_r + 1082.07T_r^2 \qquad (1\text{-}13A)$$

$$b(T_r) = 277.709 - 531.335T_r + 482.039T_r^2 \qquad (1\text{-}13B)$$

where: $0.4<T_r<0.7$, and $50<v_m<300$

The estimation of the critical temperature will be explained in Chapter Seven.

2- Polar components: If the total and the nonpolar parameters have been evaluated using one of the above methods, the polar parameter can be obtained directly from eqn. (1-6) for non-hydrogen bonded solvents. Alternatively, Bottcher's equation (47) could be used.

$$(\delta^{P})^{2} = \left(\frac{12108}{V_m^{2}}\right) \times \frac{(\phi - 1)}{(2\phi + n_D^{2})\,\mu^{2}\,(n_D^{2} + 2)} \qquad (1\text{-}14)$$

ϕ = Dielectric constant, μ = Dipole moment

3- hydrogen-bonded components: equation (1-6) can be used to obtain this parameter once the other parameters are known. For alcohols, Hansen's equation (47) may be used.

$$(\delta^{H})^{2} = \frac{5000N_H}{V_m} \qquad (1\text{-}15)$$

N_H = Number of OH groups

1-3 Solubility Measurement

A knowledge of the solubility of any given gas in a liquid is an area of active interest due to the need to know its value in designing any gas absorption process. There are many methods and apparati which could be used to determine the solubility of any gas in a particular solvent. These methods differ greatly in complexity, cost, rapidity of the operation and precision. Michael (30) has reviewed the most important ones and gave summary descriptions for the followimg methods.

- Volumetric-atmospheric pressure
- Markham and Kobe apparatus
- Microgasometric method
- The Morrison and Billett design

- Apparatus of Dymond and Hildebrand
- Modifided physical absorption apparatus
- Cook and Hanson apparatus
- High pressure solubility apparatus
- Pressure - drop method

The techniques can be separated into three major classes; physical, chemical and physochemical. In this work, only the physical absorption methods are going to be considered. Physical methods can be divided into two major classifications.

- Saturation methods:- in those method a previously well-degassed solvent is saturated with a gas under precisely controlled temperature and pressure.
- Extraction method:- wherein a previously well-saturated solvent is degassed under controlled temperature and pressure.

The factors affecting the accuracy of the measured solubility are: degree of attainment of equlibrium; incomplete degassing of the solvent; ascertaining the true amount of the dissolved gas; purity of the solvent and the gas; temperature and pressure control and measurement; and the volume determination of the solvent.

Although each of the above mentioned factors contribute in some degree to the accuracy of the measured solubility, the attainment of equilibrium and complete degassing are of prime importance. The wide divergence of the reported values of gas solubility for some mixtures are in all likelihood due to failure to either attain equilibrium or to failure to achieve complete degassing of the solvent. The equilibrium between the gas and the liquid can be achieved by one of the following approaches.

- Bubbling the gas through the liquid:- The earlier workers who used this method were O'Sullivan and Gardiner (30) and it is still used by most of the present workers.
- Flowing a film or stream of the liquid through the gas:- Hayduk (15) and King (23) have used this method.
- Shaking or stirring the mixture of the gas and the solvent:- this method has been used by Dymond (6).

A complete degassing of the solvent could be achieved by one of the following methods.

- Boiling away 10 to 20 percentage of the solvent under vacuum, this method is used if the solvent is relatively cheap.
- Pumping on the frozen solvent for an hour or more:- this method was used by Bell and described by Michael (30), and it is useful when minimizing the loss of the solvent is required.
- Spraying a solvent through a fine nozzle into evacuated chamber:- rapid and complete degassing is obtained by this technique, but it is accompanied by a considerable loss of the solvent. This method was applied by Hayduk (15)
- An improved procedure was adopted by Jenkins and Smith (20) where the pure components were degassed by boiling and condensation under vacuum.

The measurement of the amount of the dissolved gas is another vital factor which may lead to a certain amount of error in determining the solubility. The following techniques are the most well known ones.

- Gas chromatography:- applied by most people who work in this field.
- Mass spectrometry:- Cseko (4) has measured the amount of dissolved methane, oxygen, and nitrogen in water by using this method.

- Chemical methods:- this method have been applied by many people including Teng and Mather (51)
- By determining the pressure change in a gas reservoir of known volume:- this technique was used by Water and Mortimer (55).

Fogg (10) has summarized the measurements of the solubility of CO_2 in different solvents for a variety of conditions using one of the above mentioned techniques. From many experimental data Wilhelm et al. have developed an empirical formula to estimate the solubility of CO_2 in water at 1 atm for a range of temperatures between 273° K - 353° K.

$$\ln X = -159.854 + (8741.68/T) + 21.6694 \ln T - 1.10261E\text{-}3\ T \quad ......(1\text{-}16)$$

Markranczy et al. (10) have measured the solubility of CO_2 in non-cyclic alkanes at 298.2 and 313°K corrected to a partial pressure of 1 atm. Their measurements show a decrease in mole fraction solubility with increasing length of the molecule. This is not in agreement with the measurements or predictions of many other workers. Depending on the measurements carried out by King, Gjaldback and Hahduk (10) the following empirical equation was developed in the range of hexane to hexadecane which shows the increase of solubility with the molecular weight of the solvent.

$$X = 0.01156 + 9.28E\text{-}6\ C^2 \quad ....(1\text{-}17)$$

The data that were presented by Hiraoka and Hildebrand (10) show the mole fraction solubility of CO_2 in 2,2,4 trimethyl pentane at 298.2 K and a partial pressure of 1 atm to be more than that of the linear isomer. Wilcock et al. (10) have confirmed this by measuring the solubility in cyclooctane and octane, the solubilities were 0.0069 and 0.012 respectively.

The solubility of CO_2 in 2-propanone at 1 atm and for a range of temperatures between 180- 290 K can be represented by the following equation

$$\ln = -10.313 + 1905.1\ T + 0.0017 \ln T \qquad \text{.............}(1\text{-}18)$$

This equation was developed from the data of Gjaldback and Andersen. Bodor et al. (10) have shown that the solubility of CO_2 in ethylacetate is higher than that in 2-propanone.

1-4 Prediction of the Other Physical Properties

Most of the other physical properties of a solvent are as important to be known as the solubility, because of their significant role in determining investment and running costs. So, a prediction of these properties has to be made if a new solvent is to be designed, or if reliable data are not available in the pressure and temperature ranges needed for already existing liquids. Usually the estimation methods have different degrees of accuracy and the engineer must know what accuracy is required for a certain application. In this work the criterion is to use the most reliable method with sufficient accuracy for engineering purposes.

The physical properties which are required to evaluate any solvent (in addition to the solubility) are the viscosity, the vapour pressure, the thermal conductivity and the specific heat. To estimate the vapour pressure, some other properties have to be estimated, namely, the boiling point, the critical temperature, the critical pressure and the acentric factor.

There are many calculation procedures available for the prediction of the above mentioned properties. Sitthiosoth (44) has reviewed the estimation procedures for all those properties, except those for thermal conductivity and specific heat. Reid et al. (40) has given an excellent review of the latest estimation methods for all the required properties, and recommended the most reliable ones. Appendix 2 shows the most common prediction methods and those that have been used for this work, with calculation examples for prediction of the properties of acetonyl acetone.

1-5 Solvent Design and the Objective Function Derivation

It is believed that physical solvents will continue to play an increasing role as suitable liquids for gas absorption, because of the considerably lower energy requirements for the regeneration of the solvent compared with the chemical absorption ones. So the search for more suitable physical solvents has intensified recently. The general strategy of most researchers is to design a new molecule such that its estimated physical properties will meet certain required criteria. The last important research in this direction has been made by Macchietto (29) and the one before that by Sitthiosoth (44). These two have reviewed the previous works which relate to this area.

It has been mentioned before, in designing any new solvent some kind of criterion is required, so an objective function has to be set up before starting the design process. In gas absorption, the objective for solvent design is to find a new competitive molecular structure which should reduce the investment and the running costs of the gas absorption process compared with the present liquids. Unfortunately, the relationship of the physical properties of the solvent with the cost items is very complicated. Because every property relates to the cost of one (or more) items in a different way, the objective function has to include all the properties which have an effect on the capital and the running cost items, and it should also incorparate the contribution of every property to the cost of that item.

When Sitthiosoth (44) designed and selected his new solvent, he did not formulate any objective function and he did not take into account the effect of the physical properties that have an effect on the cost of the heat transfer equipment. So after the prediction of the solubilities, viscosity and the vapour pressure had been made, he depended on a mixture of logical assessment and intuition, taking into account the commercial availability of the solvent to be selected. That process led him to choose acetonyl acetone as a competitive candidate.

Macchietto (29) went one step further, when he designed a solvent by optimization to obtain the maximum value of the ratio of the solubility of the solvent to its vicosity (χ/μ). That means he suggested the ratio of the solubility to the viscosity as an objective function. Although the solubility and the viscosity play an important role in determining the size of most of the equipment and some items of the running cost, they are not the only properties which contribute to the total capital and running costs. So, Macchietto's ratio (29) can not be a comprehensive representation of the total capital and running costs. In addition to that, this ratio does not show the true contribution of the solubility and the viscosity to the cost of the different items, such as their contribution to the cost of the absorber, stripper, heat exchanger, heating steam, solvent loss, etc.

A comprehensive objective function, which includes all the effective physical properties and gives a precise definition to the role and the importance of every property has to be justified in extensive detail. The new solvent which was suggested by Sitthiosoth (44) requires considerable theoretical and practical investigation to evaluate the possibility of recommending this liquid for a pilot-plant study.

Table (1-1) Prediction of the solubility of common gases in commercial solvents using the original SPT

	Solubility, mol% at 1 atm and 298 K		
Solvent	CO_2	H_2S	COS
n-Methyl-2-pyrrolidinone (NMP Purisol solvent)	.0092 (1.45)	4.02 (17.5)	.0898 (4.24)
Tetraetylene glycol dimethyl ether (Selexol solvent)	1.07 (3.33)	12.8 (25.9)	9.17 (9.8)
Methanol (Rectisol solvent)	73E-5 (0.56)	0.34 (2.78)	.024 (3.45)

( ) Experimental data

Table (1-2) Prediction of the solubility of common gases in commercial solvents using the modified SPT

	Solubility, mol% at 1 atm & 298 K	
Solvent	CO_2	H_2S
n-Methyl-2-pyrrolidinone (NMP Purisol solvent)	0.971 (1.45)	2.3 (17.5)
Tetraetylene glycol dimethyl ether (Selexol solvent)	2.62 (3.33)	4.07 (25.9)
Methanol (Rectisol solvent)	0.653 (0.56)	2.35 (2.78)

( ) Experimental data

Table (1-3) Feddor's group additive data

Group	ΔU_i, cal/mol	V_i, cm^3/mol
CH3-	1125	54.80
-CH2-	1180	16.10
-CH-	820	-1.0
-CH=	1030	13.50
-C-	350	-19.20
-O-	800	3.80
C=O	4150	10.80
-N	1000	-9.0
5-or-6 member ring	250	16.0
n-containing ring	2500	16.0

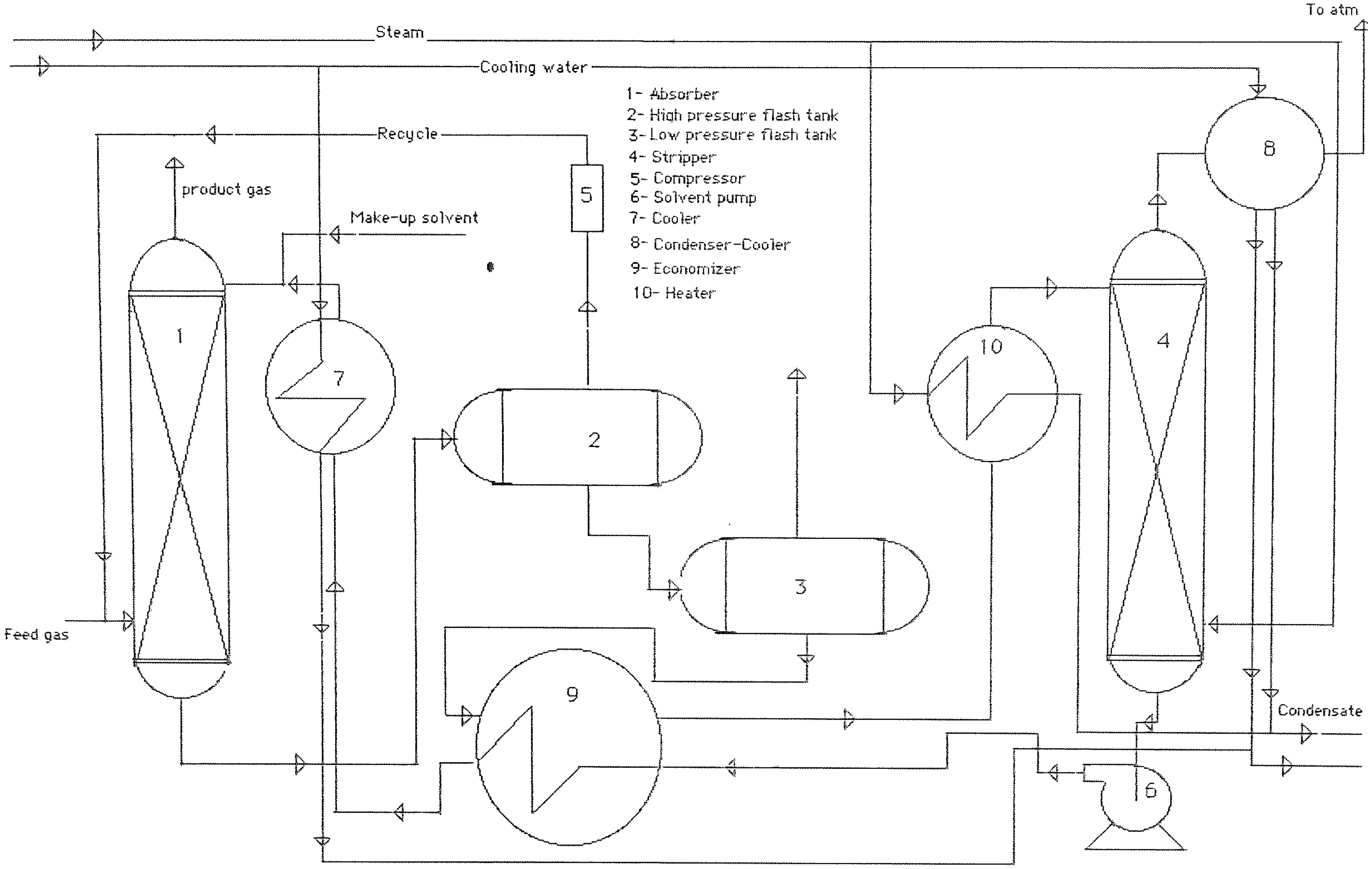
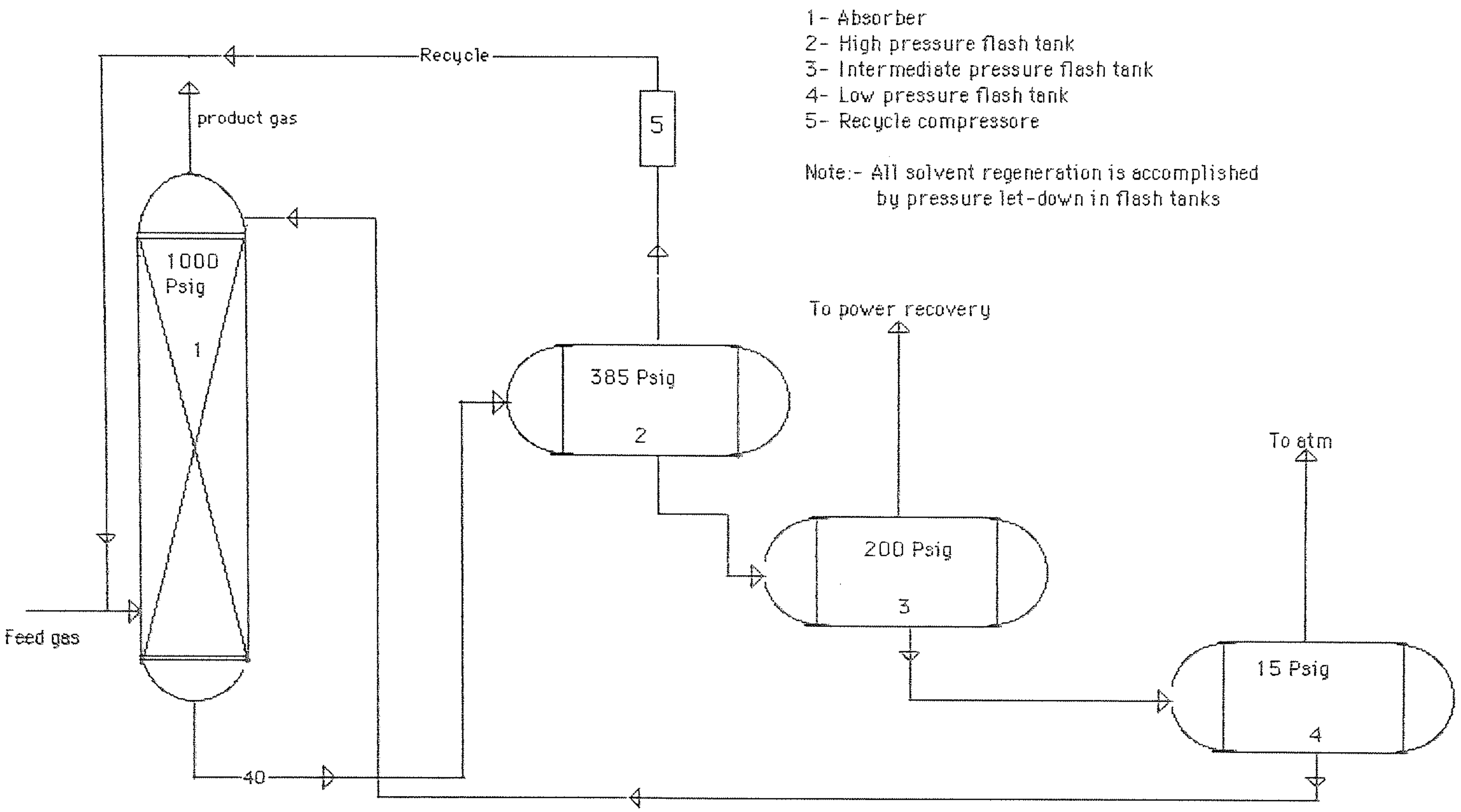


Fig. (1-1) Flow diagram of physical absorption processs to produce methane with not more than 4 ppm H2S and 3% CO2 from a mixture of 10% CO2, 1% H2S and 89% CH4



1- Absorber
2- High pressure flash tank
3- Intermediate pressure flash tank
4- Low pressure flash tank
5- Recycle compressore

Note:- All solvent regeneration is accomplished by pressure let-down in flash tanks

Fig. (1-2) Flow diagram of physical absorption process to produce methane with not more than 3.5% of CO2 from a mixture of 40% CO2 and 60% CH4

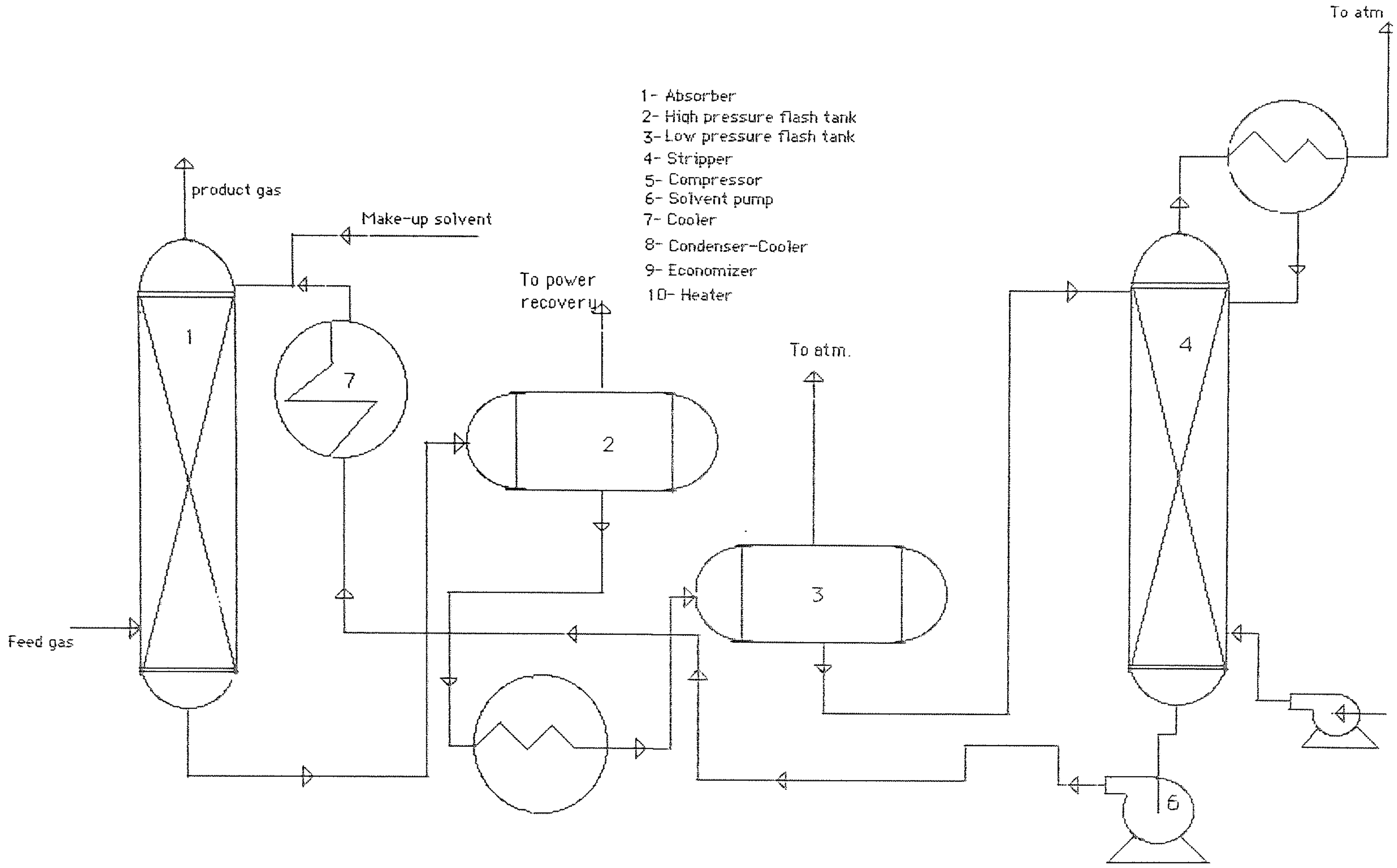


Fig. (1- 3) Flow diagram of physical absorption processs to produce methane with not more than 4 ppm H_2S and 3% CO_2 from a mixture of 10% CO_2, 1% H_2S and 89% CH_4

CHAPTER TWO

Approach to the Problem

Until recently, the commercialisation of a new physical absorption solvent has been a very expensive task. It required extensive and tedious comparisons of different solvents due to the lack of a simple method which could be used to select or design a new commercial solvent. The work described below presents a new approach whereby a solvent is selected on the basis of its physical properties or molecular structure.

2-1 Economic Evaluation of Solvents

The first step is to investigate the role of every (effective) physical property in determining the size of each main item of equipment and the cost of the required supporting utilities. Every physical property has its own effects on some design variable, and is related, in some way, to the investment cost, or running cost or both. For example, the solubility of a solvent affects the cost of many items such as the absorber, stripper, and compressing power. Another examples are the viscosity which affects the cost of the absorber, and the vapour pressure which determines the cost of the solvent loss and the size of the recovery unit.

2-1-1 The Mathematical Relationships

Direct mathematical relationships between every cost item and the effective physical properties of the solvent were derived from the principal design equations of different types of equipment. The equations have clarified two important points. The first is to obtain a precise definition of the role and importance of every physical property in determining the cost of the process. The second is to show the effect of the collection of all other factors (which are not related to the physical properties of the solvent) on the cost of the process. Unfortunately, the design equations of most chemical process equipment are fairly complicated, so assumptions are needed to simplify the derivation process, bearing in mind that some of the assumptions could cause significant deviation between the derived equation and the real relationship. It is necessary to assess the percentage and the reasons for any deviation. Some modifications may be needed to reduce the error.

2-1-2 The Use of the Mathematical Relationships

The derived equations could be used to evaluate any existing solvent or to compare between some alternatives and also could be used to design a new molecular structure. It was shown, in the previous chapter, that the physical absorption processes could have different configurations depending on the objective of the process, so it is necessary to demonstrate how these equations could be adapted to be used for any configuration. A group of physical solvents were selected, their physical properties were prepared, either from the literature or predicted using some reliable prediction technique. Table (2-1) shows a very brief description of the methods which were used to obtain these properties. It is necessary to include some successful commercial solvents within the selected group and also necessary to include any solvents which had been recommended by other people as potential competitors to the currently commercial ones. The selected solvents were evaluated for different types of process configuration by using the new suggested approach for physical solvent evaluation. The most economic solvents were identified.

Table (2-1) The principal physical properties

Property		method		Functionality
Critical Properties	(T_c, P_c)	Jobak	(40)	Group Contribution
Acentric factor	(w)	Lee-Kesler	(40)	$W = f(T_c, P_c, T_b)$
Vapour pressure	(Vp)	Lee-Kesler/G. Thodos	(40)	$V_P = f(Tc, W)$
Termal Conductivity	(KL)	Latini et al.	(40)	$KL = f(T_c, T_b, M_{w1})$
Heat Capacity	(Cp)	Missenard	(40)	Group Contribution
Viscosity	(μ)	Lewis-Sq. Ch.	(40)	Extrapolation
Solubility at high pressure	(K)	Zawaki et al.	(60)	Experimental data
Solubility at low pressure	(K1)	Sitthiosoth program	(44)	Group Contribution

2-2 Experimental Measurement of the Physical Properties of Acetonyl Acetone

Acetonyl acetone was suggested by Sitthiosoth (44) as a commercially promising physical solvent compared with the currently successful commercial ones. As we have seen, this suggestion was not fully based on the knowledge of the experimental physical properties, as some of them were measured and the others were predicted, the viscosity of acetonyl acetone at different temperatures and its solubility of CO_2 at 1 atm being measured but the vapour pressure and the solubilities of CO_2 and CH_4 at high pressure being predicted.

2-2-1 Solubility and the Selectivity Measurement

In this work, the solubilities of CO_2, CH_4 and C_3H_8 in acetonyl acetone were measured for a partial pressure range of (2 - 22) bar at 25°C. Before measuring the solubility, the solvent was purified and degassed carefully by boiling and condensation under vacuum. The degassed solvent was transferred to an equilibrium cell, where the mechanism which was used to contact the gas with the solvent was by bubbling the gas below the surface of the solvent. This contact was maintained for about four to five hours under well controlled temperature and pressure until equilibrium between the gas and the solvent was achieved.

A chemical analysis technique was used to measure the quantity of the dissolved CO_2 in the solvent. The quantity of dissolved CH_4 and C_3H_8 in the solvent were measured by using the Melzer method (1988). The central idea of this method is to determine the pressure change in a gas reservoir of known volume. The selectivity of the solvent to the CO_2 from a mixture of CO_2-CH_4 or CO_2-C_3H_8 was calculated from the measured solubilities of these gases. The experimental solubilities and selectivities of the considered gases in acetonyl acetone were compared with the predicted values and also were compared with the experimental values for Selexol.

2-2-2 The Effect of Water on the Gas Solubility in the New Solvent

Normally, the synthesis gas mixtures are saturated with water, so the transfer of some of this water to the solvent during the absorption process is unavoidable. The knowledge of the solubility of gas in a mixture of solvent-water is vital for the design of any gas absorption process. Three weight percentages of water (10, 20, & 30) in the solvent were chosen for this investigation. The solubilities of CO_2 in these three mixtures for a range of pressure of (2 -22) bar at $25^{o}C$ were measured. The effect of the contamination of the solvent with water on the solubility was presented and the maximum percentage of the water which has no significant effect on the solubility of the solvent was suggested.

2-2-3 The Vapour Pressure Measurement

The vapour pressure of acetonyl acetone was measured at different temperatures using an ebulliometer designed on the principle of the Swietoslawski (14) instrument. The Antoine correlation was formulated from the experimental data. The experimental vapour pressures were compared with the predicted data.

2-3 Re-evaluation of the New Solvent

The experimental physical properties of the proposed solvent and the new technique of evaluation of physical solvents were used to re-evaluate acetonyl acetone for different process configurations. It was found that this solvent is more economic than any other commercial solvents particularly for processes where stripper and heat exchangers are required to be used.

CHAPTER THREE

The Relationship of the Physical Properties of Solvent with the Cost of the Process

3-1 Introduction

The relationship of the cost of any equipment with any design variable depends directly upon the design equations of that equipment. Usually the design equations of most industrial chemical equipment are fairly complex, so it is not easy to derive explicit relationships between any two (or more) variables. To overcome such difficulties, some simplifying assumptions and considerations have to be made, bearing in mind that some of those assumptions could lead to a significant deviation (error) between the derived equation and the actual relationship. To assess the percentage of and the reasons behind that deviation, the actual relationship need to be presented in some way and compared with the outcome of the derived equation. Some modifications (or correction factors) may then be needed to reduce the error.

In the previous chapter, it was mentioned that different gas absorption processes could have different sets of equipment, but generally, all the possible pieces of equipment for a physical separation process are the absorber, stripper, flash tanks, heater, cooler, lean/rich exchanger and compressor. The major items of the running cost are heating and stripping steam, cooling water, solvent loss and electricity power for the compressor. In this chapter, the relationship of the cost of every equipment (or every item of the running cost) with one or more of the effective physical properties of the solvent will be derived from the design equations.

3-2 Absorber/Stripper Cost

The cost of an absorber/stripper column depends on its size. The size of the column is determined mainly by the feed rate of the raw gas and by the quantity of the component to be removed. The type of solvent also plays an important role in determining the size of the column as the gas solubility sets the quantity of the required solvent, while the viscosity affects the mass transfer rate. In the following, a direct mathematical relationship between these two variables (solubility and viscosity) and the cost of the absorber will be derived.

The following assumptions and considerations are essential to simplifiy the derivation:

1- The equilibrium and operating lines are straight.

2- The effective interfacial area is equal to the actual area of the packing material.

3- The diameter of the column is determined only by the mass flow of the feed gas and the type of the packing material.

4- The change in the flow of the solvent and the gas through the absorber due to absorption and desorption is negligible.

5- The change of solubility due to temperature increase and the solute concentration change is negligible.

6- The solvent utilized is noncorrosive and has no risk characteristics.

7- The following estimation methods have been used.

A- Onda's method (36) to estimate the overall height of transfer unit.

B- Garrett's (12) graph to calculate the cost of the column per unit length.

C- The empirical correlation of Wilke and Chang (59) to estimate the diffusivity of the solute in the solvent.

Onda (39) has published useful correlations which correlate the film mass transfer coefficients (K_L and K_G) with the physical properties of the solvent used and the type of the packing material.

The following equation is for the estimation of the liquid mass transfer coefficient.

$$K_L \left(\frac{D_L}{\mu_L g_3}\right)^{1/3} = 0.0051 \quad \left(\frac{L_W}{A_W \mu_L}\right)^{2/3} \quad \left(\frac{\mu_L}{D_L D_{L1}}\right)^{-1/2} (A_2 D_{P1})^{0.4} \qquad (3\text{-}1)$$

K_L = Liquid film mass transfer coefficient (m/s)
D_L = Density of the solvent (kg/m^3)
μ_L = Viscosity of the solvent (N s/m^2)
g_3 = Gravity constant (m/s^2)
L_W = Liquid mass flow per unit cross-sectional area (kg/m^{2}s)
A_W = Effective interfacial area of the packing per unit volume (m^2/m^3)
A_2 = Actual area of the packing per unit volume (m^2/m^3)
D_{L1} = Diffusivity of the solute in the solvent (m^2/s)
D_{p1} = packing size (m)

The absorption factor (AF) is the ratio of the slope of the equilibrium line to that of the operating line. Its reciprocal (SF) is called the stripping factor.

$$AF = \frac{K\,G}{L} \qquad (3\text{-}2)$$

AF = Absorption factor
K = Equilibrium constant
G = Inlet molar flow of the gas (kmole/s)
L = Inlet molar flow of the solvent (kmole/s)

From eqn. (3-2)

$$L_m = \frac{K\,G\,M_{w1}}{AF} \qquad (3\text{-}3)$$

L_m = Mass flow of the solvent (kg/s)
M_{W1} = Molecular wt. of the solvent.

From the definition of the mass flow rate per unit area and from eqn. (3-3) we have

$$L_W = \frac{4\,L_m}{\pi D^2} = a_1 K \qquad (3\text{-}4)$$

$$a_1 = \left(\frac{G}{AF}\right)\left(\frac{4\,M_{W1}}{\pi D^2}\right)$$

D = Diameter of the absorber (m)
L_w = Mass flow rate of the solvent per unit area (kg/s m^2)

For dilute solutions of nonelectrolytes, Treybal (52) has recommended the empirical correlation of Wilke and Chang (59) to estimate the diffusivity of a solute in a solvent.

$$D_{L1} = \frac{117.3 * 10^{-18} (\phi M_{w1})^{0.5} T}{\mu_L V_A^{.6}} \qquad (3\text{-}5)$$

$$D_{L1} = a_2 \mu_L^{-1} \qquad (3\text{-}6)$$

$$a_2 = \frac{117.3 * 10^{-18} (\phi M_{w1})^{0.5} T}{V_A^{.6}}$$

T = Absorption temperature (K)
V_A = Solute molal volume (m^3/kmole)
ø = Association factor

Substitute eqns. (3-6) & (3-4) in (3-1) and rearrange

$$K_L = a_3 K^{2/3} \mu_L^{-4/3} \qquad (3\text{-}7)$$

$$a_3 = 0.0051 \left(\frac{a_1}{A_2}\right)^{2/3} \left(\frac{1}{D_L a_2}\right)^{-1/2} (A_2 D_{P1})^{0.4} \left(\frac{D_L}{g_3}\right)^{-1/3}$$

The liquid film transfer height is

$$H_L = \frac{L_w}{M_{w1} K_L A_w C_T} \qquad (3\text{-}8)$$

H_L = Height of the liquid phase transfer unit (m)
C_T = molar density (kmole/m^3)

Substitute eqns. (3-4) and (3-7) in (3-8) and rearrange

$$H_L = a_4 K^{1/3} \mu_L^{4/3} \qquad (3\text{-}9)$$

$$a_4 = \left(\frac{a_5}{a_3}\right) \left(\frac{1}{A_2 C_T}\right) \quad \& \quad a_5 = \frac{a_1}{M_{w1}}$$

Onda's equation (36) for the gas film mass transfer coefficient is

$$\left(\frac{K_G R T}{A_2 D_v}\right) = 5.23 \quad \left(\frac{V_W}{A_2 \mu_g}\right)^{0.7} \left(\frac{\mu_g}{D_v D_g}\right)^{1/3} (A_2 D_{P1})^{-2.0} \qquad (3\text{-}10)$$

D_V = Diffusivity of the solute in the gas phase (m^2/s)
D_g = Density of the gas (kg/m^3)
R = Gas constant = 0.08206 atm (m^3/kmol K)
K_G = Gas film mass transfer coefficient (kmol/m^2s bar)
V_w = Gas mass flow per unit cross-sectional area (kg/m^2s)

$$\text{So} \qquad K_G = a_6 \qquad (3\text{-}11)$$

$$a_6 = 5.23 \left(\frac{V_W}{A_2 \mu_g}\right)^{0.7} \left(\frac{\mu_g}{D_v D_g}\right)^{1/3} (A_2 D_{P1})^{-2.0} \left(\frac{R T}{A_2 D_v}\right)^{-1.0}$$

The gas film transfer height is

$$H_G = \frac{V_w}{M_w K_G A_w P} \qquad (3\text{-}12)$$

H_G = Height of the gas phase transfer unit (m)
M_W = Average molecular wt. of the feed gas
P = Absorption pressure (bar)

$$\text{So} \qquad H_G = a_7 \qquad (3\text{-}13)$$

$$a_7 = \frac{V_w}{M_w a_6 \ A_2 P}$$

The relationship between the overall height of transfer unit (H_{OG}) and the individual height transfer unit (H_L, H_G), which are based on the concentration driving force across the gas and the liquid film, is

$$H_{OG} = H_G + \left(\frac{K G}{L}\right) H_L \qquad (3\text{-}14)$$

Substitute eqns.(3-2), (3-9), and (3-13) in (3-14) and rearrange

$$H_{OG} = a_7 + a_8 \ K^{1/3} \ \mu_L^{4/3} \qquad (3\text{-}14a)$$

$$a_8 = AF \ a_4$$

We have assumed that the equilibrium and the operating lines are straight, so the number of transfer units (N_{OG}) is

$$N_{OG} = a_9 = \left(\frac{1}{1 - AF}\right) \ln\left[(1 - AF)\left(\frac{y_1}{y_2}\right) + AF\right] \qquad (3\text{-}15)$$

The expression for the height of the packing material (Z) is

$$Z = N_{OG} H_{OG} \qquad (3\text{-}16)$$

Substitute eqns. (3-14a) and (3-15) in (3-16) and rearrange

$$Z = a_{10} + a_{11} K^{1/3} \mu_L^{4/3} \qquad (3\text{-}17)$$

$a_{10} = a_9 a_7$

$a_{11} = a_9 a_8$

If we consider the cost graph given by Garrett (1989/pp-268), the following equation represents the best fit for the relation between the cost per unit length of the column and its diameter.

$a_{12} = 139.4 + 195.09D - 25.731D^2 + 1.8775D^3$

Assume $a_{13} = (\pi/4)\, D^2\, PMC$

a_{12} = Cost of the absorber per unit length (\$/m)

PMC = Cost of the packing material per unit volume (\$/m^3)

a_{13} = Cost of the packing material per unit length of the column (\$/m)

The total cost of the absorber = cost of the column + cost of the PM

$$= Z\, a_{12}\, PF\, HF + a_{13}\, Z \qquad (3\text{-}18)$$

PF = Pressure correction factor

HF = Height correction factor

PM = Packing material

Or the total cost of the column = $a_{14} Z$ (3-19)

$a_{14} = a_{12}\, PF\, HF + a_{13}$

Substitute eqn. (3-17) in (3-19) and rearrange

The total cost of the absorber = $a_{15} + a_{16} K^{1/3} \mu_L^{4/3}$ (3-20)

$a_{15} = a_{14} a_{10}$

$a_{16} = a_{14} a_{11}$

3-3 Cooler/Heater Cost

The following assumptions and considerations were considered.

1- The heat loss is negligible.

2- The location of the solvent is chosen to be in the shellside and the cooling water or heating steam in the tube side.

3- The tube side heat transfer coefficient, the resistance of the metal tube and the dirt factors are constants.

4- The viscosity correction factor is equal to one.

5- The selected baffle cut is 25%

6- The temperature correction factor is equal to one.

7- The standard average velocities of the liquid in the shellside range from 0.3 - 1 m/s, Sinnott (43). So the velocity of the solvent is assumed to be 0.6 m/s.

8- The following estimation methods have been used.

A- Kern's method (22) to estimate the shellside heat transfer coefficient

B- Garrett (12/PP-286) graph to estimate the cost of the heat exchanger

The general equation for the quantity of the heat transfer across a surface is

$$Q = U\,A\,\Delta t_{lm} = m_s\,C_{ps}\,\Delta t_s \qquad (3\text{-}21)$$

Q = Heat transfer per unit time (W)
U = Overall heat transfer coefficient (W/m^2K)
A = Heat transfer area (m^2)
Δt_{lm} = Mean temperature difference (K)
m_s = Mass flow of the solvent (kg/s)
C_{ps} = Specific heat of the solvent (kJ/kg K)
Δt_s = Solvent temperature differance (K)

From eqn. (3-21) $A = (m_s/U)\,a_1$ (3-22)

where $a_1 = C_{ps}\,\Delta t_s\,10^3\,(1/\Delta t_{lm})$

The overall heat transfer coefficient (U) is the reciprocal of the overall resistance to heat transfer, which is the sum of individual resistances.

For a typical heat exchanger, the relation between (U) and the individual coefficient is

$$\frac{1}{U} = \frac{1}{H_o} + \frac{1}{H_{od}} + \frac{d_o \ln(\frac{d_o}{d_i})}{2\ K_w} + (\frac{d_o}{d_i})(\frac{1}{H_{id}}) + (\frac{d_o}{d_i})(\frac{1}{H_i}) \qquad (3\text{-}22a)$$

So $\frac{1}{U} = \frac{1}{H_o} + a_2 \qquad (3\text{-}23)$

$$a_2 = \frac{1}{H_{od}} + \frac{d_o \ln(\frac{d_o}{d_i})}{2\ K_w} + (\frac{d_o}{d_i})(\frac{1}{H_{id}}) + (\frac{d_o}{d_i})(\frac{1}{H_i})$$

H_o = Outside fluid film coefficient (W/m^{2}K)
H_i = Inside fluid film coefficient (W/m^{2}K)
H_{od} = outside dirt coefficient (W/m^{2}K)
H_{id} = Inside dirt coefficient (W/m^{2}K)
K_W = Themal conductivity of the tube metal (W/m K)
d_o = Tube outside diameter (m)
d_i = Tube inside diameter (m)

From eqn. (2-23) $U = \frac{H_o}{1 + a_2 H_o} \qquad (3\text{-}24)$

The heat transfer data are usually correlated by an equation of the following form, after assuming that the viscosity correction factor is equal to one.

$$Nu = J_h \ Re \ Pr^{1/3} \qquad (3\text{-}25)$$

Nu = Nusselt number ($H_o d_e/K_s$)
J_h = Heat transfer factor
Re = Reynold number ($D_L U_t d_e/ \mu_L$)
Pr = Prandtl number ($C_{ps} \mu_L/K_s$)
d_e = Equivalent (or hydraulic) diameter (m) = d_i for tube
K_s = Thermal conductivity of the solvent (W/m K)
U_t = Fluid velocity (m/s)

The relationship between the heat transfer factor (J_h) and the Reynolds number has been given by Sinnott (43/pp-546). From that relation the following equation can be obtained.

$$J_{h2} = J_{h1} \left(\frac{Re_2}{Re_1}\right)^{-0.5} \qquad (3\text{-}26)$$

1 refers to the tube side
2 refers to the shell side

or $J_h = a_3 \ Re^{-0.5}$ (3-27)

$$a_3 = J_{h1} \left(\frac{1}{Re_1}\right)^{-0.5}$$

Substitute the definitions of the Reynolds, Nusselt and Prandtl numbers and eqn. (3-27) in eqn. (3-25) and rearrange.

$$H_o = a_4 \ \mu_L^{-0.167} \qquad (3\text{-}28)$$

$$a_4 = a_3 \left(\frac{D_L U_t d_o}{10^{-3}}\right)^{-0.5} \left(\frac{D_L U_t}{10^{-3}}\right) C_{ps}^{1/3} \ K_s^{2/3}$$

Subsitute eqn. (3-28) in (3-24) and rearrange.

$$U = \frac{a_4 \mu_L^{-0.167}}{1 + a_2 \, a_4 \, \mu_L^{-0.167}} \qquad (3\text{-}29)$$

Usually a_2 is very small, so if we assume $a_2 = 0$, that means

$$U = a_4 \ \mu_L^{-0.167} \qquad (3\text{-}30)$$

From equation (3-3) the mass flow rate of the solvent was given as

$m_s = K \, G \, M_{W1}/AF = a_5 \, K$ (3-31)

$a_5 = G \, M_{W1}/AF$

Substitute eqn. (3-31) and (3-30) in (3-22) and rearrange.

$A = a_6 \ K \, \mu_L^{0.167}$ (3-32)

$a_6 = a_5 \ a_1/a_4$

The relationship between the cost of a heat exchanger with its heat transfer area was given by Garrett (12/pp-286). From that curve, the following equation can be obtained.

Cost(2) = cost(1) $(A2/A1)^{0.68}$ (3-33)

1 refer to reference cost

2 refer to the cost to be calculated

Substitute eqn. (3-32) in (3-33) and rearrange

Cost of the cooler (heater) $= a_7 \ K^{0.68} \ \mu_L^{0.1136}$ (3-34)

$$a_7 = \text{cost}(1) \ (a_6 / A1)^{0.68}$$

3-4 Lean\Rich Exchanger Cost

The following assumptions and considerations were considered.

1- The heat loss is negligible.

2- The resistance of the metal tube and the dirt factors are negligible.

3- The viscosity correction factor is equal to one.

4- The selected baffle cut is 25%

5- The temperature correction factor is equal to one.

6- The average velocity of the solvent in the shellside =1 m/S

7- The standard average velocity of the liquid in the shellside range from 0.3-1 m/s, Sinnott (43). So the velocity of the solvent is assumed to be 1 m/s.

8- The following estimation methods have been used

A- Kern's method (22) to estimate the inside and the outside heat transfer coefficient.

B- Garretts (12/PP-286) graph to calculate the cost of the heat exchanger.

The shellside heat transfer coefficient of this heat exchanger is the same as for the cooler ($H_o = a_4 \ \mu_L^{-0.167}$). The equation for estimating the tube side heat transfer coefficient is correlated in the form of ($Nu = 0.027 \ Re^{0.8} \ Pr^{0.3}$). If we use the same procedure as for the shellside heat transfer coefficient, the following equation is obtained.

$$H_i = a_8 \ \mu_L^{-0.5} \qquad (3\text{-}35)$$

$$a_8 = \left(\frac{0.027}{d_i}\right)\left(\frac{D_L\, U_t\, d_i}{10^{-3}}\right)^{0.8} C_{ps}^{0.3}\; K_s^{0.7}$$

If we assume that the resistance of the tube wall and the accumulated dirt on both sides of the tube are negligible, equation (3-22a) can be written as

$$U = \frac{H_i\, H_o}{H_i + H_o} \qquad (3\text{-}36)$$

Substitute eqns. (3-35) and (3-28) in (3-36) and rearrange

$$U = \frac{a_8\, a_4\, \mu^{-0.667}}{a_8\, \mu^{-0.5} + a_4\, \mu^{-0.167}} \qquad (3\text{-}37)$$

Substitute eqn. (3-37) and (3-31) in (3-22) and rearrange

$$A = K\,(a_9\, \mu_L^{0.167} + a_{10}\, \mu_L^{0.5}) \qquad (3\text{-}38)$$

$a_9 = a_1\, a_5 / a_8$: $a_{10} = a_1\, a_5 / a_4$

Substitute equation (3-38) in (3-33) and rearrange

$$\text{Cost of the Economizer} = a_{11}\; K^{0.68}\,(a_9\, \mu_L^{0.167} + a_{10}\, \mu_L^{0.5})^{0.68} \qquad (3\text{-}39)$$

$a_{11} = \text{cost}(1)\;(1/A1)^{0.68}$

3-5 Flash Tank Cost

The cost of a flash tank depends directly upon its weight. The weight of any tank depends on its volume and on the operating pressure as well. So, the cost of any flash tank is related to the volumetric feed flow, the residence time and the operating pressure, because the volume is a function of the feed flow and the residence time.

The following considerations are necessary to the derivation of the relationship of the cost of the tank with the solubility of the gas in the solvent.

1- The residence time of the liquid in the tank is 3 minutes.

2- The tank is running half full to ensure complete disengagement of the gas from the liquid.

3- The tank is a horizontal cylindrical vessel with length to diameter ratio of 4:1

4- Garrett's graph (12/pp-298) to estimate the cost of the tank, depending on its weight.

From eqn. (3-3) the mass flow rate of the solvent = (K G M_{W1})/AF. So

$$V_T = \left(\frac{G\,K\,M_{w1}}{AF}\right)\left(\frac{3*2*60}{D_L}\right) \qquad (3\text{-}40)$$

$$a_1 = \left(\frac{G\;M_{w1}}{AF}\right)\left(\frac{3*2*60}{D_L}\right)$$

Volume of the tank = cross sectional area times the length. So

$$V_T = (\pi/4)\, D^2\, L \qquad (3\text{-}41)$$

$$L/D = 4 \qquad (3\text{-}42)$$

From eqns. (3-40), (3-41) and (3-42) we have

$$D = a_2\, K^{1/3} \qquad (3\text{-}43)$$

$$L = 4\, a_2\, K^{1/3} \qquad (3\text{-}44)$$

$$a_2 = (a_1/\pi)^{1/3}$$

$$W = V_m\, D_m = 0.01\pi\, D\, L\, D_m = a_3\, K^{2/3} \qquad (3\text{-}45)$$

$$a_3 = 0.04\pi\, a_2^2\, D_m$$

The following equation represents the best fit for the relationship of the cost of tank with its weight. That relation was given by Garrett (12/pp-298) .

Cost of the tank = 8971.2 PF + 1.4992 PF W (3-46)

Substitute eqn. (3-45) in (3-46) and rearrange

Cost of the tank = $a_4 + a_5 K^{2/3}$ (3-47)

$a_4 = 8971.2$ PF

$a_5 = 1.4992$ PF a_3

W = Weight of the tank (kg)
V_T = Volume of the tank (m^3)
L = Length of the tank (m)
D = Diameter of the tank (m)
V_m = Volume of the metal (m^3)
D_m = Density of the metal (kg/m^3)
PF = Pressure factor

3-6 Compressor Cost

The size of the compressor depends directly on the required differential pressure and the flow of the gases to be compressed. The design capacity should be at least 10% more than the flowsheet of the recycle gases, to cover any uncertainties in the design. The flow of the recycle gases depends mainly on the capacity of the plant and on the differences between the solubilities of the product gas at the absorption and flashing pressures, and also it depends slightly on the solubilities of the component to be removed. In other words it depends on the selectivity of the solvent to the component to be separated.

The following assumptions and considerations are essential to simplify the derivation.

1- The flow of the solvent does not change due to absorption and desorption of the gases.

2- The total molar flow of the recycle = B% of the absorbed component to be removed + A% of the absorbed gas product.

3- Garrett's graph (12/pp-272) to estimate the cost of the compressor.

$$\text{Absorbed } CO_2 = X_R\, L = \left(\frac{Y_R}{K_R}\right)\left(\frac{K_R\, G}{AF}\right) = \frac{Y_R\, G}{AF} \qquad (3\text{-}48)$$

$$\text{Absorbed product} = X_p\, L = \left(\frac{1}{S_L}\right)\left(\frac{Y_P\, G}{AF}\right) \qquad (3\text{-}49)$$

$$\text{Because } S_L = \frac{K_p}{K_R}$$

$$HP = 0.0044\, P_1\, V_1 \log\left(\frac{P_2}{P_1}\right) = 0.0044\, ZNRT \log\left(\frac{P_2}{P_1}\right) \qquad (3\text{-}50)$$

From eqns. (3-48) and (3-49) we have

$$N = \left(\frac{A}{S_L}\right)\left(\frac{Y_P\, G}{AF}\right) + B\, Y_R \left(\frac{G}{AF}\right) \qquad (3\text{-}51)$$

Substitute eqn. (3-51) in (3-50) and rearrange

$$HP = \frac{a_1}{S_L} + a_2 \qquad (3\text{-}52)$$

$$a_1 = 0.0044 * A\, (ZRT)\left(\frac{Y_P\, G}{AF}\right) \log\left(\frac{P_2}{P_1}\right)$$

$$a_2 = 0.0044 * B\, (ZRT)\left(\frac{Y_R\, G}{AF}\right) \log\left(\frac{P_2}{P_1}\right)$$

From Garrett's graph (12) we have

$$\text{Cost } (2) = \text{Cost } (1) \left(\frac{HP_2}{HP_1}\right)^{0.8} \qquad (3\text{-}53)$$

1 refers to a reference cost

2 refers to the cost to be estimated.

Then the cost of the compressor $= a_3\, HP^{0.8} = a_3 \left(\frac{a_1}{S_L} + a_2\right)^{0.8}$ (3-54)

$$a_3 = \text{Cost } (1) \left(\frac{1}{HP_1}\right)^{0.8}$$

HP = Horse power

P1 = Inlet pressure

P2 = Out let pressure

V1 = Inlet flow rate
T = Compression temperature
R = Gas constant
N = Number of moles of the gas

3-7 Operating Cost

In this work the pumping power which is required to circulate the solvent is going to be ignored, only the major running cost items are going to be considered. These items are compressor power, heating steam, stripping steam, cooling water and solvent loss.

3-7-1 Electricity Cost

Electricity cost = A \$/kW hr

Eqn. (3-52) represents the required power for the compression, so

$$\text{A. E. C.} = \left(\frac{A\,\$}{\text{KW. hr}}\right)\left(\frac{0.7457\ \text{KW}}{\text{HP}}\right)(24*300) = 536A\left(\frac{a_1}{S_L} + a_2\right) \qquad (3\text{-}55)$$

3-7-2 Heating Steam Cost

The flow of the heating steam depends mainly on the flow of the solvent. So the cost of the steam is related to the solubility of the component to be removed in the solvent.

$$Q = (G\,K/AF)\,M_{W1}\,C_{ps}\,(T_1 - T_2) = LAM\,M_S \qquad (3\text{-}56)$$

From eqn. (3-56)

$$M_S = (G\,K/AF\,LAM)\,M_{W1}\,C_{ps}\,(T_1 - T_2) = a_1\,K \qquad (3\text{-}57)$$

$$a_1 = (G\,/AF\,LAM)\,M_{W1}\,C_{ps}\,(T_1 - T_2)$$

Steam cost = A \$/kg

$$\text{Annual steam cost} = (A*3600*24*300)\,a_1\,K = a_2\,K \qquad (3\text{-}58)$$

$$a_2 = (A*3600*24*300)\,a_1$$

LAM = Latent heat of steam (kJ/kg)
M_S = Mass flow of steam (kg/s)
T_1, T_2 = Inlet and the outlet solvent temperature (°C)

3-7-3 Stripping Steam Cost

The flow of the stripping gas depends on the solubilities of the gas to be removed at absorption and desorption conditions

Steam mass flow = $(L/SF\ K_1)\ M_{w2} = (K\ G/SF\ AF\ K_1)\ M_{w2} = a_1(K/K_1)$ (3-59)

$a_1 = (G/SF\ AF)\ Mw2$

Annual cost = $(A*3600*24*300)\ a_1\ (K/K_1)\ M_{w2} = a_2(K/K_1)\ M_{w2}$ (3-60)

$a_2 = (A*3600*24*300)\ a_1$

SF = Stripping factor

K_1 = Equilibrium constant at stripping conditions

L = Molar flow rate of the solvent

3-7-4 Cooling Water Cost

The required cooling water depends on the solubility of the component to be removed.

$Q = (G\ K/AF)\ M_{W1}\ C_{ps}\ (T_1 - T_2) = M_C\ \ C_{pw}\ (T_{w2} - T_{w1})$ (3-61)

$$M_c = \left(\frac{G\ K}{AF}\right) M_{w1} \left(\frac{C_{ps}}{C_{pw}}\right) \left(\frac{T_1 - T_2}{T_{w1} - T_{w2}}\right) = a_1\ K \qquad (3\text{-}62)$$

$$a_1 = \left(\frac{G}{AF}\right) M_{w1} \left(\frac{C_{ps}}{C_{pw}}\right) \left(\frac{T_1 - T_2}{T_{w1} - T_{w2}}\right) = a_1\ K$$

Cost of the cooling water = A \$/ kg

Annual cost of the cooling water = $(A)\ (3600*24*300)\ a_1\ K$
$= a_2\ K$ (3-63)

$a_2 = (A)\ (3600*24*300)\ a_1$

M_C = Mass flow rate of the cooling water (kg/s)

CP_w = Specific heat of the water (kJ/kg K)

T_{w2} ,T_{w1} = outlet and inlet temperature of the water

3-7-5 Solvent Loss Cost

The rate of the solvent loss depends on the following factors.

1- Vapour pressure of the solvent

2- Flow rate of the solvent, which means that it relates to the solubility of the gas to be removed at absorption conditions.

3- Flow rate of the stripping gas , which implies its dependence on the solubility of the gas to be stripped at stripping conditions.

$$\text{Mass rate of solvent loss} = \left(\frac{K\,G}{SF\;AF\;K_1}\right)\left(\frac{V_P}{p}\right) M_{w1} = a_1 \left(\frac{K}{K_1}\right) V_P \qquad (3\text{-}64)$$

$$a_1 = \left(\frac{G\,M_{W1}}{SF\;AF\;P}\right)$$

If the cost of the solvent = C \$/kg

Annual cost of the solvent loss = $a_2(K/K_1)$ VP C (3-65)

$a_2 = a_1$ (3600*24*300) C

V_P = Vapour pressure of the solvent (bar)

P = Operating pressure of the stripper (bar)

CHAPTER FOUR

The Accuracy of the Cost Equations

4- 1 Introduction

As mentioned before, the accuracy of derived relationships between the cost of every process item and the physical properties of the solvent have to be checked by comparing their outcome with some actual design data. So in this chapter, four steps have to be taken. The first is to select one of the well known physical separation processes, the second is to design all the equipment and estimate all the investment and running cost items, the third is to find out the actual relationships of the physical properties with the cost of every process item. The final step is to evaluate and develop the derived equations (Chapter 3) for every piece of equipment or for the operating cost items.

4-2 Selection of a Physical Separation Process

Figuger (4-1) represents the flow sheet of the selected plant. This plant is used to remove carbon dioxide and hydrogen sulfide from sour natural gas by using a well-known physical solvent called Selexol. The configuration of this process is similer to that of the commercial plant in West Germany, which includes all the major equipment for physical gas absorption. The composition of the sour natural gas depends on its source. The composition of gas from the Wyoming field, for example, is given in table (4-1). It is quite clear that the methane, carbon dioxide and hydrogen sulfide represent the major constituents, so that it is possible to assume that the sour natural gas consists only of these three materials (CH_4, CO_2, H_2S), to simplify the design process. Table (4-2) shows the assumed composition of the feed gas and the required product composition.

The raw gas at 27°C (80°F) and 68 atm (1000 psia) is contacted counter-currently with the regenerated solvent which comes with a certain composition of CO_2 and H_2S into an absorber tower which is packed with 38 mm ceramic Intalox saddles. The purified gas leaves the top of the absorber at the required methane composition. The rich (loaded) solvent leaves the bottom of the packed tower and goes directly to a flash tank which operates at 20 atm (300 psia) in order to release most of the absorbed methane with some unavoidable release of carbon dioxide and hydrogen sulfide. The released gases are recycled to the absorber after compressing them to 68 atm. From the high pressure flash tank the solvent passes into a low pressure flash tank which operates at 1.4 atm (20 psia), in order to reduce the load on the stripper by releasing most of the carbon dioxide and hydrogen sulfide. The released gases from the second flash tank goes to the exit with the off gases from the stripper. The solvent from the low pressure flash tank is pumped through an economizer to recover some of the heat contant of the hot lean solvent which leaves the stripper.

The duty of the economizer is to save some of the energy that is used in the heater by preheating the rich solvent and precooling the lean solvent. The loaded solvent leaves the economizer to enter the heater, where steam is used, to increase its temperature to the operating temperature of the stripping process. The solvent is fed in at the top of the stripper while the steam enters the stripper from the bottom. The remaining absorbed gases (CO_2, H_2S, CH_4) must be removed by the steam to leave the solvent clean. The concentration of the carbon dioxide and hydrogen sulfide in the clean solvent must not be more than 500ppm for CO_2, and 18ppm for H_2S. The clean solvent is pumped through the economizer and the cooler, to decrease its temperature to 27°C (80°F) before entering the top of the absorber. The steam with the stripped gases comes out from the top of the stripper into the cooler/condenser to condense the steam and send it back to the boiler for reuse. The uncondensable gases togather with the released gases from the low pressure flash tank go to exit.

4-3 Process and Equipment Design

Figure (4-1) with table (4-3) represent the process flow diagram of the selected process, while Appendix 1 shows the full design details and the estimated investment, running and process cost for every cost item.

4-4 The effect of the Physical Properties on the Process Cost

A primary assesment of the effect of every property on the cost of every item has been made. It was found that the solubility and the viscosity of the solvent could change the investment cost dramatically, because the size of most of the equipment is determined by their values. That does not mean the role of the other properties is unimportant, but their effect is limited to the size of a certain equipment and on some items of the operating cost. In other words, the vapour pressure affects the quantity of the solvent loss while the selectivity dominates the size of the compressor and the power required to run it. But the solubility and the viscosity (together or individually) determine the sizes of the columns, heat exchangers, flash tanks, compressor, the quantity of the stripping and heating steam, cooling water and solvent loss.

To find out the real role of the solubility and the viscosity and their effects on the cost of the process, the same design programs, shown in Appendix 1, were used for a range of equilibrium constants (0.7 - 0.25) at eight values for the viscosity. The output of those calculations is shown in figures (4-2) to (4-6). Figure (4-7) shows the effect of the solubility on the cost of the flash tanks. The relationships of the selectivity with the cost of the compressor and the required power are shown in Figure (4-8), while Figure (4-9) explains the role of the solubility (at absorption and stripping conditions) and the vapour pressure on the cost of the solvent loss.

4-5 The Optimum Cost Equations

The optimum relationships, for every unit and for some items of the running cost, have been found by using a nonlinear optimization programe called GRG2. GRG2 is a Fortran program which is available from the computer network centre/Aston University, and any student can have access to this program. This program has been used to find the optimum fitting equation for certain data. Those equations can be seen underneath each graph.

By comparing the derived equations (Chapter 3) with those resulting from the actual design data, a clear similarity was found between the equations for the same equipment, although there are some differences between the values of the coefficients due to the simplified assumptions that were made. To reduce the error due to the assumptions made, the coefficients of the derived equations have to be refined by fitting to the actual design data. So, the new suggested equations for every process item are as follows.

Cost of the absorber = $a_1 + a_2 K^{0.962} \mu^{1.43}$ (4-1)

Cost of the stripper = $a_3 + a_4 K^{0.81} \mu^{1.143}$ (4-2)

Cost of the flash tank = $a_5 + a_6 K^{2/3}$ (4-3)

Cost of the cooler = $a_7 K^{0.624} \mu^{0.2}$ (4-4)

Cost of the heater = $a_8 K^{0.624} \mu^{0.2}$ (4-5)

Cost of the economizer = $a_9 K^{0.68} (a_{10} \mu^{0.7} + a_{11} \mu^{0.3})^{0.7}$ (4-6)

Cost of the compressor = $a_{12} (a_{13}/S_L + a_{14})^{0.8}$ (4-7)

Annual C.P.C@ = $a_{15} (a_{13}/S_L + a_{14})$ (4-8)

Annual S.S.C@ = $a_{16} K/K_1$ (4-9)

Annual H.S.C@ = $a_{17} K$ (4-10)

Annual C.W.C@ $= a_{18} K$ (4-11)

Annual S.L.C@ $= a_{19} (K/K_1) V_p C$ (4-12)

@C.P.C = Compressing power cost
S.S.C = Stripping steam cost
H.S.C = Heating steam cost
C.W.C = Cooling water cost
S.L.C = Solvent loss cost

The constants (a_1, a_2, ...a_{19}) are related mainly to the type of the process. More details about these constants will be considered in the next chapter.

Table 4-1 Example of natural gas compositions

Component	Wyoming (mole%)
H_2	0.28
N_2	4.2
C_1	71.15
C_2	2.01
C_3	0.49
i-C_4	0.07
n-C_4	0.23
C_5	0.25
CO_2	17.56
H_2S	3.76
COS	Traces

Table 4-2 Composition of the feed and the required product

Component	% in the feed	% in the product
CO_2	10.0	3.0
H_2S	1.0	4.0 ppm
CH_4	89.0	Balance
Total	5000 kmole/hr	To be calculated

Table (4-3) The process flow diagram of the Selexol process

Line number	**10**	**20**	**30**	**40**
Total flow (kg/hr)	94704	8238	102945	648501
Density (kg/m^3)	65.5	80.8	66.54	1021
Pressure (atm)	68			
Temperature (°C)	27			
Flow of CO_2 (kg/hr)	21954	4051	26007	20575
Flow of H_2S (kg/hr)	1699	46.0	1745	1746.6
Flow of CH_4 (kg/hr)	71051	4141	75192	5564.5
Flow of Selexol (kg/hr)				620615
Flow of steam (kg/hr)				
Flow of water (kg/hr)				

Line number	**50**	**60**	**70**	**80**
Total flow (kg/hr)	621094	75550	640263	15539
Density (kg/m^3)	1021	54.8	1021	2.7
Pressure (atm)		68	20	1.4
Temperature (°C)		27	27	25
Flow of CO_2 (kg/hr)	489	5921	16524	13559
Flow of H_2S (kg/hr)	1.36		1700	579
Flow of CH_4 (kg/hr)		69628	1423	1401
Flow of Selexol (kg/hr)	620603	0.0213	62061	
Flow of steam (kg/hr)				
Flow of water (kg/hr)				

Line number	**90**	**100**	**110**	**120**
Total flow (kg/hr)	624740	3478	7660	620555
Density (kg/m^3)	1021	1.88	1.1	1021
Pressure (atm)	1.4	1.4	1.4	1.4
Temperature (°C)	27	127	127	71
Flow of CO_2 (kg/hr)	2966		2479	487
Flow of H_2S (kg/hr)	1122		1120.65	1.35
Flow of CH_4 (kg/hr)	22		22	
Flow of Selexol (kg/hr)	620630		563	620067
Flow of steam (kg/hr)		3478	3477	
Flow of water (kg/hr)				

Line number	**130**	**140**	**150**	**160**
Total flow (kg/hr)	536	996828	3285	33890
Density (kg/m^3)	1021	995	995	1.8
Pressure (atm)	1.4	1.7	1.1	1.05
Temperature (°C)	27	15	15	138
Flow of CO_2 (kg/hr)				
Flow of H_2S (kg/hr)				
Flow of CH_4 (kg/hr)				
Flow of Selexol (kg/hr)	536			
Flow of steam (kg/hr)				33890
Flow of water (kg/hr)		996828	3285	

Table (4-4) The general equations suggested with their coefficients for the Selexol process

Cost Item	Eqn. No.	Actual Cost $	Fitting Cost $	$(Par)_1$	$(Par)_2$	$(Par)_3$	%Error
Absorber	4-1	420187	421453	37548	50809	....	0.3
Stripper	4-2	70325	70469	23249	66106	....	0.2
H.P.F.T	4-3	64000	64514	17942	65466	....	2.3
L.P.F.T	4-3	32000	32257	8971	33430	....	2.3
Cooler	4-4	125000	110665	119165	....	....	11
Heater	4-5	99450	88611	113713	....	....	6.7
Economizer	4-6	190414	171602	1055	530.2	637.3	9.8
Compressor	4-7	105000	116909	3485	43	....	10
Elect.power	4-8	139166	156653	3485	43	....	11
Stripping S.	4-9	553419	544774	1.362E7	....	....	1.5
Heating S.	4-10	5392577	5405345	9008908	....	....	0.25
Cooling W.	4-11	315795	325971	543286	....	....	3.1
Solvent L.	4-12	34740	46635	9293545	....	....	25
T. Equip. C.	....	1106376	1087924	....	....	....	2.0
T. Running C.	....	6435697	6479379	....	....	....	0.7

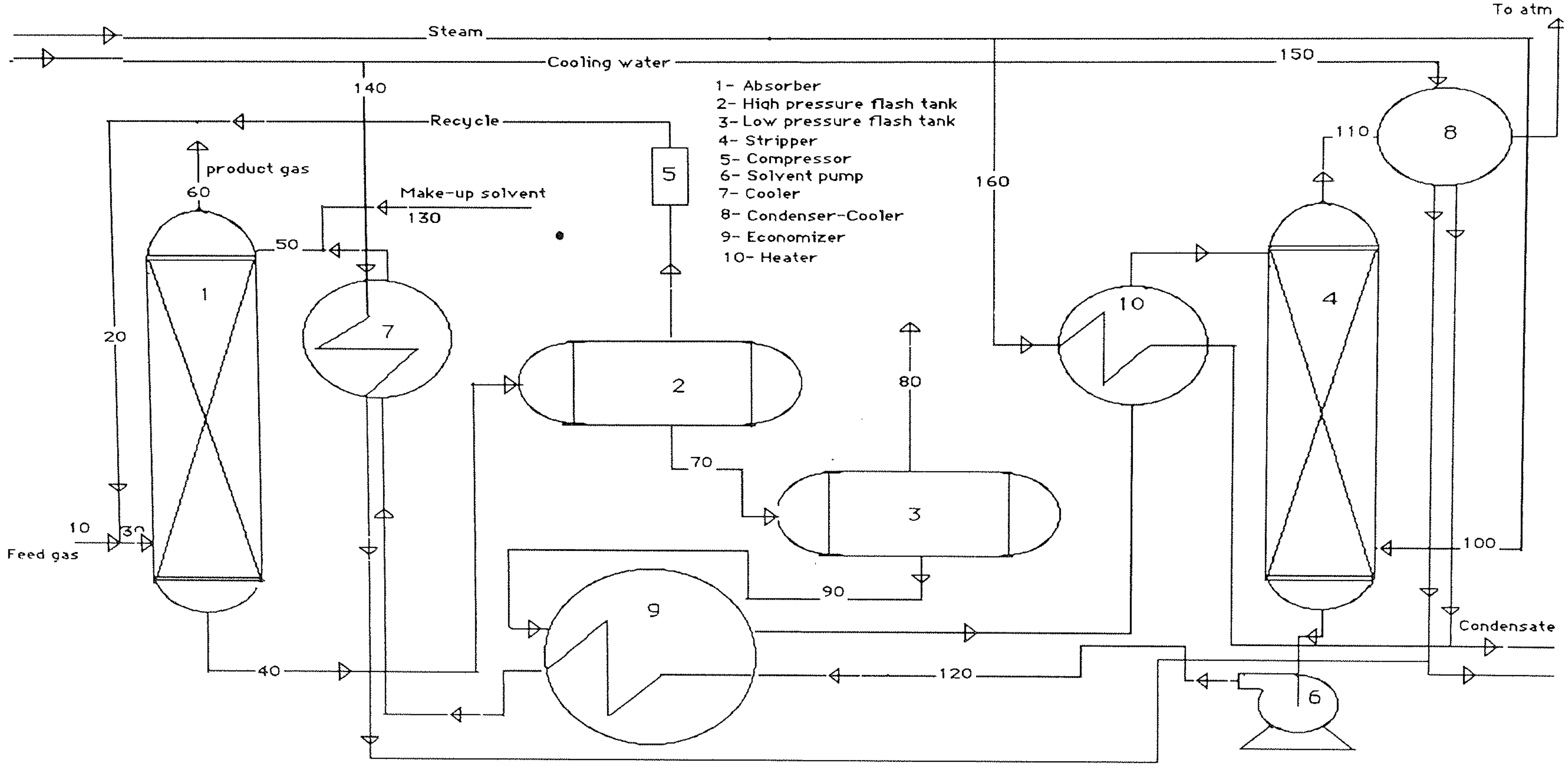


Fig. (4-1) The flow sheet of the selected process for CO2 and H2S separation from CH4 by Selexol

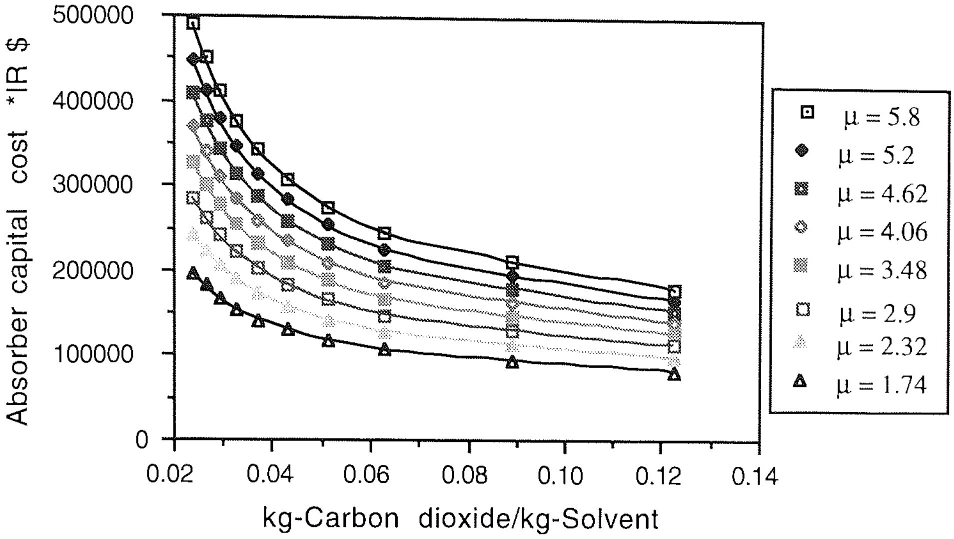


Fig. (4-2) The effect of the solubility and the viscosity of the solvent on the cost of the absorber

The derived equation (Chapter 3)

Cost of the absorber = $a_1 + a_2 K^{1/3} \mu^{4/3}$

If we consider the Selexol process a_1 = 37548

a_2 = 50809

cost = $ 484126 %error = 13.2

The resulting equation from curve fitting to the design data

Cost of the absorber = $43000 + 53000\ K^{.962} \mu^{1.43}$

Cost = $ 443460 %error = 5.25

The suggested general equation

Cost of the absorber = $a_1 + a_2 K^{.962} \mu^{1.43}$

Cost = $ 421453 %error = 0.3

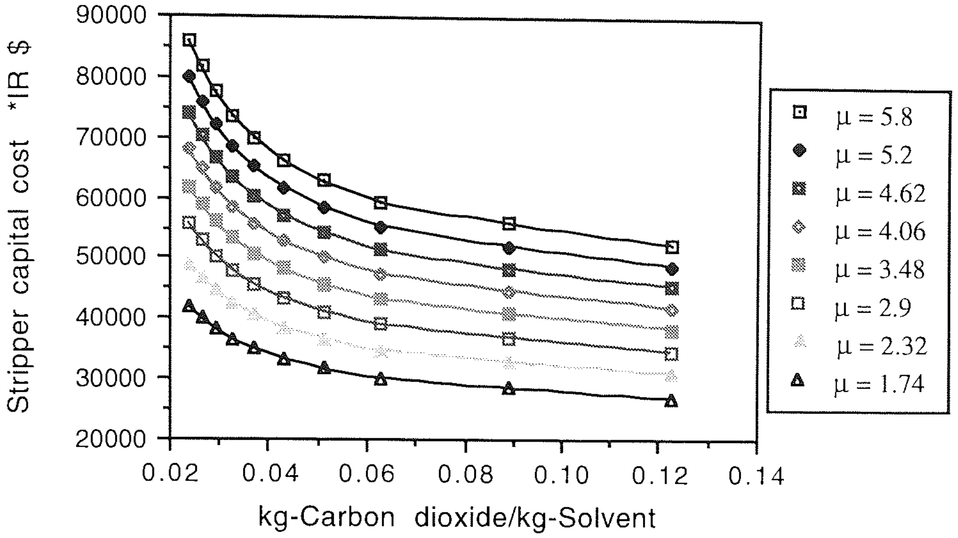


Fig. (4-3) The effect of the solubility and viscosity of the solvent on the cost of the stripper

The derived equation (Chapter 3)

Cost of the stripper = $a_1 + a_2 K^{1/3} \mu^{4/3}$

If we consider the Selexol process a_1 = 23249

a_2 = 66106

cost = \$ 84268 %error = 16.5

The resulting equation from curve fitting to the design data

Cost of the stripper = $25000 + 74000 \ K^{.81} \mu^{1.143}$

= \$ 77859 %error = 9.7

The suggested general equation

Cost of the stripper = $a_1 + a_2 K^{.81} \mu^{1.143}$

Cost = \$ 70469 %error = 0.2

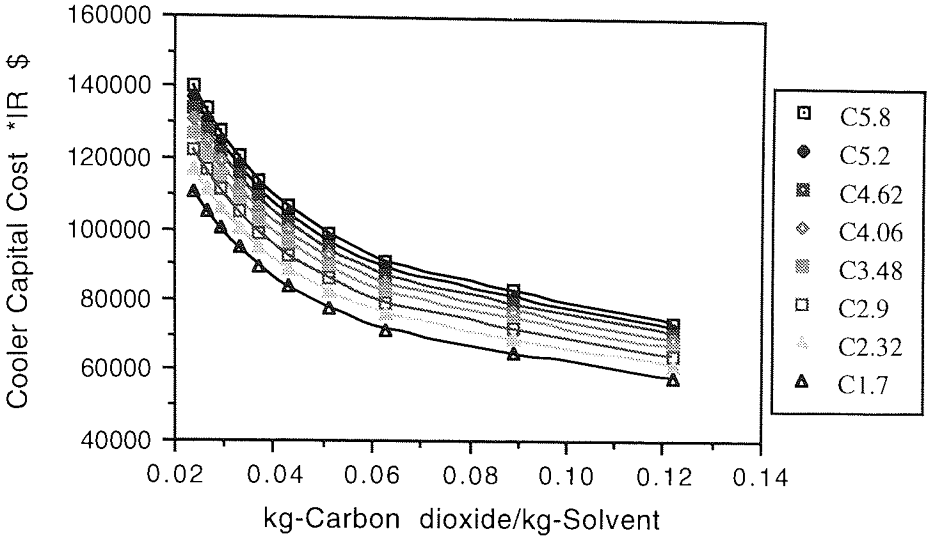


Fig. (4-4) The effect of the solubility and viscosity of the solvent on the cost of the cooler

The derived equation (Chapter 3)

Cost of the cooler = $a_2 K^{.68} \mu^{.1136}$

If we considered the Selexol process $a_1 = 119165.4$

Cost = \$ 96754 % error = 22.6

The resulting equation from curve fitting to the design data

Cost of the cooler = $137414 \; K^{.624} \mu^{.2}$

Cost = \$ 127613 %error = 2.0

The suggested general equation

Cost of the cooler = $a_1 K^{.624} \mu^{.2}$

Cost = \$ 110665 %error = 11.0

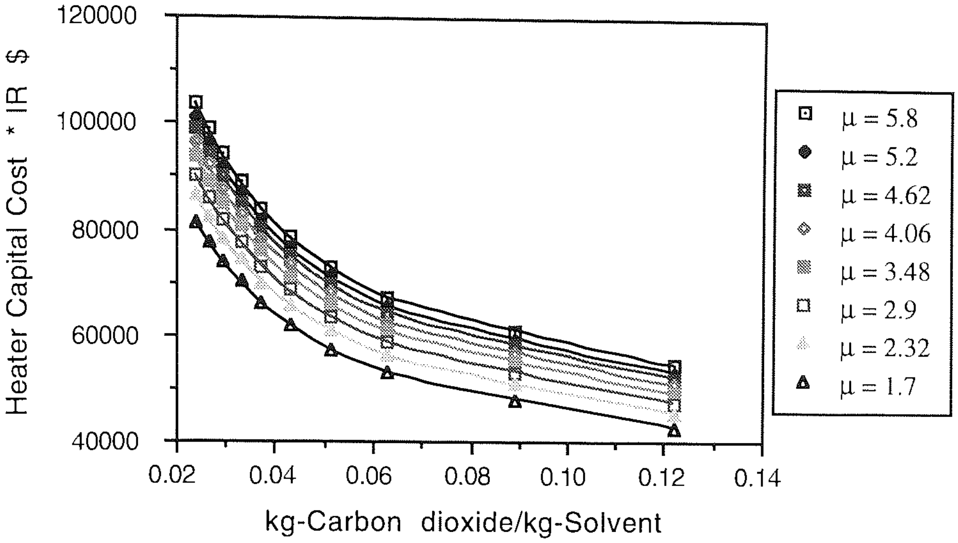


Fig. (4-5) The effect of the solubility and viscosity of the solvent on the cost of the heater

The derived equation (Chapter 3)

Cost of the heater = $a_2 K^{.68} \mu^{.1136}$

If we consider the Selexol process a_1 = 113713

Cost = $ 83474 %error = 16

The resulting equation from curve fitting to the design data

Cost of the heater = 121089 $K^{.624} \mu^{.2}$

Cost = $ 94167 %error = 5.3

The suggested general equation

Cost of the heater = $a_1 K^{.624} \mu^{.2}$

Cost = $ 88611 %error = 11

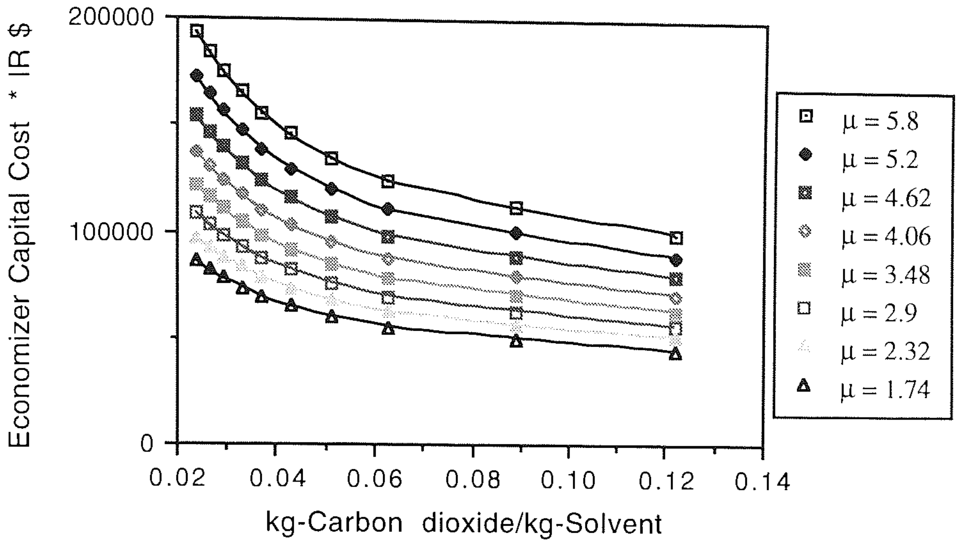


Fig. (4-6) The effect of the solubility and viscosity of the solvent on the cost of the economizer

The derived equation (Chapter 3)

$$\text{Cost of the economizer} = a_1\, K^{.68}\, (\, a_2\, \mu^{.5} + a_3\, \mu^{.1136}\,)^{\,0.68}$$

If we consider the Selexol process $a_1 = 1055$

$a_2 = 530.2$

$a_3 = 637.3$

Cost = \$ 114401 %error = 40

The resulting equation from curve fitting to the design data

$$\text{Cost of the economizer} = 1440 + 80848\ K^{.65}\, \mu^{1.0}$$

Cost = \$ 175455 %error = 7.8

The suggested general equation

$$\text{Cost of the economizer} = 1.5a_1\, K^{.68}\, (\, a_2\, \mu^{.5} + a_3\, \mu^{.1136}\,)^{\,0.68}$$

Cost = \$ 171602 %error = 9.8

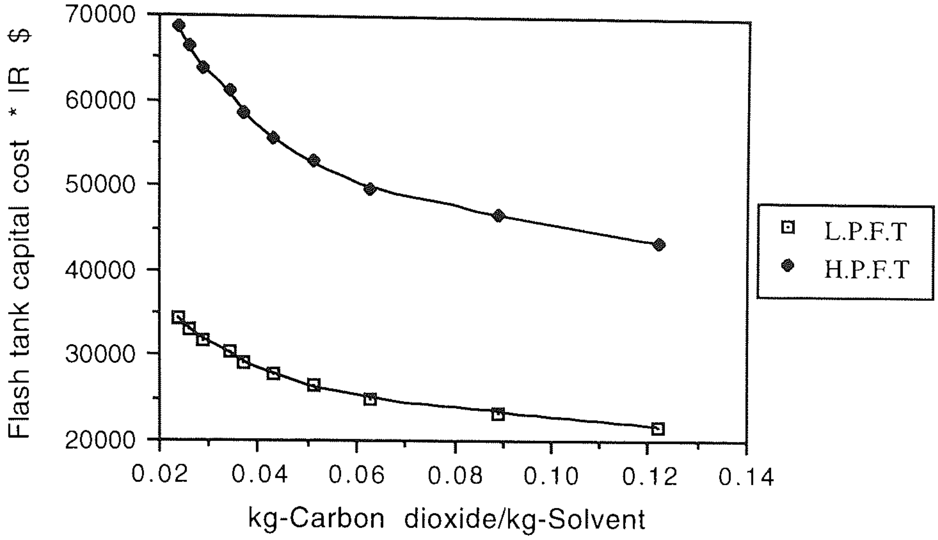


Fig. (4-7) The effect of the solubility of the solvent on the cost of the flash tanks

The derived equation (Chapter 3)

$$\text{Cost of the flash tank} = a_1 + a_2 K^{2/3}$$

If we consider the Selexol process $a_1 = 8971$

$a2 = 32733$

Cost = \$ 32257

The suggested general equation

$$\text{Cost of the flash tank} = a1 + a_2 K^{2/3}$$

Cost = \$ 32257

%error = 2.3

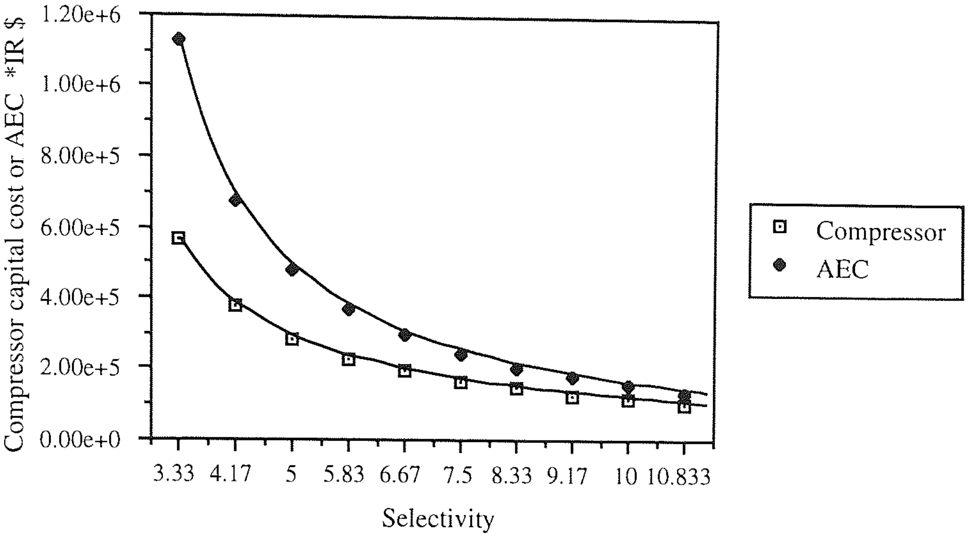


Fig.(4-8) shows the relationship of the Selectivity with the cost of the compressor and the AEC

The derived equation (Chapter 3)

Cost of the compressor $= 1043\,[(a_1/SL) + a_2]^{0.8}$

$a_1 = 3485$

$a_2 = 43$

Cost = \$ 116909 %error = 10.0

Annual Electricity Cost $= 429.52\,[(a_1/SL) + a_2]$

$a_1 = 3485$

$a_2 = 43$

Cost = \$ 156653 %error = 11.0

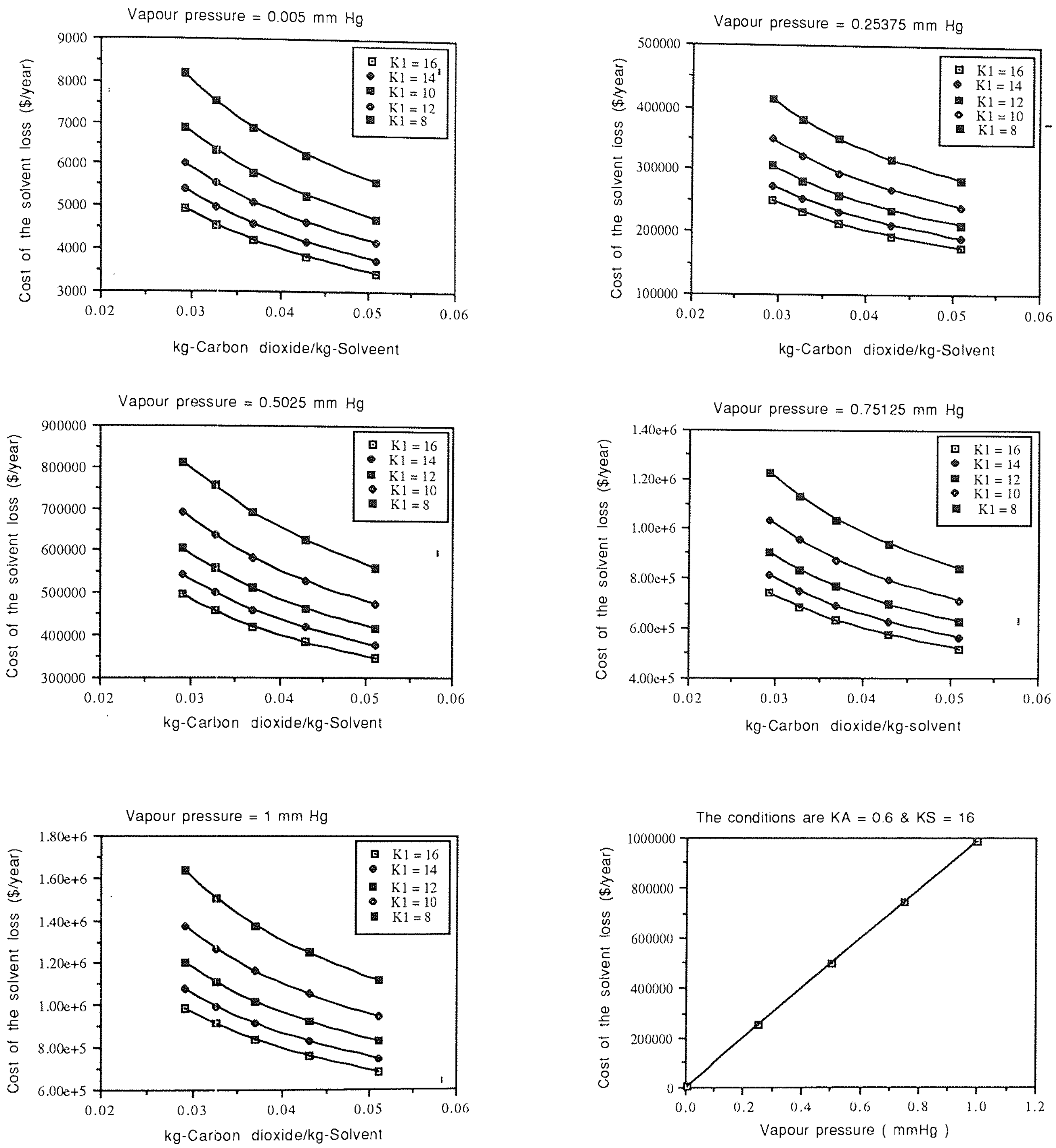


Fig. (4-9) The relationship of the solvent loss with the vapour pressure and the solubility of the solvent

The derived equation (chapter two)

$$\text{Annual Solvent Loss Cost} = a_1 \, (K/K_1) \, V_p \, C$$

CHAPTER FIVE

An Objective Function for Solvent Design

5-1 The Cost Equations

From table (4-4), it is easy to see that the heating steam and the cooling water cost represents a very high percentage of the total operating cost. The heat exchanger cost also represents a significant percentage of the total capital cost. This demonstrates the important influence of the physical properties of the solvent which are related to the heat transfer process, in addition to those which already affect the mass transfer process. The properties of a solvent which affect the capital and the running cost of heat transfer equipment are the heat capacity and thermal conductivity. The heat capacity plays an important role in determining the required heating or cooling fluid in addition to its effect on the size of the heat exchanger. The thermal conductivity (with some other properties) determine the heat transfer coefficient. The heat transfer coefficient and the mass circulation rate are the major factors that determine the size of the heat exchanger.

In Chapter 3, when the optimum cost equations were derived, it was assumed that the heat capacity, the thermal conductivity and the molecular weight of the solvent are constants. These assumptions do not affect the coefficients of the absorber and the stripper cost equations, but it affects the coefficient values of all the other cost equations. If we consider those new properties as variables and review the derivation of those equations, we may obtain coefficient values which are independent of the solvent used.

According to this approach and by rederiving the optimum cost equations (for the capital and operating cost items) the following new set of equations have been obtained.

Cost of the absorber = $a_1 + a_2 K^{0.962} \mu_1{}^{1.43}$ (5-1)

Cost of the stripper = $a_3 + a_4 K^{0.81} \mu_3{}^{1.143}$ (5-2)

Cost of the flash tank = $a_5 + a_6 (K * M_{w1})^{2/3}$ (5-3)

Cost of the heat exchanger = $a_1 (K M_{w1})^{0.68} \mu_2^{0.2} (\frac{S_p}{K_L})^{0.453}$ (5-4)

Cost of the compressor = $a_8 (\frac{a_9}{S_L} + a_{10})^{0.8}$ (5-5)

Annual C. P. C. $= a_{11} (\frac{a_9}{S_L} + a_{10})$ (5-6)

Annual S.S.C@ $= a_{12} (K/K_1) M_{w2}$ (5-7)

Annual H.S.C@ $= a_{13} K S_p M_{w1}$ (5-8)

Annual C.W.C@ $= a_{14} K S_p M_{w1}$ (5-9)

Annual S.L.C@ $= a_{15} C (K/K_1) V_p M_{w1}$ (5-10)

@C.P.C = Compressing power cost
S.S.C = Stripping steam cost
H.S.C = Heating steam cost
C.W.C = Cooling water cost
S.L.C = Solvent loss cost

5-2 The Coefficients of the Cost Equations

The cost of a physical gas absorption process is related to two factors, as can be seen from the cost equations derived above. The first is the physical properties of the solvent. The second is the collection of all other factors affecting the cost of the process which are not related to the physical properties of the solvent. The second factor is represented by the coefficients of the cost equations. In this work, the main objective is to investigate the role of every physical property of the solvent used in determining the cost of the process, so it is necessary to assume that the coefficients of the equations are constants. The values of these constants are determined by the following factors.

- Flow rate of the feed gas and its physical properties
- Degree of separation required
- Operating conditions of the absorber and the stripper (temperature and pressure)
- Type of the packing material
- Pressure of the first flash tank
- Geometry of the heat exchanger and its operating conditions

The coefficients can be estimated, from their definitions which were shown in chapter three, for any selected process. A simple computer program has been written for this purpose, and used to calculate the coefficients of the selected process, which was mentioned in the previous chapter. The values of the coefficients for that process are shown in table (4-1).

5-3 The Objective Function of Every Cost Item

Equations (5-1) to (5-10) highlight the fact that the objective function for every cost item can be represented by one or more of the physical properties of the solvent to a certain power. For example the objective function of the absorber cost is a function of the equilibrium constant and the viscosity at absorption conditions. The powers on these two properties (0.962 for K and 1.43 for μ) represent the role or the contribution of each one to the cost of the absorber.

Figures (5-1) and (5-2) show the relationship of every cost item with its objective function. These two figures demonstrate the following points.

- The vital role of the solubility in determining the cost of the most important items, like the cost of the absorber, heat exchangers, heating steam and solvent loss.

- The role of the viscosity is vital in determining most of the items of capital cost but it has no effect on the running cost items (if we ignore the pumping cost).
- The solvent loss cost could represent a very high percentage of the total operating cost especially when the vapour pressure of the solvent is very high .
- The effect of the selectivity is limited to the cost of the compressor and the power required to run it.
- The specific heat of the solvent has a reasonable effect in determining the quantity of the heating steam and the cooling water in addition to its effect on the size of the heat exchanger.
- The thermal conductivity role in determining the cost of the heat exchangers.

It is difficult to put the properties in their order of importance because the degree of the importance of any property depends on the type of the process, but we can suggest the following sequence as representative of their importance for the selected process.

1- Solubility
2- Vapour pressure
3- Viscosity
4- Selectivity
5- Specific heat
6- Thermal conductivity

5-4 The Total Objective Function

The setting up of the objective function is a necessary step before starting the design of any new molecule. No one, so far, has set a comprehensive objective function in terms of the effective physical properties of the solvent, because these properties are related to the cost of the process in a very complicated relationship. From the previous paragraph we have seen that every cost item has its own objective function, so if it is wanted to minimize, for example, only the cost of the absorber the function ($K^{0.962}\ \mu_1^{1.43}$) has to be minimized or if we wanted to minimize only the cost of the heat exchanger, the function ($M_{W1}^{0.68}\ K^{0.624}\ \mu_2^{0.2}\ (S_P/K_L)^{0.453}$) has to be minimized. Normally, minimizing the total cost of the process is desired more than minimizing only one cost item, so the objective function which has to be minimized can be represented by the best combinations of those physical properties which have a part in forming the individual objective functions. An optimization program is required to find out the best combination between the effective physical properties which minimizes the total cost of the process. It is obvious, that such a program would be complicated and require much effort to make it work, due to the complexity of the problem. Establishing such a type of optimization program represents an advanced step in the direction of physical solvent design, and this is left for future work.

5-5 Solvent Evaluation

The evaluation of any solvent can be made provided two things are known. The first is the objective which is to be achieved by the process; from the objective, the configuration of the process can be designed. The second is the required physical properties of the solvent. Ten solvents have been chosen for evaluation. The selected solvents include three important solvents, the first one is Selexol, which represents the currently most successful one, the second is acetonyl acetone, which has been suggested by Sitthiosoth (44) as a potentially credible alternative to the currently successful solvents due to its low viscosity and high solubility, and the third one is n-formyl morpholine which had been suggested by Zawacki (60) as an alternative because of its high selectivity and its low vapour pressure. The basis for the selection of the other seven solvents was essentially the availability of the required properties. The selected solvents are shown in table (5-

2). To make precise evaluations for those solvents, several steps have to be taken. These are as follows:

A- Select or design a suitable process configuration to suit the objective which is to be achieved. From the process configuration the individual cost items can be named. In this work, the process, shown in Chapter 4 was chosen. The duty of that process is to produce methane gas with not more than 3% of CO_2 and 4 ppm H_2S from 5000 kmole/hr of a gas mixture with 10% CO_2 and 1% H_2S at 68 atm. The configuration of this process has already been designed.

B- All or some of the following physical properties for the solvents considered have to be obtained either by collecting them from the literature or by estimating them using a reliable estimation method or by direct measurement.

1- The solubilities of CO_2, H_2S and CH_4 at different pressures and temperatures.
2- Viscosity at different temperatures.
3- Vapour pressure at different temperatures.
4- Thermal conductivity at different temperatures.
5- Normal boiling point.
6- Molecular weight.
7- Specific heat at different temperatures.
8- Critical temperature and pressure.
9- Acentric factor.
10- Cost per unit mass.

In this work, some of the data required were collected from the literature as experimental data and the others were estimated. Appendix 2 shows the calculation procedures for the estimation of the thermal conductivity, specific heat and viscosity. In Chapter 6 the estimation methods of the vapour pressure, critical properties (temperature and pressure) and the acentric factor were reviewed. Table (2-1) shows a very brief description of the methods which were used for the estimation, and table (5-2) gives the predicted or the measured physical properties for all the selected solvents.

C- The values of the parameters of the cost equations can be calculated from their definitions as shown in Chapter 3. Then the total equipment, running and process costs can be estimated from equations (5-1) to (5-10). For this work table (5-1) shows the values of the parameters for the selected process and table (5-4) shows the costs of all the individual items in addition to the total equipment, running and total process cost. The methods which were used to calculate the total process cost are shown in Appendix 1.

D- Select the solvent which has the most competitive process costs.
From table (5-4) we can see that the process costs obtained by using methyl ethyl ketone, ethyl acetate, methanol and acetone are very high compared with the other solvents. So these four solvents have to be taken out of the evaluation. By considering the remaining six solvents, the total equipment, running and process costs have been represented in figures (5-3A), (5-4A) and (5-5A). These figures show the significant importance of the running cost compared with the capital cost. Dimethyl acetamide and dimethyl formamide also have to be taken out of the evaluation, although their capital costs are very low. The other four solvents represent the best ones in the selected group. At this stage and before selecting the cheapest process, a hazard anaylsis for every one has to be considered. From Janssen Chimica catalogue (1993) the following description of the risk of each solvent has been given.

1- Selexol:- no risk.
2- Acetonyl acetone:- irritant to eyes, respiratory system and skin
3- n-Formyl morpholine:-irritant to eyes, respiratory system and skin.

4- Methyl pyrrolidone:- corrosive and causes burns.

So methyl pyrrolidone has to be excluded because of its hazardous nature which means additional expenditure to meet the safety requirements. The risks from using acetonyl acetone and n-formyl morpholine are not so significant and can easily be minimised. So acetonyl acetone is the best one due to its lower running, capital and total process costs. The weak points of n-formyl morpholine are its high viscosity and low solubility compared with Selexol, that is why its capital cost is about twice Selexol's. The running cost of the n-formyl morpholine is slightly less than that of Selexol. But if we include the pumping cost for both solvents, the increase in the capital and running costs of n-formyl morpholine process will be more than that of Selexol due to the high viscosity of the n-formyl morpholine.

5-6 The effect of the Configuration of the Process on the Selected Solvent

In the previous example, it was shown that acetonyl acetone was the the most economic solvent for the configuration shown in figure (4-1). It is necessary to consider another example of process configuration to see how that would affect the economic position of the same selected group of solvents. Let us assume that it is required to produce a methane stream with not more than 3.5% impurity of CO_2 from a feed gas mixture of 13535 kmole/hr with 40% CO_2 and 60% CH_4. In this case, there is no need to use strippers or heat exchangers. Figure (1-2) is the suitable process configuration to achieve this objective. The cost items for this process are the absorber, the flash tanks, the compressor, the electricity to run the compressor and the lost solvent. The same solvents (excluded methyl pyrrolidone) which were evaluated in the first example will be re-evaluated for this new configuration. The values of the parameters of equations (5-1), (5-3), (5-5) were calculated from their definitions (Chapter 3) and are shown in table (5-

3). The cost of the absorber, flash tanks, compressor and electricity were calculated for the nine different solvents from equations (5-1), (5-3), (5-5) and (5-6) respectively and are shown in table (5-5). Unfortunately, for this particular process, the cost of the solvent lost can not be calculated from equation (5-10) as this equation was derived to calculate the cost of the solvent lost from the stripper only. The rates of solvent loss in this particular process were calculated from simple material balances for the nine selected solvents and are shown in table (5-6). The capital, running and total process costs were calculated and are shown in table (5-5). From this table, it is reasonable to exclude ethyl acetate, methyl ethyl ketone, acetone and methanol from the comparision due to their very high process costs. The equipment, running and total process costs are represented in figures (5-3B), (5-4B) and (5-4B) respectively to present a clear picture about the differences in the costs of using these solvents. For this particular configuration (example two), Selexol is the best solvent followed by n-formyl morphyline then acetonyl acetone.

From these two examples it can be concluded, that there is no universal solvent which is the best for any configuration, but there is a best solvent for any particular configuration.

Table (5-1) The parameters of the cost equations for Example 1

Parameter	Value	Parameter	Value
a_1	37548	a_2	50809
a_3	23249	a_4	66106
a_5	26914	a_6	2341.5
a_7	3231	a_8	1043
a_9	3485	a_{10}	43
a_{11}	429.52	a_{12}	756667
a_{13}	13989	a_{14}	843.6
a_{15}	33191		

Table (5-3) The parameters of the cost equations for Example 2

Parameter	Value	Parameter	Value
a_1	72896.3	a_2	106275
a_5	8971.2	a_6	1710
a_8	1043	a_9	3988.6
a_{10}	841.5	a_{11}	429.52

Table (5-2) The physical properties of the solvents considered

Solvent	Properties 1	2	3	4	5	6	7	8	9	10	11
Selexol	0.6	16.3	280	10.83	5.8	3.2	1.07	2.3	0.173	0.013	9.65
Acetonyl acetone (B2)	0.6	30.6	114	5	1.75	1.13	0.4	2.11	0.114	1.655	16
Ethyl acetate	0.97	31.1	88.11	2.65	0.42	0.31	0.14	2.17	0.146	274.1	8.86
n-Formyl morpholine	1.42	31.9	115.1	17.5	6.79	4.11	0.94	1.73	0.062	0.089	47.5
Acetone	1.29	31.8	58.1	7.48	0.3	0.23	0.11	2.7	0.138	603	2.96
Dimethyl acetamide	1.17	27.4	87.12	8.41	1.95	1.24	0.4	2.104	0.179	8.06	8.32
Dimethyl formamide	1.17	37.7	73.1	11.6	0.85	0.59	0.23	1.913	0.188	13.3	7.84
Methanol	2.64	38.9	32.04	5.93	0.514	0.372	0.16	2.99	0.169	411.2	3.2
Methyl ethyl ketone	1.05	28.9	72.1	6.25	0.37	0.275	0.125	2.23	0.138	254.6	10.17
Methyl pyrrolidone	1.24	26.2	99.13	11.8	1.67	1.08	0.36	1.85	0.188	0.971	6.84

1- Equilibrium constant at 1000 psia and 25 C (K)
2- Equilibrium constant at 20 psia and 127 C (K1)
3- Molecular weight of the solvent (Mw1)
4- Selectivity of the solvent (KCH4/KCO2)
5- Viscosity at absorption conditions (μa)
6- Viscosity at heat exchange conditions (μh)
7- Viscosity at desorption conditions (μs)
8- Heat capacity of the solvent, Cp (kJ/kg K)
9- Thermal conductivity of the solvent, KL (W/m K)
10- Vapour pressure of the solvent, VP mmHg
11- Cost per unit weight $/kg

Table (5- 4) The cost for every item by using different solvents for Example 1

	Cost Item ($) or ($/year)						
Solvent	Absorber	Stripper	F. Tank	H.Exch.s	Comp.	T.E.C	
Selexol	421454	70469	98205	441875	116909	1148912	
Acetonyl acetone	106742	38584	66076	226325	205911	643639	
Ethyl acetate	51819	30065	72346	179019	334732	667982	
n-Formyl morpholine	1139128	105073	96922	610393	84273	2035789	
Acetone	49152	29767	68537	172099	152610	472167	
Dimethyl acetamide	191111	49590	78008	237126	140126	695960	
Dimethyl formamide	84387	37243	72367	169924	111424	475344	
Methanol	87460	41116	72033	188814	181196	570619	
Methyl ethyl ketone	50397	29634	68817	166577	174247	489672	
Methyl pyrrolidone	167654	47726	84801	240923	110100	651205	
Solvent	A. E. C.	A.C.W.C	A.S.S.C	A.S.L.C	A.H.S.C	T.O.C	T. P. C.
Selexol	156652	325972	544774	46635	5405345	6479378	8279340
Acetonyl acetone	317853	121753	267046	1964608	2018947	4690208	5698576
Ethyl acetate	583445	156459	424783	2.215 E8	2594436	2.253 E8	2.263 E8
n-Formyl morpholine	104049	238597	606253	715874	3956482	5621257	8810659
Acetone	218579	170715	552483	1.396 E8	2830843	1.434 E8	1.441 E8
Dimethyl acetamide	196461	180922	581556	8280086	3000100	1.224 E8	1.333 E7
Dimethyl formamide	147520	138026	422669	7851505	2288782	1.085 E7	1.159 E7
Methanol	270902	213359	924295	9.496 E7	3537968	9.99 E7	1.008 E8
Methyl ethyl ketone	257979	142420	494821	2.236 E8	2361651	2.2684 E8	2.276 E8
Methyl pyrrolidone	145333	191841	644580	1034247	3181155	5197155	6217377

A. E. C. = Annual compressing power cost
A.S.S. C = Annual stripping steam cost
A.H.S.C = Annual heating steam cost
A.C.W.C = Annual cooling water cost
A.S.L.C = Annual solvent loss cost
T.E.C = Total capital cost
T.O.C = Total operating cost
T.P.C = Total process cost

Table (5- 5) The cost of every item by using different solvents for Example 2

	Cost Item			
Solvent	Absorber	F. Tank	Compressor	T. E. C
Selexol	875895	305179	305080	1486154
Acetonyl acetone	217626	187858	389035	794519
Ethyl acetate	102747	210752	518418	831918
n-Formyl morpholine	2377022	300493	276455	2953971
Acetone	97168	196846	337942	631957
Dimethyl acetamide	394096	231426	326301	951823
Dimethyl formamide	170867	210830	300160	681858
Methanol	177294	209610	365095	751999
Methyl ethyl ketone	99771	197866	358437	656074
Solvent	A. E. C.	A. S. L. C.	T. O. C.	T. P. C.
Selexol	519571	47764	567335	2895643
Acetonyl acetone	704068	9317645	1.0022E+7	1.12665E+7
Ethyl acetate	1008042	2.5435E+9	2.5445E+9	2.5458E+9
n-Formyl morpholine	459367	2128201	2587568	7215456
Acetone	590448	1.56E+9	1.5606E+9	1.56158E+9
Dimethyl acetamide	565133	5.2E+7	5.2565E+7	5.40563E+7
Dimethyl formamide	509119	7.48E+7	7.5309E+7	7.63774E+7
Methanol	650332	4.566E+8	4.5715E+8	4.5833E+8
Methyl ethyl ketone	635541	2.53E+9	2.53064E+9	2.53166E+9

Table (5-6) The rate of solvent loss for the nine solvents considered in Example 2

Solvent	v. p. at 25C	S. L. I. F. T.	S. L. L. F. T.	T. A. S. L.
Selexol	.0008	.0364	0.651	4949.82
Acetonyl acetone	.26	5.022	75.86	582353
Ethyl acetate	87	3094.06	36777.7	2.8708 E8
n-Formyl morpholine	.009	0.39342	5.829392	44804.23
Acetone	222	4380.34	68894.27	5.276 E8
Dimethyl acetamide	1.7	52.45	814.512	6242114
Dimethyl formamide	3.0	81.3585	1244.136	9543563
Methanol	121	1119.12	18692.61	1.4264 E8
Methyl ethyl ketone	83.2	2139.906	32382.27	2.4856 E9

S. L. I. F. T. = Solvent loss in the intermedaite pressure flash tank (kg/hr)
S. L. L. F. T. = Solvent loss in the low pressure flash tank (kg/hr)
T. A. S. L. = Total annual solvent loss (kg/year)

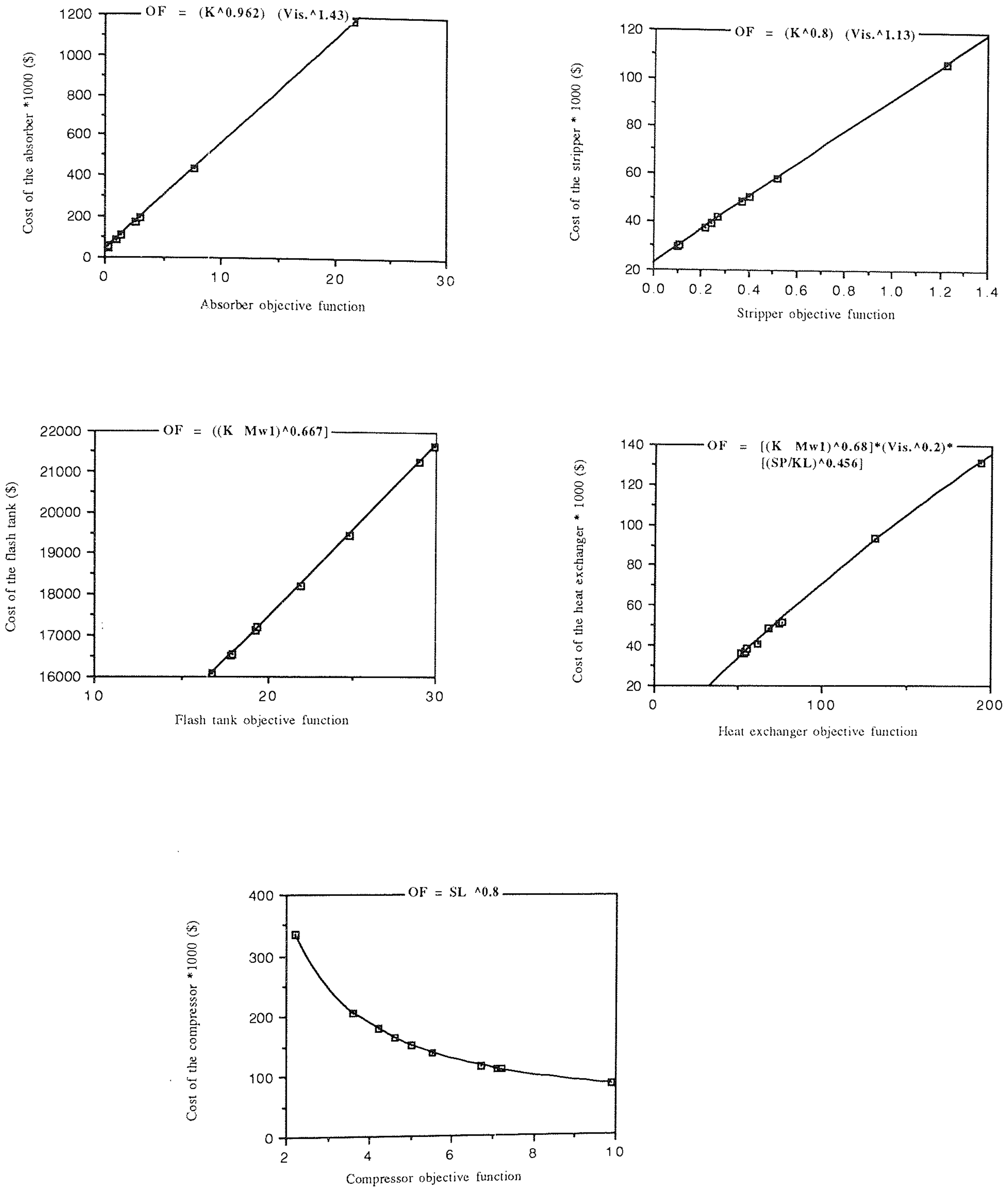


Figure (5-1) The relationship of every equipment cost with its objective function

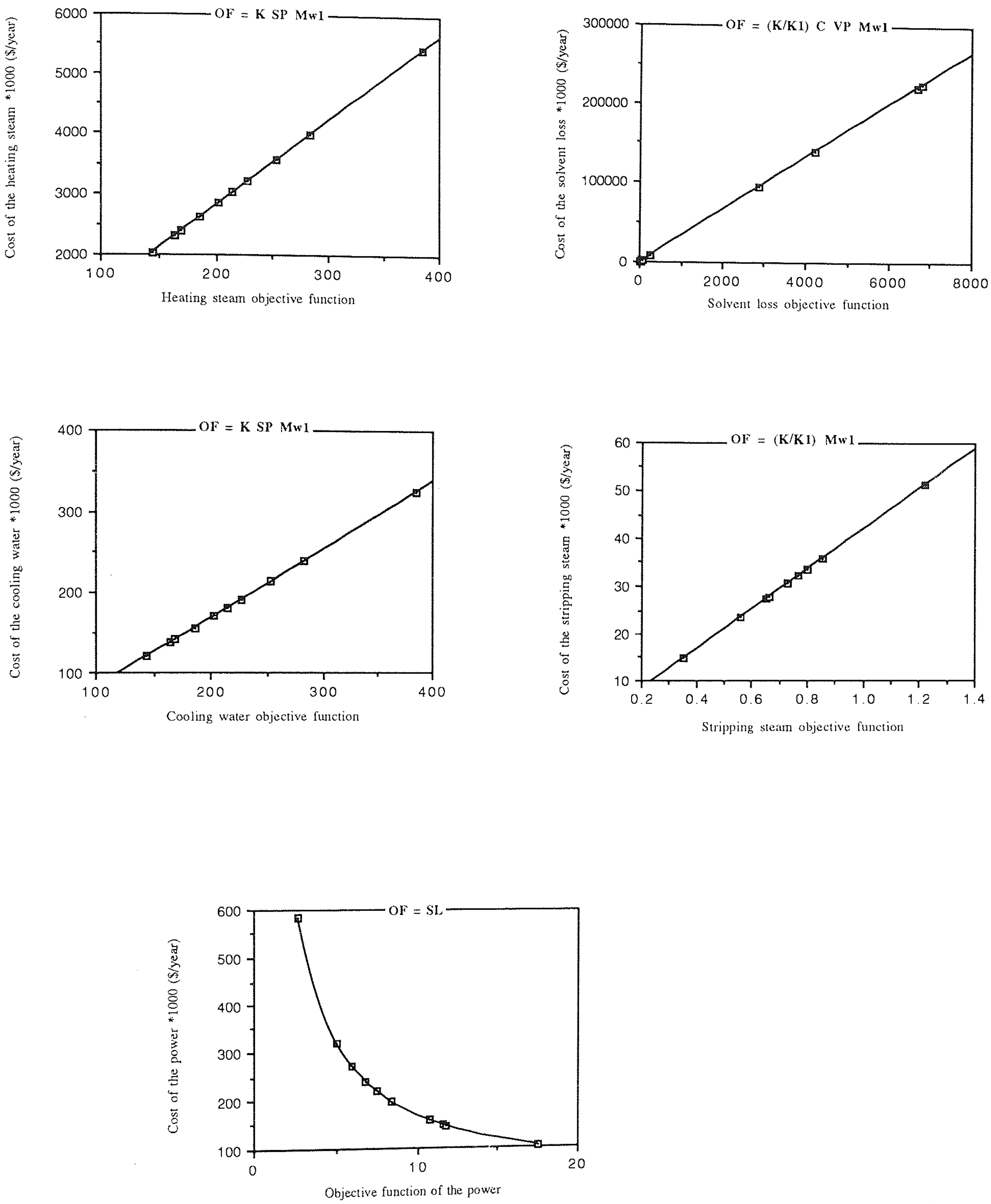
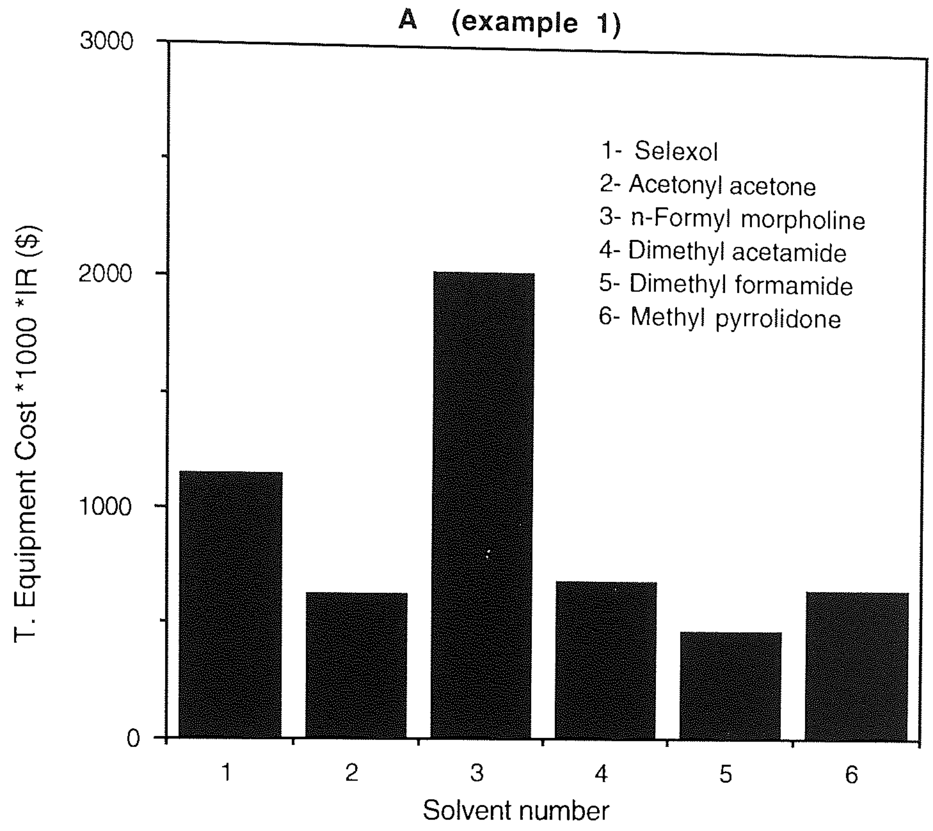


Figure (5-2) The relationship of every running cost item with its objective function



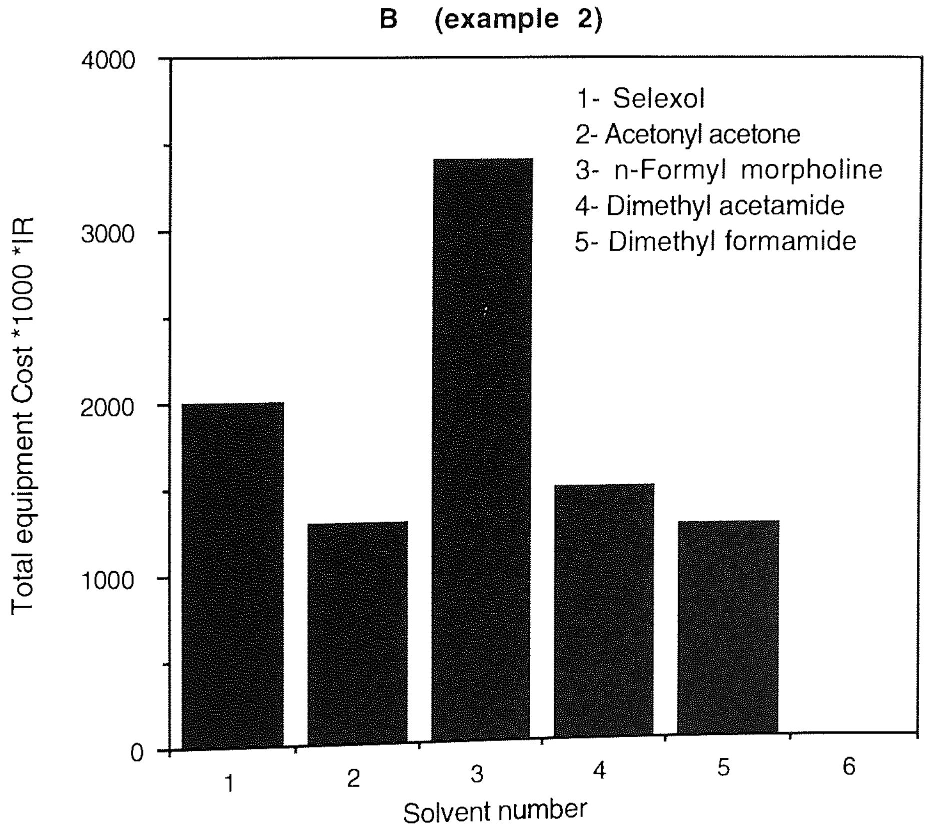
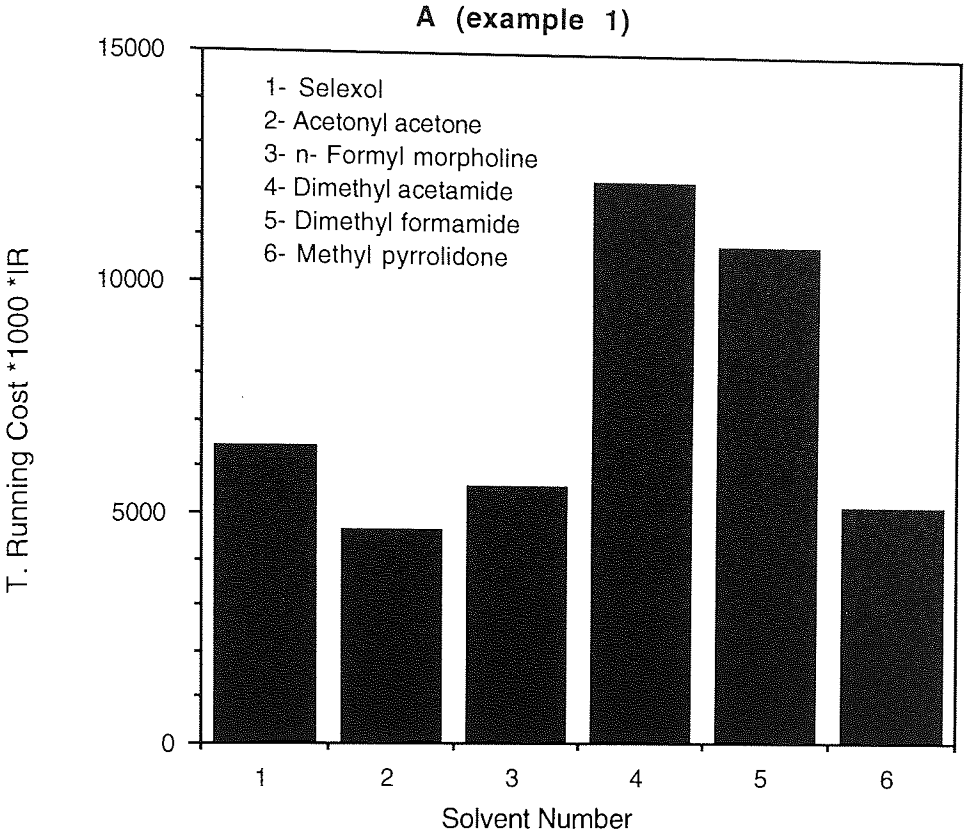


Fig. (5-3) The effect of the solvent type on the cost of the equipment



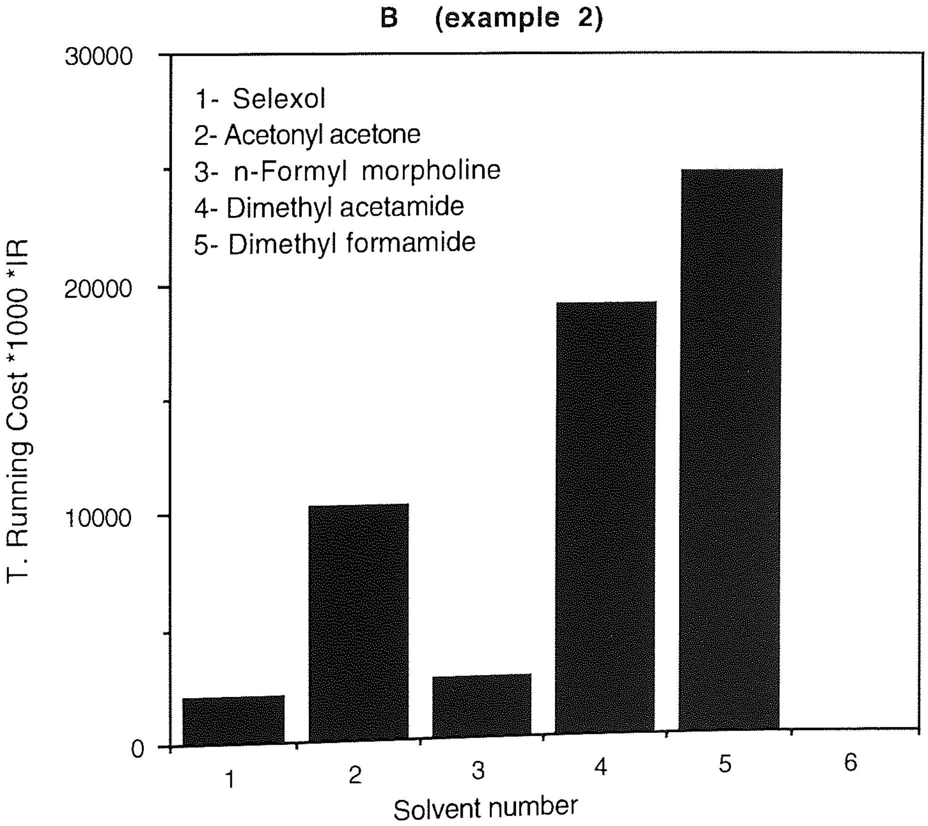


Fig. (5-4) The effect of the type of the solvent on the running cost

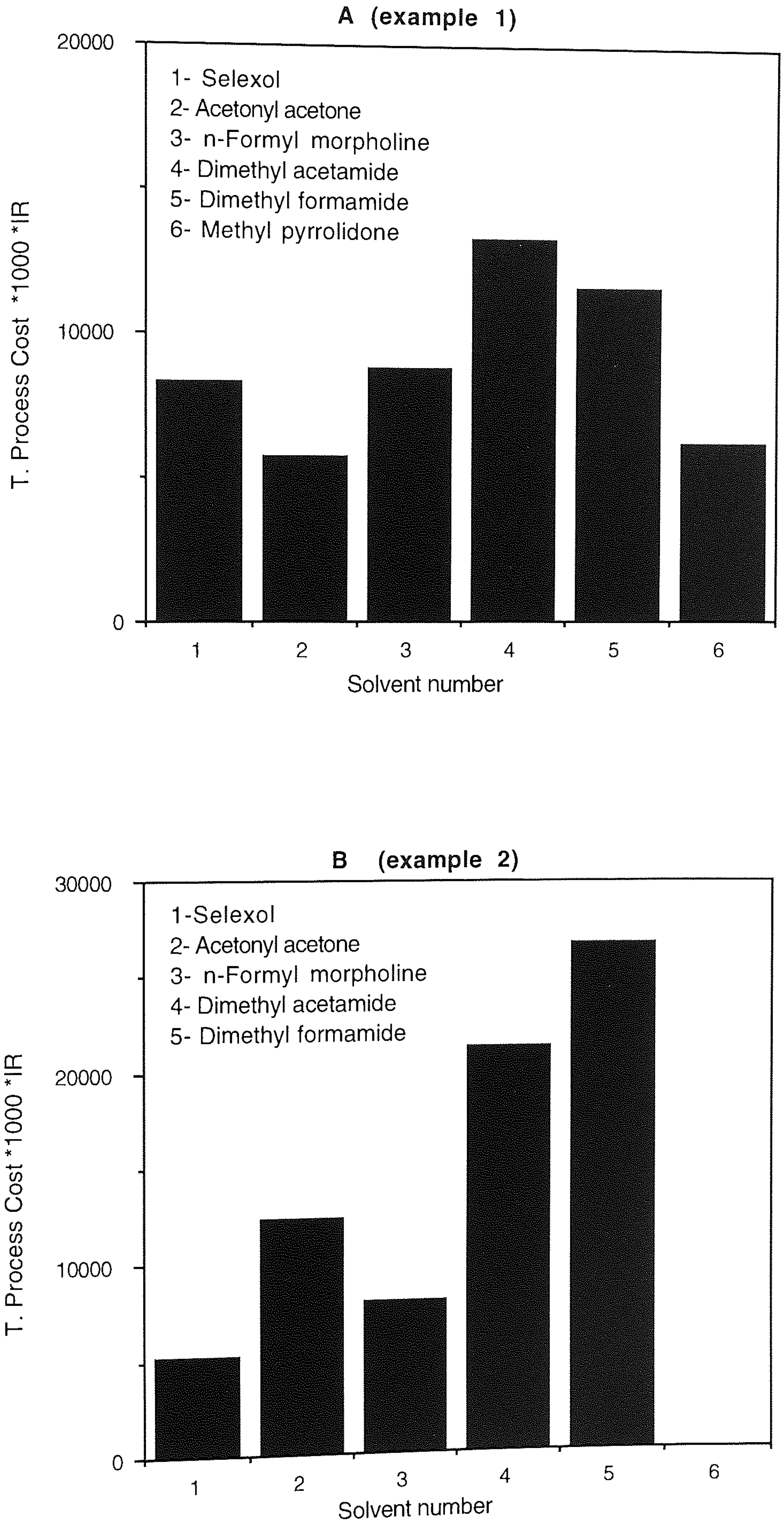


Fig. (5-5) The effect of the type of the solvent on the process cost.

CHAPTER SIX

Measurement and Estimation of the Vapour Pressure of Acetonyl Acetone

It was seen in the previous chapters that the vapour pressure of the solvent affects the running cost of the gas absorption process significantly. In this chapter, the theories of estimating and measuring of the vapour pressure of liquids will be reviewed. The vapour pressure of acetonyl acetone will be both estimated and measured.

6-1 Estimation of the Vapour Pressure

The molecules of any gas are conceived as having completely random motion within the container of the gas. There are two factors which affect the motion of the molecules, if the action of external force fields are not considered. The first factor is the kinetic energy of the molecules, which is affected by the temperature changing. The second one is the intermolecular forces, which could be attractive or repulsive forces. When the gas is compressed the intermolecular attractive forces increase due to decreased distances between the molecules, so at a certain distance these forces reach a maximum. At a certain point of the gas compression process, where the value of the attractive forces become greater than the value of the kinetic energy, the molecules will join together converting the gas state to a liquid state.

The existence of the liquid-phase of any molecules depends upon several related factors, mainly, the potential energy, kinetic energy, temperature and the pressure. The substance can not be liquefied, if its kinetic energy is greater than that of the potential energy, no matter what pressure has been applied. The temperature at which the attractive forces of the molecules are equal to that of their kinetic energy is called the critical temperature. The critical temperature is the temperature at which the gas and the liquid phases can not be distinguished. The minimum pressure required to liquefy a gas at its critical temperature is called the critical pressure. The molar volume of a material at its critical point is called the critical molar volume.

In practice, a liquid of any material contains some molecules whose kinetic energy is higher than their attractive forces. These molecules could leave the surface of the liquid and fly in the space above it forming a phase of vapour. Some of the vapour molecules have a potential energy higher than their kinetic energy. These molecules can return to the liquid surface (condensation). A system at constant temperature is at equilibrium if the number of the molecules leaving the liquid surface is equal to the number returning. The pressure of the vapour phase of the equilibrium system is called the vapour pressure of the substance.

Over the years, many techniques have been used to estimate the vapour pressure of different materials. Most of these techniques were derived from the integration of the Clausius-Clapeyron equation, which arises from the equality of the chemical potential, temperature, and pressure for both liquid and vapour phases.

$$\frac{d\ \ln P_{vp}}{d(1/T)} = -\frac{\Delta H_v}{R\,\Delta Z_v} \qquad \text{..........(6-1)}$$

ΔH_v and ΔZ_v refer to the difference in the enthalpies and compressibility factors of the saturated vapour and the saturated liquid. To integrate the above equation some assumptions have to be made regarding the dependence of the heat of the vaporisation and the compressibility factor on the temperature. Also, one vapour pressure-temperature point is needed to calculate the constant of integration. Over small temperature ranges it is possible to assume that the group

($\Delta H_v/R\ \Delta Z_v$) is constant, and the following equation can be obtained from the integration of equation (6-1)

$$d\ \ln P_{vp} = A - \frac{B}{T} \qquad \text{..........(6-2)}$$

where $B = \frac{\Delta H_v}{R\,\Delta Z_v}$ and A is the constant of integration. Equation (6-2) shows a linear relationship between ln P_{vp} and (1/T), which is only true in a narrow range of temperatures, so its results are approximate for a wide range of temperatures.

6-1-1 Antoine Correlation

Many semi-empirical equations have been proposed to correlate more accurately data for the vapour pressure. One of these equations was developed by Antoine (40), which could be used over a limited range of temperatures.

$$\ln P_{vp} = A - \frac{B}{T + C} \qquad \text{..........(6-3)}$$

When C = 0, equation (6-3) reverts to equation (6-2). The constant C can be determined either from experimental data or calculated from the following empirical equations.

- For hydrocarbons with n carbon atoms

$$C = 271 - 7.2\ n \qquad \text{............(6-3A)}$$

- For elements (monatomic vapours) and for substances with boiling point lower than -150°C

$$C = 264 - 0.034\ T_b \qquad \text{.............(6-3B)}$$

- For other substances

$$C = 240 - 0.19\ T_b \qquad \text{.............(6-3C)}$$

where T_b is the normal boiling point in ^oC

Reid et al. (40) state that the above rules for estimating the value of the constant C are not reliable, so they have tabulated the values of A, B, and C for several materials derived from experimental data.

6-1-2 Lee and Kesler Equations

To achieve higher accuracy, several investigators have suggested three-parameter forms. The Lee-Kesler technique is one of the most successful.

$$\ln p_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \qquad \text{..........(6-4)}$$

The functions $f^{(0)}$ and $f^{(1)}$ have been expressed in analytical form as follows:

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862 \ln T_r + 0.169347\, T_r^6 \qquad \text{..........(6-5)}$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.472 \ln T_r + 0.43577\, T_r^6 \qquad \text{..........(6-6)}$$

$$T_r = \frac{T}{T_c} \qquad \text{..........(6-6A)}$$

6-1-3 Gomez-Thodos Equation

Gomez-Nieto and Thodos have proposed the following equations for estimating vapour pressures.

$$\ln p_{vpr} = \beta\left[\frac{1}{T_r^m} - 1\right] + \lambda (T_r^7 - 1) \qquad \text{..........(6-7)}$$

Compounds are divided into three classes: non-polar, polar and hydrogen bonded. The estimation procedure for eqn. (6-7) and its coefficients are different for each class.

<u>A- For non polar compounds</u>

$$\beta = -4.267 - \frac{221.79}{h^{2.5}\exp(.0384h^{2.5})} + \frac{3.8126}{\exp(2272.44/h^3)} + \Delta^* \qquad \text{..........(6-8)}$$

$$m = 0.78425 \exp(.089315h) - \frac{8.5217}{\exp(0.74826h)} \qquad ....(6\text{-}9)$$

$$h = T_{br} \frac{\ln (P_c/1.01325)}{1 - T_{br}} \qquad ....(6\text{-}10)$$

$$\lambda = ah + b\beta \qquad ....(6\text{-}11)$$

where $a = \frac{1 - 1/T_{br}}{T_{br}^7 - 1}$ and $b = \frac{1 - 1/T_{br}^m}{T_{br}^7 - 1}$

Δ^* = 0 except for He (Δ^* = 0.41815), H_2 (Δ^* = 0.19904) and Ne (Δ^* = 0.02319)

B- For polar compounds (except for alcohols and water)

$$m = 0.466\, T_c^{0.166} \qquad ....(6\text{-}12)$$

$$\lambda = 0.08594 \exp(7.452 \times 10^{-4}\, T_c) \qquad ....(6\text{-}13)$$

For water and alcohols

$$m = 0.0052\, M^{.29}\, T_c^{.72} \qquad ....(6\text{-}14)$$

$$\lambda = \frac{2.464}{M} \exp(9.8 \times 10^{-6}\, M\, T_C) \qquad ....(6\text{-}15)$$

where M = mol. wt.

6-1-4 Reid's Recommendations

Ried et al. (40) have recommended the following points.

- The Clapeyron-Clausius equation could be used for a narrow range of temperature, where ($\Delta H_v/R\ \Delta Z_v$) can be considered constant in addition to the availability of one vapour pressure-temperature point to evaluate the constant A.
- If the constants of the Antoine equation for a particular compound are available in the literature, then the Antoine equation could be used.
- For reduced temperatures below 0.5 the Lee-Kesler technique may be used
- For polar compounds at reduced temperature between (0.5 - 1.0) the Gomez-Thodos method is recommended.

So according to the above recommendations we will use Gomez-Thodos method for high temperatures and Lee-Kesler for low temperatures to estimate the vapour pressure.

6-2 Estimation of the Critical Properties

The methods of vapour pressure estimation require the critical properties of the solvent considered to be estimated. There are many methods to estimate these properties, Reid et al. (40) have reviewed the most reliable ones. All methods of critical properties estimation depend upon group contribution techniques.

6-2-1 Ambrose Method

Ambrose (40) has developed the following equations to estimate the critical properties.

$$T_c = T_b\left[1 + (1.242 + \Sigma\Delta T)^{-1}\right] \quad ....(6\text{-}16)$$

$$P_c = M\,(0.339 + \Sigma\Delta P)^{-2} \quad ....(6\text{-}17)$$

ΔT and ΔP represent the contribution of the different groups of the molecule to the considered property. The values of these Δ quantities had been estimated by Ambrose and are given on page 13, Reid et al. (40).

6-2-2 Joback Modification of Lydersen's Method

This method is considered one of the most successful techniques which was developed by Lydersen (40). This method was re-evaluated by Joback (40) using additional experimental data determined in the intervening years to add several functional groups. His proposed relations are

$$T_c = T_b\left[0.584 + 0.965\Sigma\Delta T - (\Sigma\Delta T)^2\right]^{-1} \quad ....(5\text{-}18)$$

$$P_c = (0.113 + .0032n_A - \Sigma\Delta P)^{-2} \quad ....(5\text{-}19)$$

n_A is the number of atoms in the molecule. The values of Δ quantities are shown on page 15, Reid et al. (40). We have chosen this method to estimate the required critical properties for this work.

6-3 Acentric Factor

The acentric factor is another property which has to be estimated before the estimation of the vapour pressure. This factor represents the acentricity of the nonsphericity of the molecule. For monatomic gases the value of ω is zero, however it is very small for methane (.011) . Its value increases with increasing molecular weight and the polarity of the molecule. Reid et al. (40) have tabulated the values of the acentric factor for many compounds, but for those compounds not covered in the literature, Lee and Kesler have formulated an empirical expression to estimate the acentric factor.

$$\omega = \frac{\alpha}{\beta} \qquad \text{..........(6-20)}$$

$$\alpha = -\ln P_c - 5.92714 + 6.09648\theta^{-1} + 1.28862 \ln \theta - 0.169347\,\theta^{6} \qquad \text{..........(6-21)}$$

$$\beta = 15.2518 - 15.6875\,\theta^{-1} - 13.4721 \ln \theta + 0.43577\,\theta^{6} \qquad \text{..........(6-22)}$$

$$\theta = \frac{T_b}{T_c} \qquad \text{...........(6-23)}$$

6-4 Prediction of the Vapour Pressure of B2 at 50°C

$\Sigma\Delta T = 2(CH_3) + 2(CH_2) + 2(>CO=) = 2(.0141) + 2(.0189) + 2(.038)$

$= 0.142$ page - 15, Reid et al. (40)

$\Sigma\Delta P = 2(CH_3) + 2(CH_2) + 2(>CO=) = 2(-.0012) + 2(0) + 2(.0031)$

$= 0.0038$ page - 15, Reid

$T_b = 464$ K for B2

$T_c = 662$ K Eqn. (6-18) $P_c = 36$ Bar Eqn. (6-19)

$\theta = 0.701$ Eqn. (6-23) $\beta = -2.291$ Eqn. (6-22)

$\alpha = -1.291$ Eqn. (6-21) $\omega = 0.5635$ Eqn. (6-20)

$T_r = 0.45$ Eqn. (6-6A) $f^{(0)} = -6.5861$ Eqn. (6-5)

$f^{(1)} = -8.841$ Eqn. (6-6)

$V_p = 2.17787\ 10^{-3}$ Bar $= 1.655$ mmHg Eqn. (6-4)

6-5 Measurement of the Vapour Pressure

Measurement of the vapour pressures of any liquid means the determination of the boiling points of that liquid at different pressures. At the normal boiling point, the vapour pressure of any liquid is equal to one atmosphere. One of the oldest methods was suggested by Beckmann, who used essentially a container of boiling liquid into which a thermometer is immersed. This method is accompanied with a high percentage of error mainly due to two reasons. The first is that the boiling liquid is always superheated as the surface tension of the liquid resists the release of small bubbles of the vapour, which means that the pressure of these bubbles have to be slightly higher than the operating pressure to overcome this resistance. The second is that the liquid at the bottom of the vessel must be superheated because of the hydrostatic pressure of the liquid.

There are mainly three basic techniques to measure the vapour pressures of pure liquids. The first one is the dynamic technique in which the mixture of the two phases (liquid and vapour) are driven from the boiling vessel to a compartment where the thermometer is placed. In this compartment the equilibrium between the vapour and the liquid is accomplished. The second method is the static technique in which the equilibrium between the vapour and the liquid occur in the boiling vessel. The third one is called the micro method which is used only to measure the normal boiling point, so this technique (third one) is not going to be considered in this work.

6-5-1 Dynamic Methods

At the beginning of this century, Cottrell (14) developed a method for precise measurement of the boiling point. His instrument is called the Cottrell ebulliometer, figure (6-3). This ebulliometer is formed basically from a wide test-tube (A) in which a narrow vertical tube is placed (B). The vertical tube is known as a Cottrell pump. The mixture of the vapour and the liquid are lifted through the Cottrell pump, flows to a horizontal plate and from it on to the thermometer which is placed in the vapour space. So the equilibrium temperature between the liquid and the vapour will to be established on the thermometer.

Washburn (14) also developed an ebulliometer at the same time as Cottrell, working on the same principles as shown in figure (6-6). The mixture of the two phases is pumped from the bottom of the vessel (A), through the narrow vertical tube (B), to above the level of the liquid in the vessel. The vertical tube is branched into two or three arms, where the thermometer is placed. So the mixture of the vapour and the liquid will spurt onto the thermometer.

Swietoslawski (14) and his school have rendered the greatest service in developing and perfecting the method of precision measurement of the vapour pressure. By using a Swietoslawski ebulliometer, the precision of the measured temperature is better than 0.001°C if the pressure of the system is held constant. Swietoslawski's ebulliometer, figure (6-7) is a modification of the Cottrell pump, and is widely used. The main characteristics of this ebulliometer is the thimble (2) in which the thermometer is placed. The wall of the thimble is fitted with an external glass spiral which slows down the run-off of the liquid. So the mixture of vapour and liquid spurts on to the wall of the thimble where the equilibrium between the two phases is going to be established.

6-5-2 Static Methods

Smith and Menzies (14) have proposed the isoteniscopic method to measure the vapour pressure of pure substance, as shown in figure (6-5). The liquid being tested fills about two-thirds of the bulb (A) and one-third of the U-tube (B). The temperature of the liquid is controlled by immersing the isoteniscope in a thermostat. A condenser is inserted into the tapered joint, and the pressure measuring and regulating system is connected to the condenser. When the pressure of the system is reduced, the vapour of the substance drives the air from the system, then at the given temperature of the system the pressure is raised until the levels of the liquid in the U-tube equalise. At this point the pressure of the system is equal to the vapour pressure of the liquid under test.

Another type of the isoteniscope, figure (6-4), was designed by Booth and Halbedel (14). In this version the instrument is connected to the vacuum system through the flange (A) and after evacuation, pure mercury is added to the bulb (C). The instrument is again pumped down and the mercury is heated until no further bubbles are evolved. After that the liquid under test is vacuum distilled into the bulb (E), which is immersed in liquid air. A little of the liquid is boiled off to drive out the air and the cock (B) is then closed. Then the instrument is inclined and the mercury is poured into the U-tube. At a certain temperature, when the levels of the mercury in the both arms of the U-tube are equal, the pressure of the system is equal to the vapour pressure of the liquid under consideration.

6-6 Measurement of the Vapour Pressure of Acetonyl Acetone

The instrument which was used in this work had been constructed by the Chemical Engineering Department, Aston University. The design of this instrument is based on that of the Swietoslowski ebulliometer. Figure (6-1) shows a schematic diagram of the Aston ebulliometer with its pressure regulating and measurement system. The instrument functions as follows: The solvent is fed into the vessel (A) through the feeding point (B). This liquid is heated by an immersed electrical heater rod (C). The bubbles of vapour with some slugs of liquid flow through the tube (D) to the thimble (E) in which a type K thermocouple is placed (F) . The wall of the thimble is fitted with an external glass spiral which is to help in slowing down the run-off of the liquid. Normally the liquid which is spurting on the wall of the thimble is superheated. The superheat is removed from the liquid by vaporisation of some of the liquid as it flows down the thimble. Its temperature is reduced to the equilibrium temperature which is measured by the thermometer at the pressure of the system. At this point the pressure of the system is equal to the vapour pressure of the solvent. The vapours of the solvent are condensed in the condenser (G). The condensate from it flows back to the vessel (A) through the drop counter (H). The drop counter is used to check the rate of vaporisation by means of the number of the drops per minute. For organic liquids the number of drops per minute must be more than 25. The walls of the tube (D) with the thimble must be well insulated to minimise the heat losses and prevent supercooling the liquid.

6-7 Results and Data Analysis

The relationship between the vapour pressure of acetonyl acetone and the temperature has not been published previously, so both estimation and measurement were therefore made to provide the necessary data. Table (6-1) shows these data, while figure (6-2) represents them graphically. From this graph, we can note the agreement between the experimental data and the theoretical data at high temperature. This demonstrates the good accuracy of the empirical equations proposed by Lee-Kesler and Gomez-Thodos at high temperature.

We have mentioned at the beginning of this chapter that Reid et al. (40) have tabulated the values of Antoine constants (A, B, C) for many liquids. These constants were derived from experimental data. There are no experimental data for acetonyl acetone in the literature, hence the values of the Antoine constants were untabulated. Therefore they have to be estimated from our experimental data using least squares method. The values of the constants are

A = 18.218

B = -1809.8

C = 80

The Antoine correlation fitted to the acetonyl acetone data is

$$\ln P_{vp} = 18.218 - \frac{1809.8}{t + 80} \qquad (6\text{-}24)$$

Table (6-1) The measured and estimated vapour pressure of the acetonyl acetone

Temp. (C)	E.PV (Pa)	T.VP (Pa)	1000/T+80	ln E.PV	ln T.VP
79.4	824	1695	6.274	6.714	7.43
82.2	1180	1951	6.165	7.073	7.576
91.6	2400	3067	5.828	7.783	8.028
98.8	3302	4259	5.593	8.102	8.356
105.9	5022	5804	5.379	8.522	8.666
121.1	10250	10775	4.973	9.235	9.285
138.2	21600	20269	4.583	9.98	9.916
152	31700	32325	4.31	10.364	10.384
158.3	40250	39541	4.196	10.603	10.585
165.2	50716	48924	4.078	10.834	10.798
170.3	60010	56979	3.995	11.002	10.95
175.4	70020	66093	3.915	11.157	11.0988
181.4	80093	78311	3.826	11.291	11.268
185.2	90100	86960	3.771	11.409	11.37
191.5	97526	103003	3.683	11.488	11.543

E.VP = Experimental vapour pressure (Pa)

T.VP = Theoretical vapour pressure (Pa)

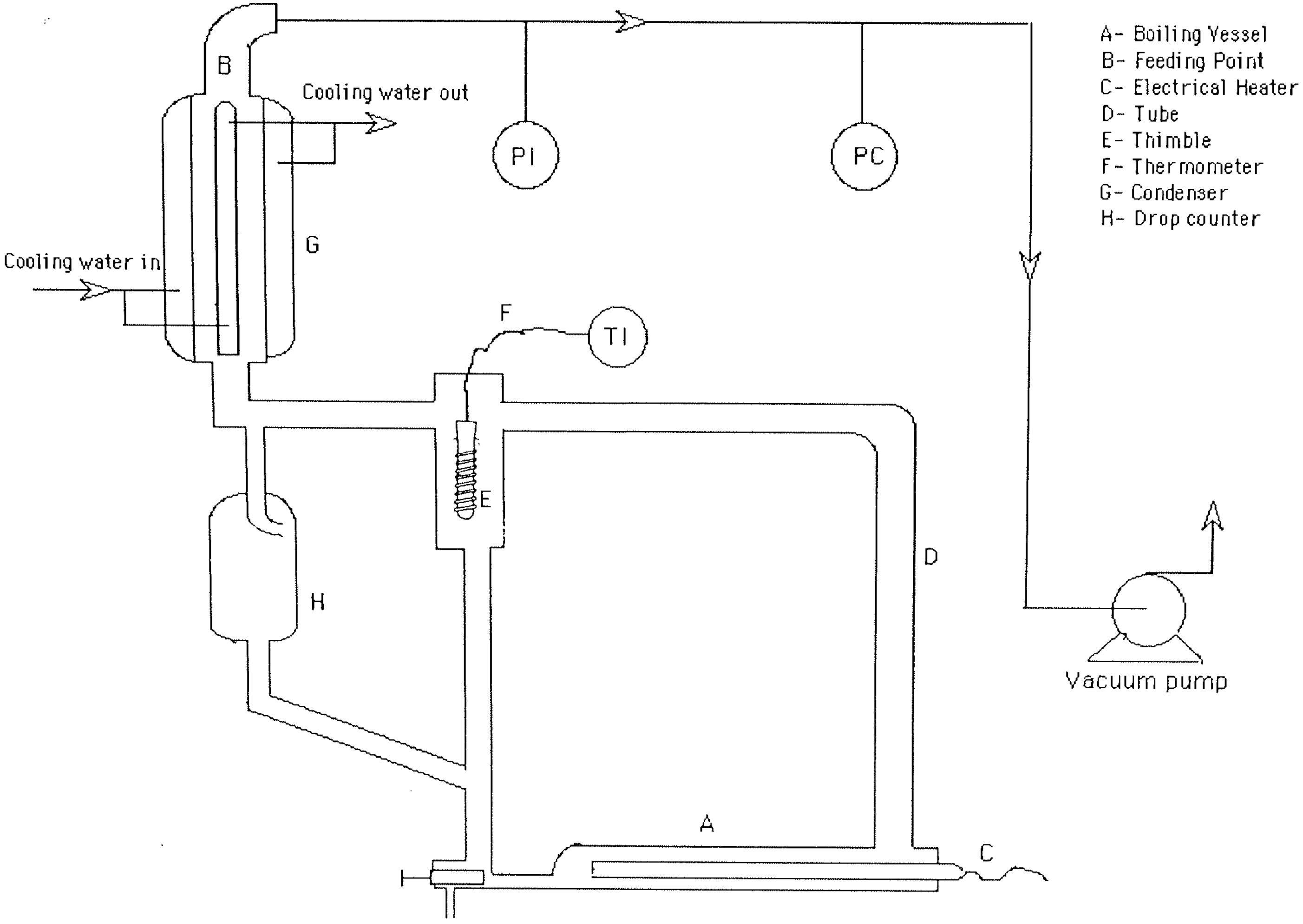


Figure (6 -1) The ebullimeter which was used to measure the vapour pressure of acetonyl acetone

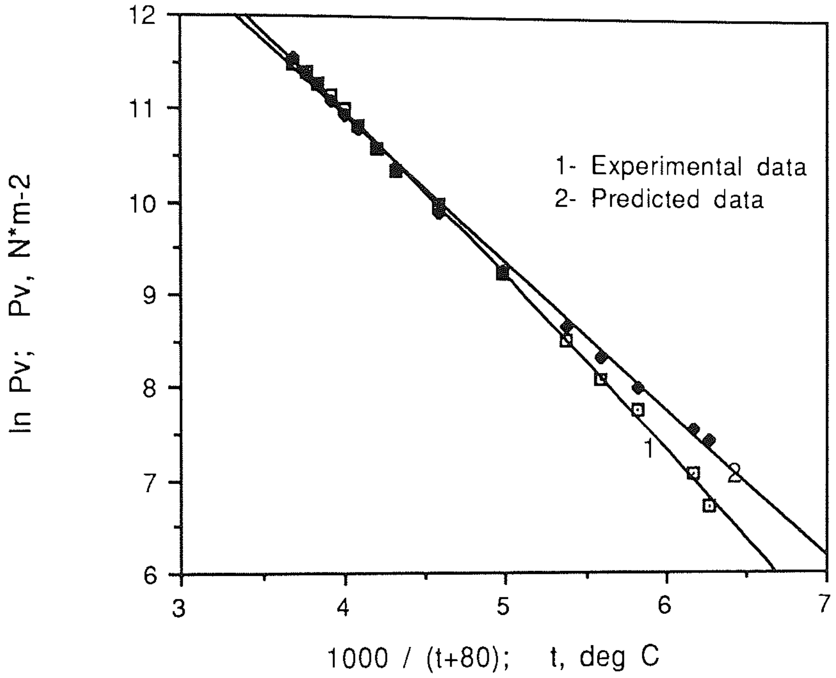


Figure (6-2) The measured and estimated variation of acetonyl acetone vapour pressure with temperature

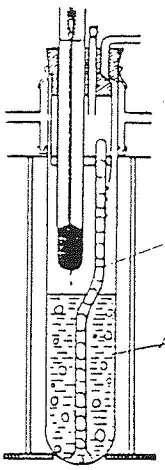


Figure (6-3)
Cottrell ebulliometer
A- Test- tube
B- Cottrell pump
C- Thermometer

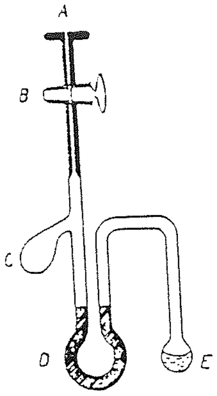


Figure (6-4)
Booth -Halbedel Isotensicope
A- Flange
B- Cock
C- Mercury-bulb
D- U-tube
E- Liquid-bulb

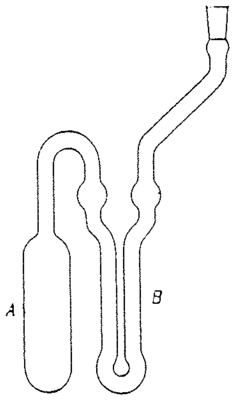


Figure (6-5)
Smith-Menzies Isoteniscope
A- Liquid container
B- U-tube

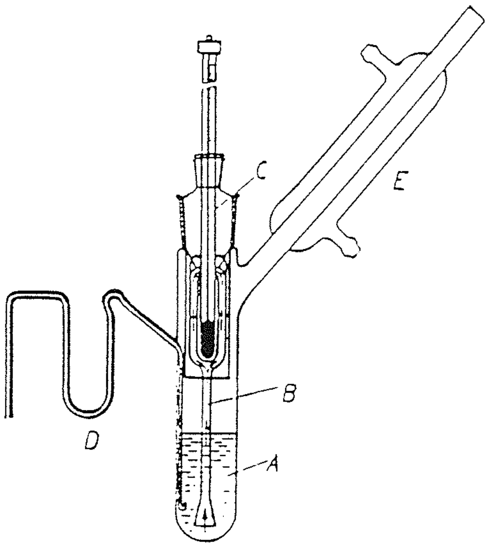


Figure (6-6) Washburm edulliometer
A- Test- tube
B- Cottrell pump
C- Thermometer
D- Sampler
E- Cooler

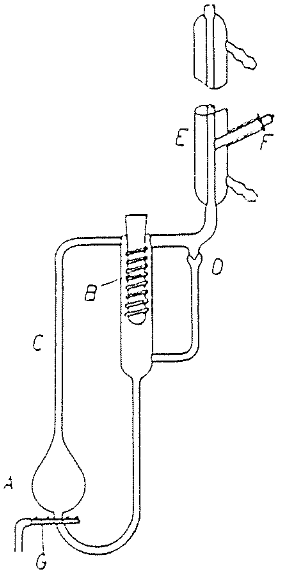


Figure (6-7) Swietoslawski ebulliometer
A- Liquid container
B- Thimble
C- Test-tube neck
D- Drop counter
E- Cooler
F- Feeding point
G- Gas fire

CHAPTER SEVEN

Solubility Measurement for CO_2, CH_4 and C_3H_8 in Acetonyl Acetone

7-1 Introduction

In Chapter 5, equations were developed and used to evaluate some selected solvents. The conclusion was that acetonyl acetone (B2) is the most attractive candidate for commercial applications. Experimental data for all the required physical properties were not available, so during the evaluation process, we used some estimated properties where no experimental data existed. In particular Sitthiosoth (44) had measured the solubility of CO_2 in B2 at low pressures, its viscosity and boiling point, while he predicted the other properties. It is not reasonable to recommend any new solvent for commercial applications or for a pilot plant study if all its effective physical properties have not been measured. In this chapter the other effective properties were measured, namely the solubility at high pressure, the selectivity, and the effect of water on the gas solubility is described.

7-2 The Solubility of CO_2 in B2

Acetonyl acetone was purchased from the Aldrich Company with a purity of 97%, while carbon dioxide was obtained from the British Oxygen Company (BOC). Its properties are as follows.

- Critical temperature = 304.3 K
- Critical pressure = 73.9 bar
- Critical volume = 0.094 m^3/mol
- Relative molecular mass = 44.009

Density at 273.15 K and 1.013 bar = 1.977 gm/m^3

The following simple Antoine type equation approximately fits the vapour pressure of CO_2 in the range (273 - 303)K

$$\log P_{vp} = 5.696 - \frac{1519}{T + 91.9} \qquad (7\text{-}1)$$

where: T = temperature (K)

P_{vp} = vapour pressure (bar)

The experimental procedure of the measurement of the solubility of CO_2 in B2 can be summarized into the following three main steps.

A- Solvent degassing:- Before measuring the solubility, the solvent was purified and degassed carefully under vacuum. The unit which was used for this purpose is shown in figure (7-1). It consisted of three parts, the preliminary degassing section, the main degassing section and the storage and feeding section. In this unit the solvent was degassed by repeated boiling and condensation under vacuum.

B- Preparing a sample of solvent in equilibrium with the gas:- After the degassing, the solvent was transfered to the equilibrium cell which is shown in figure (7-2). The mechanism used to contact the B2 with CO_2 is by bubbling the gas below the surface of the solvent. This contact was maintained for about four to five hours under well controlled temperature and pressure until the equilibrium between the gas and the solvent was achieved.

C- Measurement of the sample composition:- A combination of absorption of CO_2 in 0.1N sodium hydroxide followed by back titration with 0.1N of hydrochloric acid was used to determine the quantity of CO_2 in a known amount of loaded solvent. Figure (7-3) shows the glassware arrangment which was used for the reaction of CO_2 with

NaOH. The details of the above three main steps will be considered in the following pragraphs.

7-2-1 Degassing Process

The removal of the impurities or any other dissolved gases from a solvent is an essential step before determining the solubility of a specific gas in that solvent. Poorly decontaminated solvent could be the cause of misleading figures.

In Chapter 1 we have reviewed the various degassing techniques which were reported in the literature. In this work, the improved technique adopted by Jenkins and Smith (20) has been used. In this technique the degassing process is achieved by boiling and condensation of the solvent under vacuum in two separated steps. Figure (7-1) shows the flow diagram of the degassing apparatus which was made by Rafaquat (62) in accordance with the Jenkins and Smith design. Rafaquat checked the reliability of this apparatus by measuring the saturated vapour pressure of absolute ethanol and water at different temperatures, he then compared the values obtained with those published in the literature.

The Jenkins and Smith (20) apparatus is comprised of three main parts. The first part (A) is, where the preliminary degassing is performed, while the second part (B) represents the main part of the degassing unit and the third part (C) is used as a reservoir to store the degassed solvent. All these parts are connected to a vacuum pump, to remove the noncondensable gases built up during the boiling and condensation process.

Part A consists of a 500 ml three-necked glass round bottom flask, isomantle heater and double surface condenser. The upper neck of the bottom flask is connected to the condenser, while the left one is joined to part B and the third neck provides the inlet for the feed.

Part B is formed from a 250 ml flask with a thermosiphon boiler, double surface condenser and Electrothermal Hot-rod (as a heating element) immersed into the heating compartment. The flask is connected to the condenser from the top, and joined to the bottom and the upper part of the heating compartment by two arms. The upper part of the condenser is connected to part C. The dimensions of the heating compartment were such that the heating element of the hot rod is almost immersed in the solvent to ensure the whole of the heating surface is in contact with the boiling liquid.

Part C consists of a 250 ml roundbottom flask with a long neck and finger condenser. A modified microburrette is connected to the bottom of the storage flask as a precision dispensing system. Cooling water to stage B is shut off and the vapour is pulled by vacuum to impinge on the finger condenser. The condensed vapour runs down the finger condenser and is stored in the 250 ml round bottom flask. Once the solvent is judged to have been degassed it is transfered to the reservoir where it is stored for subsequent introduction to the equilibrium cell. At this stage the solvent can be kept for the duration of the experiment, so it is necessary that the reservoir be leak tight. A modified microburette is used to transfer a precise volume of the solvent from the reservoir to the equlibrium cell.

7-2-1-1 The Operation of the Degassing Apparatus

The following general technique is used to degas the acetonyl acetone.

A- 500 ml of solvent was transfered to the 500 ml round bottom flask, through the feed neck. It was then heated to its boiling point by the Isomantle heater. The solvent vapour produced by the boiling liquid was condensed on the Liebeg condenser and allowed to run back into the boiling vessel. This boiling/condensing operation was maintained for about four hours. Noncondensable gases were removed from above the liquid by periodically applying vacuum to the boiling flask.

B- Vacuum was applied to the boiling flask of the second stage and used to draw some of the liquid over from the first stage boiling flask. The solvent was heated by the immersed heating element, and the vapour produced was condensed onto the surface of the condenser and returned to the reboiler flask. This operation lasted for about 8 to 6 hours. The liquid is completly degassed when a characteristic cracking noise is heard as the vapour bubbles collapse against the wall of the reboiler. The cracking noise of the acetonyl acetone was more subtle than that of water.

C- Finally, the solvent was transfered from the reboiler to the storage flask by stopping the cooling water of the reboiler while the cooling water of the cold finger is running and allow the solvent vapour to condense onto the surface of the cold finger above the storage flask. During the period of the condensation, a little vacuum was applied to remove any residual dessolved gasses.

7-2-1-2 Degassing Procedure

The practical procedure of the degassing was attained as follow

A-First stage of the degassing

- The valves V1, V2, V3, V4, V5, V6, V7, and V8 were closed.

- Pour the liquid into the 500 ml three-necked flask through the inlet neck, then close it with the stopcock.

- Energise the vacuum pump.

- Let the cooling water flow through condenser (1).

- Open V1 to evacuate the space above the solvent for 15 minutes then close it.

- Energise the isomantle heater. So the vapour liquid starts to arise, condense and fail back into the flask.

- From time to time open V1 to remove any build-up of noncondensable gases. Care has to be taken when applying the vacuum as a large quantity of the solvent may rise into the condenser and may be flashed out of the flask. This process should continue for at least three to four hours.

B- The second stage of the degassing

- While V1 is closed, open V2 to create a vacuum in the reboiler unit, then close V2.

- Let the cooling water flow through the condenser (2).

- Open V8 slowly to let the solvent drip into the reboiler unit until almost full, then close V8.

- Energise the immersed heating element.

- Allow the solvent to boil under reflux, and apply the vacuum from time to time until a chacteristic cracking noise could be heard, which means a good degassing of the liquid has been achieved.

C- The storage of the degassed solvent

- Open V5, V4 and V3.

- Stop the flow of the coolant through condenser (2), and let it flow through condenser (3). This permits the liquid vapour to impinge on the cold finger condenser, then to condense and fell down into the storage flask, while the traces of remaining uncondensable gases flow through V4 to outside under the effect of the vacuum pump.

- When most of the solvent is transfered from the reboiler unit to the storage flask, turn the immersed heating element off.
- Close V5, V4 and V3 and stop the flow of the cooling water through the condenser (3). Now the solvent is ready to be charged to the cell.

7-2-2 Preparing a Sample of B2 in Equilibrium with CO_2

The apparatus which was used in this work is shown in figure (7-2). It consists mainly of the following items:-

- Stainless steel equilibrium cell.
- Stainless steel sampler
- Two remote drive Graphite Gear pumps.
- Pressure measurement and control system, which consists of a pressure transducer, millivoltmeter, pressure indicator and controller and N_2 gas cylinder.
- Temperature measurement and control system, which consists of an electrical heater, temperature controller, thermocouple with temperature display device and cooling system.
- Vacuum system, which mainly consists of vacuum pump and cold trap.
- Carbon dioxide gas cylinder.
- Finally a net work of pipes, fitting and valves.

The volume of the equilibrium cell with the tubing and fittings is 56 ml. This cell was maintained in a constant temperature air bath by maintaining it inside a Pye 104 chromotograph oven. The temperature inside the cell and the temperature of the air bath were controlled within $0.1^{o}K$, on $298^{o}K$ for the whole course of the test, using the temperature controller of the chromotography oven.

The volume of the stainless steel sampler is 12 ml, it is provided with two valves to facilitate its separation from the loop. The solvent is circulated between the cell and the sampler by a graphite gear micropump (P1).

The duty of the micropump (P1) is to fill the sampler with the saturated solvent through the circulation process of the solvent. The second micropump (P2) is used to take the gas from the top of the cell to bubble it below the surface of a measured quantity of the solvent.

The pressure system which was used in this work consists mainly of the following four parts.

- Appleby and Ireand DPT type A1.741.MD.07.A.S.01.01.8
- Druck pressure indicator and controller type DPI 500.
- Millivoltmeter type Comark 1201 which is used as a read-out device.
- cylinder of N_2 gas supplied by British Oxygen Company (BOC).

The accuracy of this system is determined by the performance of the pressure transducer. This transducer was placed inside the air bath to maintain its temperature constant. The pressure transducer consists of two compartments separated by a diaphragm, the first compartment to contain the N_2 gas while the other for the gas under consideration. The cell pressure is transmitted to the transducer by a capillary tube and this causes deflection in the diaphragm of the transducer. If the pressures in the two sides of the transducer are the same, the reading of the millivoltmeter should be on the null position, i.e., zero read-out is obtained.

The N_2 gas was used for two main purposes, the first is the measurement and control of the pressure of the cell by using it in the other side of the pressure transducer to balance the pressure of the cell. The second is to check for leaks in the cell and in the associated capillaries before measuring the solubility.

The duty of the temperature measurement and control system is to keep the temperature of both the cell and the air bath at 298 K through the whole course of the experiment. This system was formed from the following.

- Pye 104 chromatograph oven with its temperature controller
- Type K thermocouples with temperature display devices (type Norma D1401)
- Cooling system which was formed from a cooling coil installed around the cell, water pump type STL 210, a water reservoir and the required piping and fittings.

The chromatography oven is designed to work at elevated temperatures, but to adapt it to work at 25°C, cooling water at a temperature about 0°C was circulated through a cooling coil within the air bath. Ice was always kept in the reservoir with the water during the saturation process to maintain the temperature of the cooling water at about 0°C.

The vacuum system is an important auxillary unit which is used for two purposes, the first is to achieve the vacuum needed for the degassing procedure while the other is to pump down the cell and the associated capillaries to about 0.1 mmHg. This system consist of three parts, an Edward's rotary vacuum pump, cold trap and the well-sealed lines.

7-2-2-1 Procedure of the Solubility Measurement

This procedure includes nine main steps as follows.

1- Getting the null position on the millivoltmeter:-

- Open the valves of the cell vent V4, V5 & V6 and the valve of N_2 vent V13 which means having atmospheric pressure on both sides of the transducer's diaphram.
- Set the pointer of the millivoltmeter on null position.
- Close V4, V5, V6 & V13.

2- Checking for leaks within the absorption section:-

- Check the pressure of the N_2 cylinder's regulator which has to be set on 23 bar.
- Open V3 & V1 and all the other valves have to be closed.
- Set 23 bar on the pressure controller (PIC) then put its selector on read position, this will feed the N_2 to both sides of the transducer and to the cell.
- Note the pointer of the millivoltmeter, it should be on zero position.
- Close V1 and watch the pointer of the millivoltmeter, if it does not shift from the null position that means there is no leak within the cell section and vice versa.
- Release the pressure from the cell.

3- Emptying the cell:-

- Open V1, V2, V4, V10, V14, V15 and V11 and all the other valves have to be closed.
- Put some dry ice in the cold trap.
- Put the vacuum pump on.
- Watch the decreasing of the pressure on (PI1) until it is below 0.0004 bar.
- Close V1 and V2 and switch the vacuum pump off.

4- Feeding the solvent to the cell:-

- Open V6 (of the degassing unit) and fill the Metrohm microburette with the solvent.

- Close V6 and open V7 (of the degassing unit) with V12.

- Charge the solvent to the cell.

- Close V12.

5- Setting the temperature controller:-

- Put the heater on.

- Set the temperature on 25°C on the controller.

- Put water and ice in the cooling water reservoir.

- Open V8 and V9 then put the pump (P3) on.

6- Setting the pressure controller:-

- Close V3.

- Set the pressure as required on the (PIC) then change the selector to read position.

- Note the big deflection of the millivoltmeter pointer from the null position.

7- Feeding the carbon dioxide to the cell:-

- Check there is enough gas pressure in the CO_2 gas cylinder.

- Close V4 and open V7 then increase the pressure of the CO_2 up to the required pressure using (PI2) as indicator.

- Open V4 and note the return of the millivoltmeter to the null position, then close V4.

8- Getting the equilibrium point:-

- Put the pumps P1& P2 on and monitor the deflection from the null position.

- Record the temperatures of the cell and the air bath and also the pressure of the cell every 15 minutes.

- The valve V4 has to be opened from time to time to charge some more CO_2 to the cell.

- Continue to recording the temperatures and the pressure until they settle down to final values i.e., the equilibrium has been reached between the gas and the solvent. This process may take from 4 to 6 hours.

9- Dismantle the sampler:-

- Close V10 and V11.
- Switch the pumps P1, P2, P3, and the heater off.
- Vent the pressure from the cell.
- Dismantle the sampler from the loop to remove the saturated sample for chemical analysis.

7-2-3 Chemical Analysis

Chemical analytical techniques can often be used to determine the concentration of the solute in the solvent. In this work 0.1N sodium hydroxide was used to determine the quantity of CO_2 that had dissolved in the acetonyl acetone. As shown in figure (7-3), CO_2 exits from the sampler to bubble into the solution due to the difference in the pressure between the bulk of the sampler and the bulk of the flasks. Sodium hydroxide reacts with CO_2 according to the following equation.

$$2NaOH + CO_2 = Na_2CO_3 + H_2O$$

Once bubbling ceases, the solution would contain the excess of the NaOH, the sodium carbonate produced and water. This solution is titrated against 0.1N hydrochloric acid. The following reactions would take place during the titration.

$$NaOH + HCl = NaCl + H_2O$$

$$Na_2CO_3 + HCl = NaHCO_3 + NaCl$$

$$NaHCO_3 + HCl = NaCl + H_2O + CO_2$$

So the titration process is performed in two steps. The first step, where phenolphthalein is used as indicator, gives the amount of soduim hydroxide plus half the amount of the sodium carbonate present. In the second titration methyl orange is used as the indicator, this reaction is, in effect, the determination of the bicarbonate formed in the first titration, and gives a result corresponding to half the amount of carbonate present. So multiplying the second reading by two gives the number of moles of sodium carbonate which is equal to the moles of the reacted CO_2.

7-2-3-1 Procedure of the Analysis

- Arrange the flasks, the sampler and the manometer in the way shown in figure (7-3)
- Prepare 0.1N sodium hydroxide and 0.1N hydrochloric acid.
- Put 400 ml of soduim hydroxide in the flasks and fill the burette with hydrochloric acid.
- Start to open the valve very slowly and carefully in a way not to allow any bubbles in the third flask and watch the increase in the pressure in the manometer.
- The valve must be opened bit by bit until the valve is fully open
- Wait for some hours until the pressure in the manometer goes back to the starting pressure.
- Mix the solution of all three flasks.
- Pipette 25 ml from the solution and put 2-3 drops of phenolphthalein and titrate it with HCl until the disappearance of the red colour. Put down the reading of the burette, then put 2-3 drops of methyl orange and continue the titration until the first appearance of the red colour, again record the reading of the burette.
- Repeat the above step three times
- Get the average of the first and the second readings
- Multiply the second reading by two to obtain the amount of carbon dioxide reacted with the NaOH. Then subtract the second reading from the first reading to obtain the amount of excess NaOH.

7-3 The Effect of Water on the Solubility of CO_2 in B2

During the absorption process, contamination of the solvent with water is inevitable, due to two reasons. Most synthesis gas mixtures are saturated with water, some of this water would transfer to the solvent during the absorption, and in some absorption processes, steam is used as a stripper, which means the unavoidable condensation of some of that steam, which mixs with the solvent. So the knowledge of the solubility of a gas in a mixture of solvent with water is vital for the design of any gas absorption process.

The apparatus described in sections (7-1) and (7-2) was used to measure the solubility of CO_2 in water-B2 mixtures of different compositions. Three weight percentages of water (10, 20, and 30) were chosen for this investigation. A type Unicam model 204 gas chromatograph analyser was used to detemine the percentage of water in the solvent after saturation.

7-4 The Solubility of Methane and Propane in B2

The knowledge of the selectivity of any solvent is vital for the design of any physical gas absorption process, as it gives a numerical picture about the following cost items.

- The quantity of the gas product which may be lost.
- The size of the compressor which is needed to recycle the gas stream from the first flash tank to the absorber.
- The cost of the power which is required to run the compressor.

The selectivity of any solvent to a certain gas is the ratio of the solubility of that gas to the solubility of the gas product. Methane and propane, very often, are the components from which carbon doxide must be removed. So the solubility of these two components at elevated pressure were measured.

Methane and propane were purchased from the British Oxygen Company (BOC). Their properties are as follows.

	Methane	Propane
Critical temperature	191.05 K	369.95 K
Critical pressure	46.42 bar	42.57 bar
critical volume	0.099 L/mol	0.2 L/mol
Molcular weight	16.043	44.017
Density *	0.71683 gm/L	2.02 gm/L

* at 273.13 K & 1.01 Bar

For CH_4 $$\log P_{vp} = 8.3077 - \frac{746.61}{T + 23.74} \qquad (7\text{-}2)$$

For C_3H_8 $$\log P_{vp} = 10.7611 - \frac{2897.6}{T + 42.46} \qquad (7\text{-}3)$$

It was mentioned earlier in this chapter, that the solubility measurement of any gas in a solvent includes three main steps, degassing the solvent, getting the equilibrium point between the solvent and the gas and ascertaining the composition of the gas in the solvent. The technique used to perform the first two steps are similar to those for the measurement of solubility of CO_2 in the solvent. But the methane and the propane do not react with sodium hydroxide or any other solution. So the following technique was used for analysis.

7-4-1 Finding the Quantity of CH_4 and C_3H_8 in B2

The central idea of the technique which was used to determine the concentration of CH_4 and C_3H_8 in a given volume of saturated B2, is to determine the pressure change in a gas reservoir of known volume. This method had been used by several workers like Melzer (1988) to determine the solubilities of CH_4 and C_3H_8 in a solvent mixture of n,n-dimethylformamide, n-methyl-2-pyrrolidone and water.

Figure (7-4) shows the apparatus which was utilized in this work. It consists of the following items.

- 550 ml container.
- Mercury manometer.
- Edward's rotary vacuum pump.
- Cold trap and well sealed lines.

After saturation of the solvent with the gas, the 12 ml sampler was dismantled from the loop of the equilibrium cell and connected to the apparatus of the pressure change measurement. The 550 ml container with the associated lines was pumped down to about 0.5 mmHg, then the vacuum pump was separated from the loop by closing the valve (V3). Valve (V2) was opened to allow the solvent to degas, then the pressure of the reservoir was recorded. From the difference between the initial pressure and the final pressure, the quantity of the gas which was dissolved in 12 ml of B2 was calculated.

7-5 Safety Precautions

Methane and propane are flammable gases, therefore, safety precautions were taken before, during and after the experimental run. Before the experimental run all the electrical devices have been well earthed, to reduce the chance of sparking. During the experimental run, the air bath of the cell was purged continuosly by low pressure N_2 to separate the cell from the oxygen (air). After the equilibrium process, the cell was normally at high pressure, so an empty 100 ml steel bomb was connected to the gas feeding line to discharge the gas from the cell into this bomb. This vessel was disconnected from the cell loop and taken it to a fumehood to discharge the gas there. This step was repeated several times until the pressure of the cell became about one atmosphere.

7-6 Gas Solubilities Results

The solubilities of CO_2, CH_4, and C_3H_8 in the B2 were measured in this work. The solubility was expressed in grammes of gas per kg of solvent at 25°C for different pressures. Table (7-1) shows the effect of the pressure on the solubilities of the gases considered in B2. The numerical smoothing method of least squares was utilized to find the best fitting equations which represent the above data.

$$X_{BE1} = 7.4299 + 3.4603P + 0.29391P^2 \qquad \text{..........(7-4)}$$

$$X_{BE2} = -0.062702 + 0.1433P + .0029976P^2 \qquad \text{..........(7-5)}$$

$$X_{BE3} = 0.57802 + 5.998P + 0.3617P^2 \qquad P <= 8.5 \qquad \text{..........(7-6)}$$

X_{BE1} = gm of CO_2 per kg of B2

X_{BE2} = gm of CH_4 per kg of B2

X_{BE3} = gm of C_3H_8 per kg of B2

P = Pressure (bar)

From the above equations the solubilities of these gases in B2 was calculated at 3, 6, 10, 14, 18, 22 bar and were represented by the figures (7-5), (7-6) and (7-7).

The simultaneous effect of the contamination of B2 with water and the pressure on the solubility of CO_2 in B2 was also investigated by using different concentrations of water in B2. Three weight percentages of water were chosen, 10 wt%, 20 wt% & 30 wt%. But because the concentration of the water would change after equilibrium was reached with the gas, due to different in the vapour pressures for B2 and the water, the concentrations of H_2O in B2 was measured again by chromatography. The above concentrations changed to 10.3 wt%, 20.6 wt%, 30.1wt% respectively. Table (7-2) shows the solubilities of CO_2 in the mixtures, and from these data the best fitting equations were derived by the least squares method. The solubility of CO_2 in pure water was taken from the literature and is quoted here for comparision purposes. Figure (7-8) shows how the presence of the water reduces the solubility of CO_2 in B2.

X_{ME1} = - 0.76169 + 5.0681P + 0.10871P^2 10.3wt% .....(7-7)

X_{ME2} = 2.4071 + 5.0204P + 0.045203P^2 20.6wt% .....(7-8)

X_{ME3} = 0.33711 + 2.9975P + 0.0088034P^2 30.1wt% .....(7-9)

X_{WE} = 0.91088 + .09466P +0.0045117P^2 Pure water .....(7-10)

X_{ME1} = gm of CO_2 per kg of mixture of 10.3wt%

X_{ME2} = gm of CO_2 per kg of mixture of 20.6wt%

X_{ME3} = gm of CO_2 per kg of mixture of 10.3wt%

X_{WE} = gm of CO_2 per kg of water

It was mentioned at earlier stages of this report that one of the main purposes of this work is to find out the possibility of recommending B2 for commercial applications. So these data have to be compared with those for Selexol, which represents one of the most successful commercial physical solvents currently available. The following equations represent the solubilities of the three gases considered in Selexol.

X_{SE1} = 8.4204 + 0.9195P + 0.30492P^2 ......(7-11)

X_{SE2} = .0015864 + 0.13746P + .0036829P^2 ......(7-12)

X_{SE3} = 1.5818 + 4.9229P + 0.45816P^2 P <= 8.5 bar ......(7-13)

X_{SE1} = gm of CO_2 per kg of selexol

X_{SE2} = gm of CH_4 per kg of selexol

X_{SE3} = gm of C_3H_8 per kg of selexol

Sitthiosoth (44) predicted the solubility of CO_2 and CH_4 in B2 at high pressures by using the group contribution equation of state method (GCEOS). It is worthwhile to compare our experimental results with his prediction to see the reliability of the GCEOS method for prediction of the solubility of the gases. The following equations represent his prediction.

$$X_{BT1} = 23.077 + 8.1020P + 0.50922P^2 \qquad \text{..........(7-14)}$$

$$X_{BT2} = 2.6068 + 0.69169P + .0043P^2 \qquad \text{..........(7-15)}$$

X_{BT1} = gm of CO_2 per kg of B2

X_{BT2} = gm of CH_4 per kg of B2

Figures (7-5), (7-6) and (7-7) show a comparision between these data. From the figures we see that the solubility in B2 for the three considered gases is more than that in Selexol with about 27% for CO_2 and CH_4, while it is more by about 2.11% for C_3H_8. Also it is obvious that the solubility prediction by using GCEOS method is much higher than the reality.

7-7 The Selectivity of the Acetonyl Acetone

The selectivity of B2 to the CO_2 from a mixture of CO_2-CH_4 is the ratio of the solubility of CO_2 to that of CH_4. The selectivity increases as the partial pressure of the component to be removed increases. A mixture of CO_2-CH_4 at 50 bar was considered, then the selectivities were calculated for different partial pressures of CO_2 in this mixture (see table 7-3). Another mixture of CO_2-C_3H_8 was considered at a total pressure range of 7.5 - 25 bar, then the selectivities were calculated for different partial pressures of CO_2 (see table 7-4). The same procedure was used to calculate the following.

- The selectivity of B2 from the predicted solubilities of CO_2 and CH_4.
- The selectivity of Selexol from the experimental solubilities of CO_2, CH_4 and C_3H_8.

The results of all these calculations were presented in figures (7-9) and (7-10).

Table (7-1) The solubilities of CO_2, CH_4 and C_3H_8 in acetonyl acetone at high pressure

CO_2		**CH_4**		**C_3H_8**	
Pressure	gm CO_2/kg B2	Pressure	gm CH_4 / kg B2	Pressure	gm C_3H_8 / kg B2
2.68	16.673	3.53	0.495	0.87	5.73
5.83	39.558	5.66	0.857	2.07	15.03
9.29	67.41	9.25	1.473	3.3	24.44
13.27	103.96	13.12	2.28	4.12	31.64
17.54	157.95	16.76	3.323	5.31	41.9
20.25	193.4	19.98	3.93	6.11	50.47
22.25	234			6.71	57.66

Table (7-2) The effect of water on the solubility of CO_2 in acetonyl acetone

Pure B2		10.3 wt% H_2O		20.6 wt% H_2O		30.1 wt% H_2O	
1	**2**	**1**	**2**	**1**	**2**	**1**	**2**
2.68	16.67	1.53	6.623	1.55	5.97	2.03	5.7
5.83	39.56	2.96	15.58	3.36	13.4	3.96	12.04
9.29	67.41	5.69	31.98	5.22	21.7	5.88	18.6
13.27	104	8.16	48.14	7.07	30.4	7.86	25.13
17.54	158	11.62	72.69	10.8	49.56	10.38	34.1
20.25	193.4	16.15	108.6	18.09	70.8	14.88	46.3
22.25	234	19.65	141.7	20.31	82.6	19.83	59.5
						22.51	75.0

1- pressure (bar), **2**- gm of CO_2/kg of mixture.

Table (7-3) The selectivity of B2 for CO_2 from a mixture of CO_2-CH_4

P_{CO_2} (bar)	P_{CH_4} (bar)	gm CO_2/kg B2	gm CH_4/kg B2	Selectivity
2.5	47.5	17.92	13.51	1.3
5	45	32.1	12.5	2.6
10	40	71.42	10.5	6.8
15	35	125.46	8.6	14.55
20	30	194.2	6.93	28.02

Table (7-4) The selectivity of B2 for CO_2 from a mixture of CO_2-C_3H_8

P_{CO2} (bar)	P_{C3H8} (bar)	gm CO_2/kg B2	gm C_3H_8/ kg B2	Selectivity
2.5	5	17.92	39.62	0.34
5	5	32.1	39.62	0.81
10	5	71.42	39.62	1.8
15	5	125.46	39.62	3.17
20	5	194.2	39.62	4.9

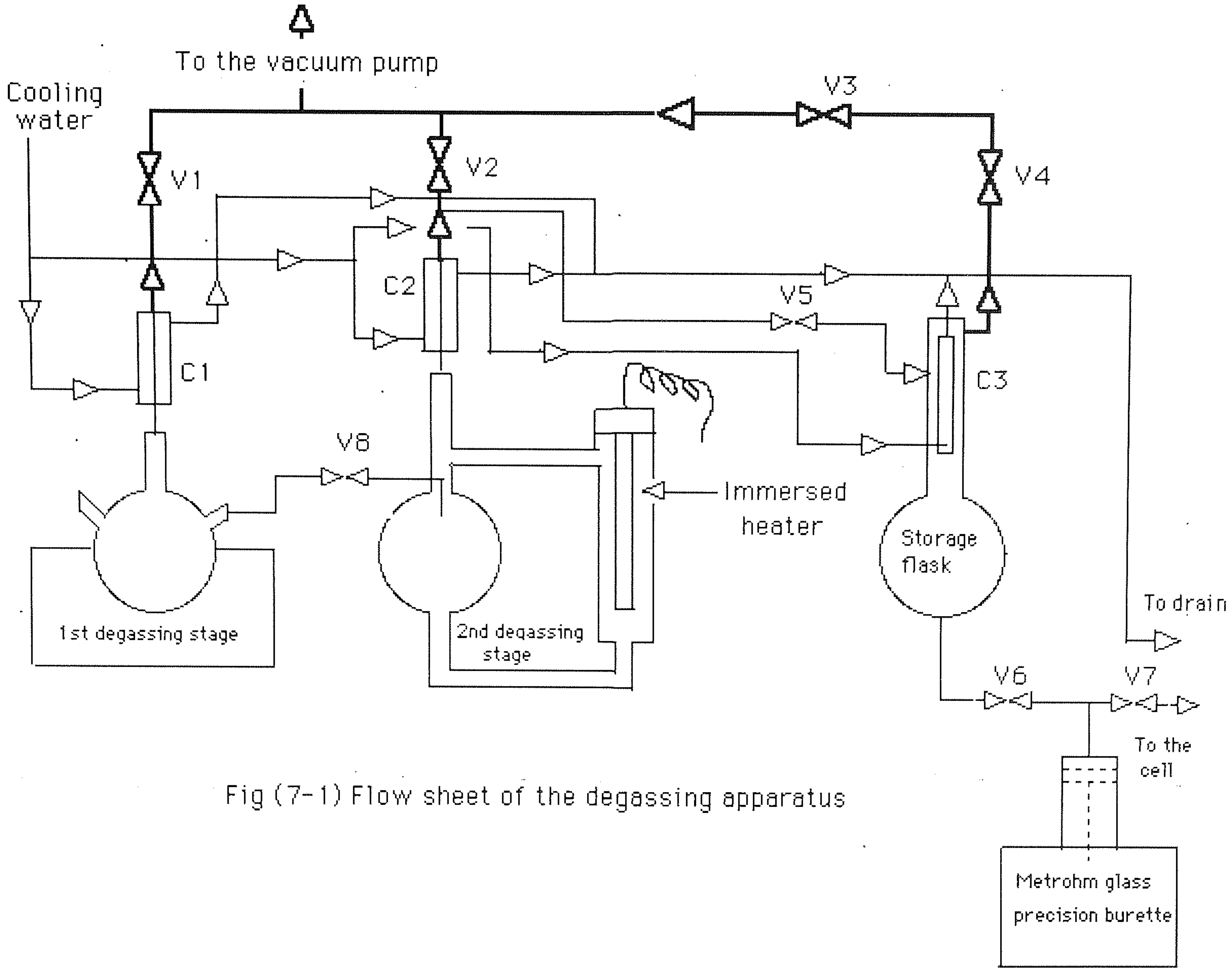


Fig (7-1) Flow sheet of the degassing apparatus

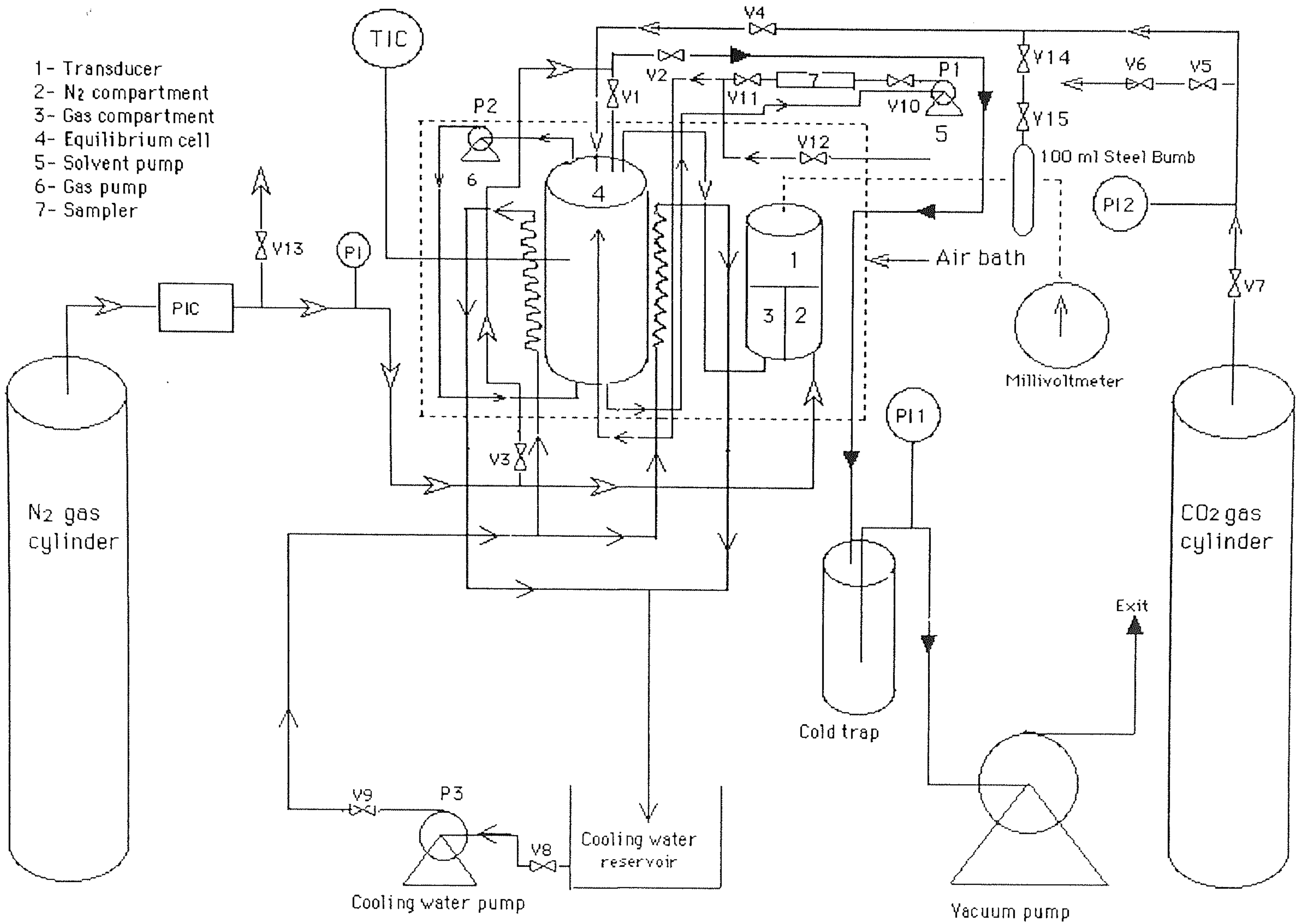


Figure (7-2) The flow sheet of the equilibrium cell

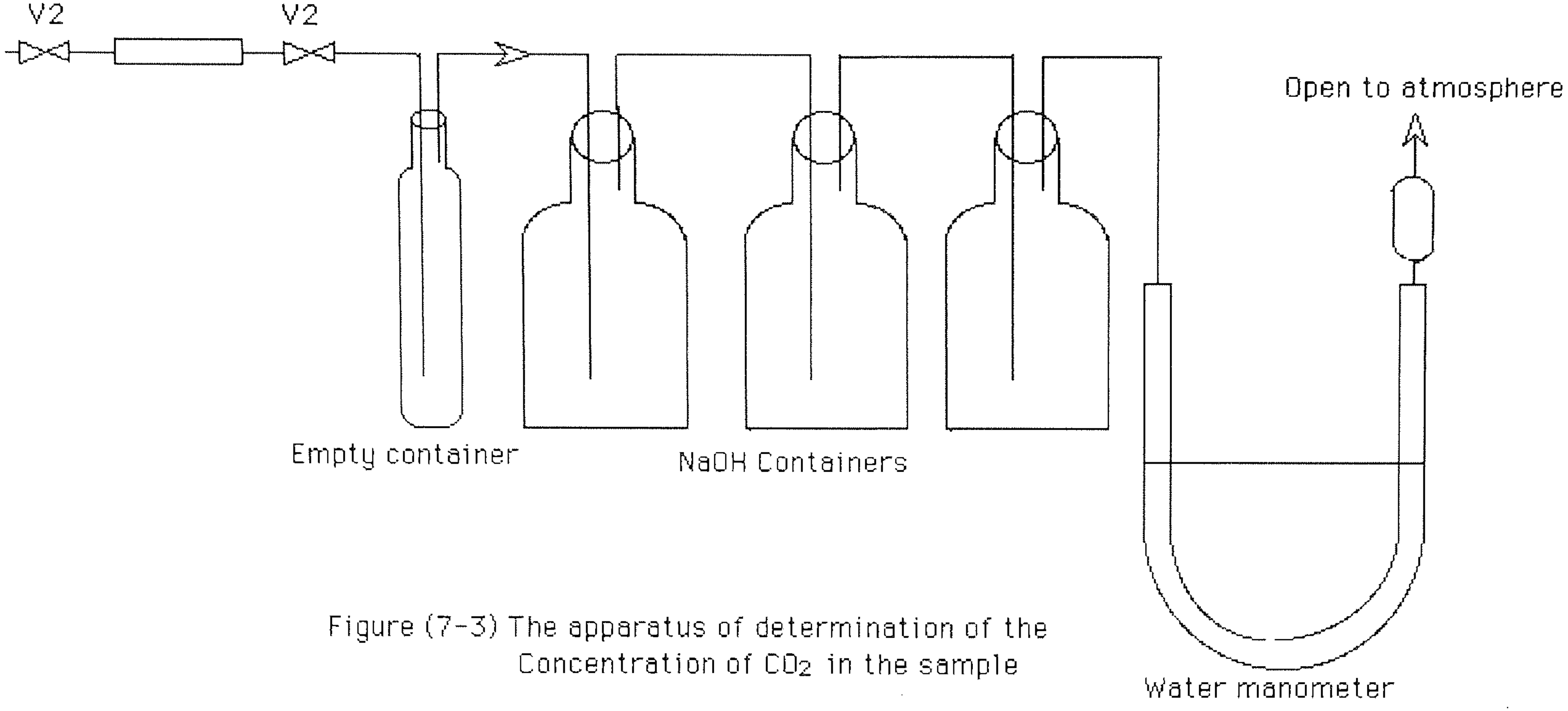


Figure (7-3) The apparatus of determination of the Concentration of CO_2 in the sample

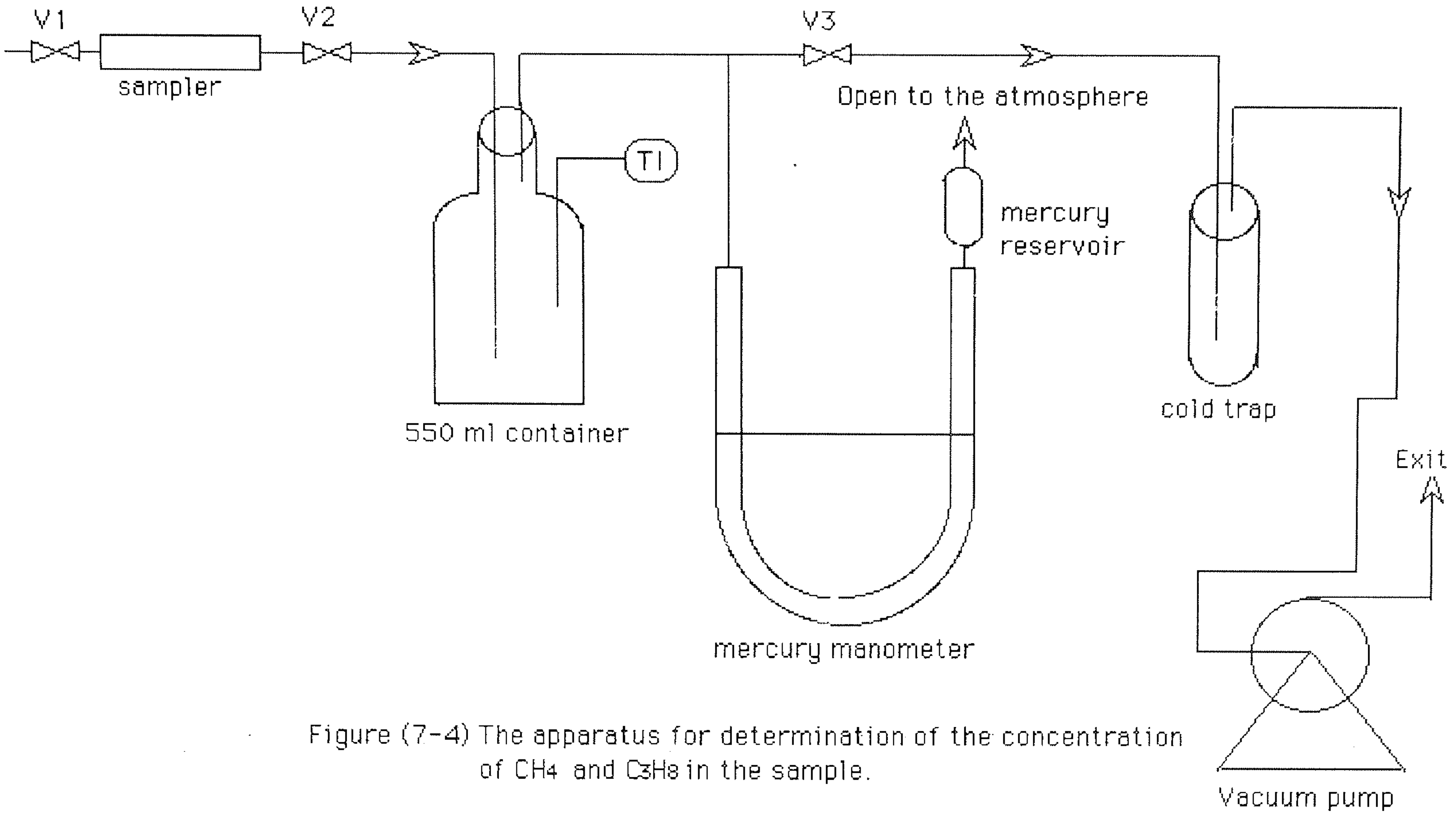


Figure (7-4) The apparatus for determination of the concentration of CH_4 and C_3H_8 in the sample.

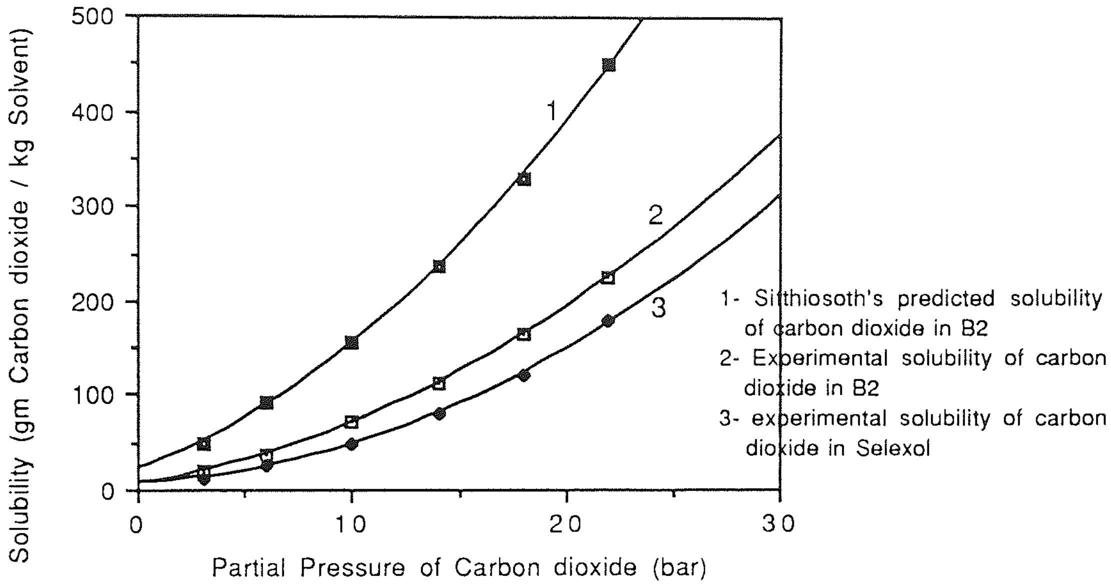


Figure (7-5) Comparision between the solubility of carbon dioxide in B2 with that in Selexol and with Sitthiosoth's prediction

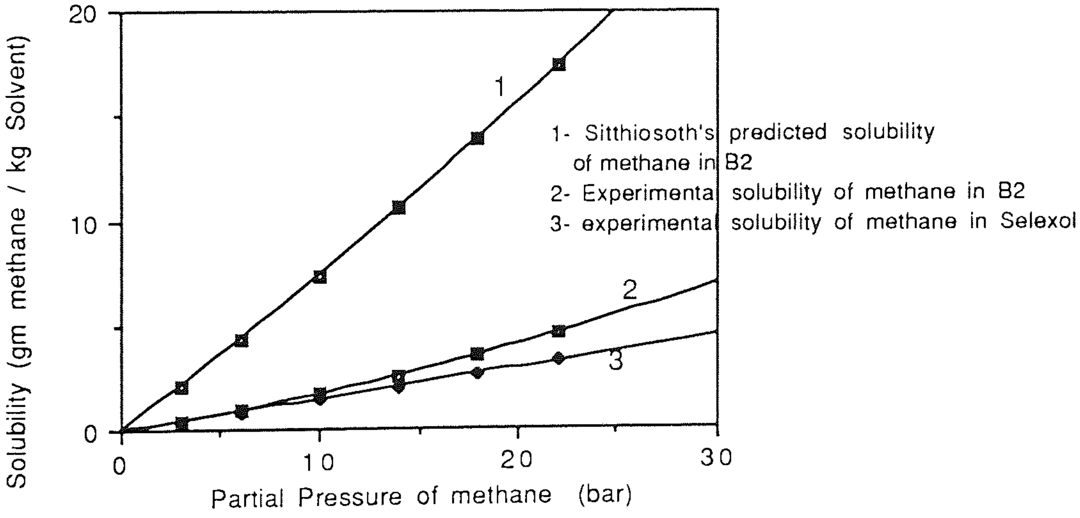


Figure (7-6) Comparision between the solubility of methane in B2 with that in Selexol and with Sitthiosoth's prediction

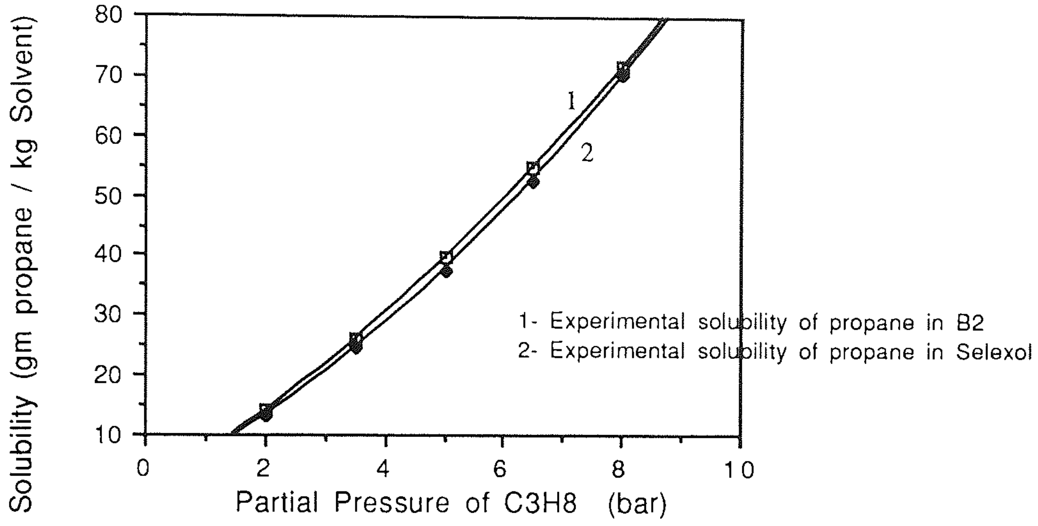


Figure (7-7) Comparision between the solubility of propane in B2 with that in Selexol

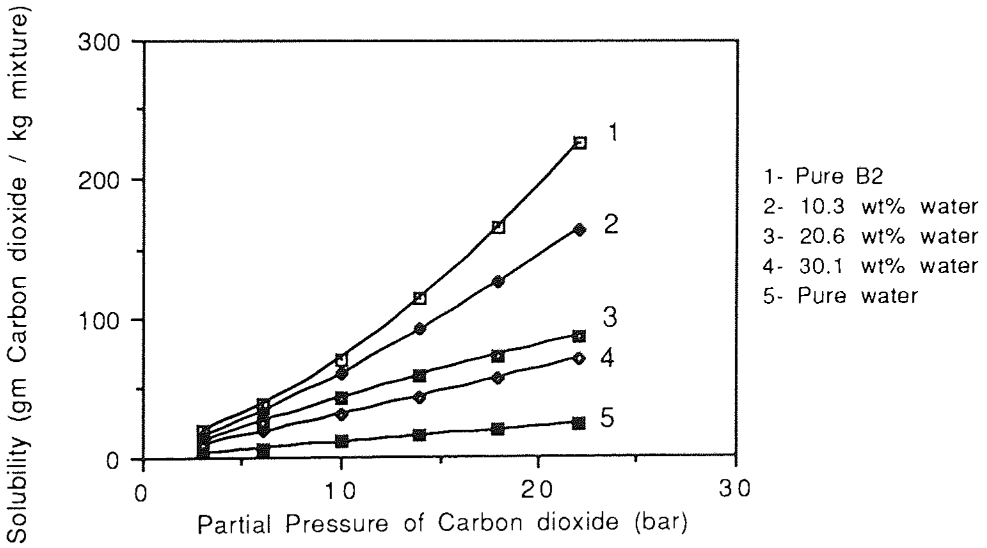


Figure (7-8) The effect of the contamination of B2 with water on the solubility of carbon dioxide in the mixture

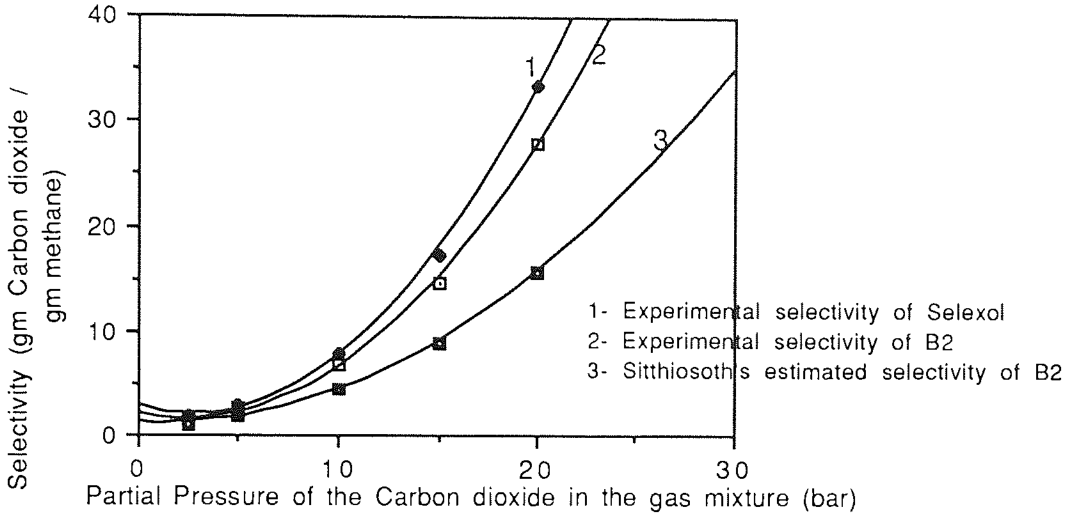


Figure (7-9) The experimental and predicted selectivity of B2 for carbon dioxide from a mixture of carbon dioxide and methane

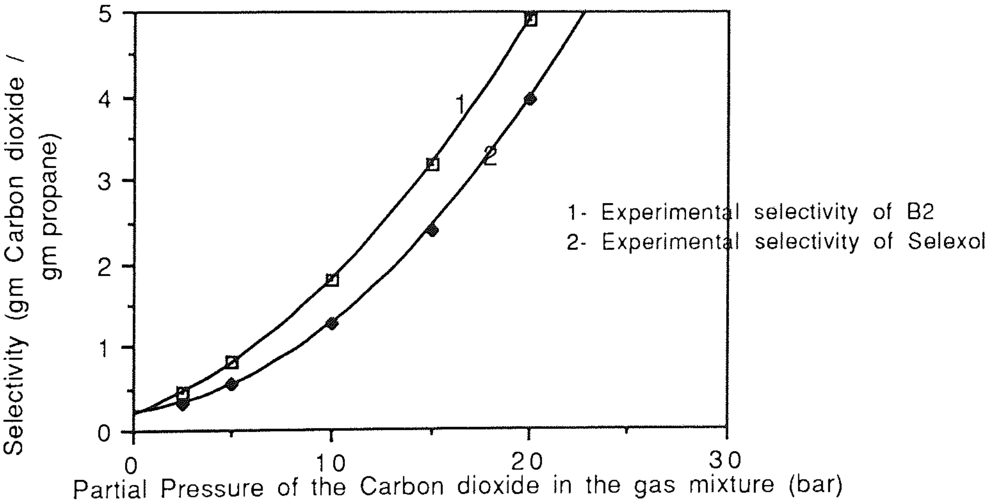


Figure (7-10) The selectivity of B2 and Selexol for carbon dioxide from a mixture of carbon dioxide and propane

CHAPTER EIGHT

Re-evaluation of Acetonyl Acetone

8-1 Introduction

In Chapter 5, some physical solvents have been evaluated. The conclusion from that chapter was that acetonyl acetone is more competitive than Selexol. That study was based on estimated values of the vapour pressure of the solvent and also of the solubilities of carbon dioxide and methane in the solvent. After measuring the properties experimentally, it was found that the experimental results were not in satisfactory agreement with the estimated ones. Table (8-1) shows that the experimental solubility of carbon dioxide and methane in the solvent and also its vapour pressure are less than the estimated ones. Re-evaluation of acetonyl acetone has to be made depending on the experimental data rather than the predicted figures.

The evaluation of any solvent can be made either by using the cost equations presented in Chapter 5 or by complete process design and cost calculations. The first method is quick and straight forward but it includes a certain percentage of error, while the second method is more complicated and time consuming but it is more accurate. In this work we are going to use both methods as complete design calculations have already been made. This means we can use the same design programs, that were shown in Appendix 3, to calculate the total cost of the process by using acetonyl acetone instead of Selexol. These two evaluation methods will be applied to both process configurations {examples (1) and (2)} which were considered in Chapter 5. A comparison will be made between Selexol and the new solvent.

8-2 The Design Method

The design of the equipment has been achieved by running the following programs given in Appendix 3.

- Program A to design the absorber/stripper columns. Tables (8-6), (8-7), (8-13) and (8-14) show the design parameters of these columns.
- Program B to design the high, medium and low pressure flash tanks. Tables (8-8), (8-9) and (8-15) to (8-20) show the flow and the composition of the in/outlet streams in addition to the volume of the tanks.
- Program C to design the cooler, economizer and the heater. Tables (8-10) to (8-12) show the design variables of these heat exchangers.

The same procedures for the cost calculation which are shown in Appendix 1 were used to calculate the cost of all the above mentioned equipment and also the cost of the running cost items.

Table (8-2) shows a comprehensive comparison between the design variables, the cost of the equipment, the running cost items, total capital cost, total running cost and total process cost of the acetonyl acetone process and that of the Selexol process for configuration (1). From this table it can be seen that the investment, the running and the total process cost will be reduced by 36%, 21%, & 25% respectively, when Selexol is replaced by acetonyl acetone. Table (8-3) shows the same comparison for configuration (2). From this table, it can be seen that using Selexol for this particular configuration is more economic than acetonyl acetone. From tables (8-2) and (8-3), it can be seen that the advantages of using acetonyl acetone are smaller sizes of the absorber, stripper and heat exchangers. Also the required heating steam and cooling water are less than that for Selexol. The main weak points of acetonyl acetone are its vapour pressure, and to some extent its selectivity .

8-3 The Cost Equations Method

The cost equations shown in Chapter 5 were used to estimate the cost of the equipment and the running cost items for both configurations considered. It has been mentioned that using the cost equations requires the availability of the physical properties of the solvent used and the values of the coefficients for the configuration considered. The experimental physical properties of Selexol are shown in table (5-2), while table (8-1) shows those of the new solvent. The values of the coefficients were calculated in Chapter 5 and shown in table (5-1) and (5-3) for configurations (1) and (2) respectively. By using these figures, the cost items for both configurations were estimated and are shown in tables (8-4) and (8-5). In the same table the actual design data were quoted to compare with the estimated figures. From these tables, it can be seen that the errors associated with each item of the cost are sometimes large. However the error in the total estimated process cost is less than 10%. This demonstrate the accuracy of the simplified cost equations. The cost equations distinguish correctly between Selexol and acetonyl acetone for configuration (1), because the total process cost by using acetonyl acetone is 25% less than that of Selexol, which is greater than 10% (the accuracy of the cost equation). For configuration (2) the difference in the total process cost is about 8%, within the accuracy of the cost equations. This means it is impossible to distinguish between the two solvents.

Table (8-1) The difference between the estimated and the experimental physical properties of B2.

Physical property	Estimated	Experimental
Solubility of CO_2 at 7.5 bar (gm of CO_2/kg of solvent)	112.5 ($K_{CO2} = 0.6$)	50 ($K_{CO2} = 0.96$)
Solubility of CH_4 at 60.5 bar (gm of CH_4/kg of solvent)	57.6 ($K_{CH4} = 3$)	19.6 ($K_{CH4} = 7.26$)
Selectivity (gm of CO_2/gm of CH_4)	1.953 ($S_L = 5$)	2.55 ($S_L= 7.56$)
Vapour pressure (mmHg) at 50C	1.655	0.56

$S_L = K_{CO2}/K_{CH4}$

Table (8-2) Comparison between the process cost of Selexol with that of acetonyl acetone for configuration (1).

	By using B2			By using Selexol			% Reduction		
Equipment	D (m)	H (m)	Cost $	D (m)	H (m)	Cost $	%R of D	%R of H	%R
Absorber	2.6	7.4	156475	3	15.26	420187	13.3	51	62
Stripper	2.2	9	48705	2.52	9.74	70325	12.7	7.6	31
		L (m)			L (m)			%R of L	
H.P.F. Tank	2.43	9.7	56000	2.717	10.87	64000	10.6	10.7	12
L.P.F. Tank	2.43	9.7	28000	2.717	10.87	32000	10.6	10.7	12
	H.T. A.(m2)		Cost $	H.T.A. (m2)		Cost $	%R H.T.A		%R
Cooler	762		95000	1166		125000	35		24
Economizer	939		110801	2080		190414	55		42
Heater	515		73648	801		99450	36		26
	H. power			H. power			%RH. power		
Compressor	368		135000	324		105000	-13.6		-14.3
R. Cost Items	Flow(kg/hr)		Cost $/year	Flow(kg/hr)		Cost $/year	%R Flow		
Heatin steam	19267		3065765	33890		5392577	43		43
Cool. water	604464		191494	996828		315797	39.4		39.4
Strip. steam	2715		432011	3478		553419	22		22
Solvent Loss	10.5		1209600	0.6		41688			
	H. Power			H. Power			%RH. Power		
Comp. power	368		158065	324		139166	-14.0		-14.0
T. Runn. Cost			5056935			6442647			21.5
T.Equip Cost			703629			1106376			36
T.Proc. Cost			6159287			8175969			24.7

Table (8-3) Comparison between the process cost of Selexol with that of acetonyl acetone for configuration (2).

	By using B2			By using Selexol			% Reduction		
Equipment	D (m)	H (m)	Cost $	D (m)	H (m)	Cost $	%R of D	%R of H	%R
Absorber	4.4	11.2	421682	5	14.6	629143	12	23	33
		L (m)			L (m)			%R of L	
H.P.F. Tank	3.5	13	115200	4	15	139200	12.5	13	17
I.P.F. Tank	3.5	13	74400	4	15	89900	12.5	13	17
L.P.F. Tank	3.5	13	48000	4	15	58000	12.5	13	17
	H. power			H. power			%RH. power		
Compressor	1530		360000	1530		360000	0		0
Com. power	1530		657170	1530		657170	0		0
	Flow(kg/hr)		Cost $/year	Flow(kg/hr)		Cost $/year	%R Flow		
Sol. Loss	45468 kg/y		727493	4950 kg/y		47764			
T. Equ. Cost			1019282			1276243			21
T.Runn. Cost			1384663			704934			- 49
T.Proc. Cost			2981538			2704381			9.3

Table (8-4) Comparison between the estimated and the actual costs of the different cost items for configuration (1).

	By using acetonyl acetone			By using Selexol		
Equipment	Estimated	Actual	% Error	Estimated	Actual	%Error
Absorber	146298	156475	6.5	421453	420187	0.3
Stripper	45689	48705	6.2	70469	70324	0.2
Flash Tanks	80487	84000	4.2	98205	96000	2.3
H.Exchangers	303462	279449	8.0	441875	414864	6.5
Compressor	151399	135000	11.0	116909	105000	10.0
Heatin steam	3230314	3065765	5.1	5405345	5392577	0.25
Cooling water	194805	191494	1.7	325972	315797	3.1
Stripp. steam	427274	432011	1.1	544774	553419	1.5
Solvent Loss	1063619	1209600	12.0	46635	41688	11.0
Comp. power	216413	158065	14.0	156652	139166	11.0
T. Runn. Cost	5132425	5056935	1.5	6479378	6442647	1.0
T.Equip Cost	727337	703629	3.4	1148912	1106376	3.7
T.Proc. Cost	6271920	6159287	1.8	8279340	8175969	1.2

Table (8-5) Comparison between the estimated and the actual costs of the different cost items for configuration (2).

	By using acetonyl acetone			By using Selexol		
Equipment	Estimated	Actual	% Error	Estimated	Actual	% Error
Absorber	300364	421682	28.7	875894	629143	28.0
Flash Tanks	240480	237600	1.2	305179	287100	6.0
Compressor	336806	360000	6.5	305080	360000	15.2
Comp. Power	587968	657170	10.5	519571	657170	21.0
Solvent Lost	727493	727493	0.0	47764	47764	0.0
T. Runn. Cost	1315461	1384663	5.0	567335	704934	19.5
T.Equip Cost	877651	1019282	13.9	1486154	1276243	16.4
T.Proc. Cost	2690447	2981538	9.7	2895643	2704381	7.1

Table (8-6) The calculated design parameters of the absorber using B2 for configuration (1)

```
     VAPOUR DATA                                          LIQUID DATA
     -----------                                          -----------

  FLOW(kg/hr)          = 102944.6                          410252.6
  DENSITY(kg/m^3)       = 66.59867                         973.0004
  VISCOSITY(CP)        = .011                              1.1
  MOL. WT.             = 19.27142                          113.8

                                TOWER DIAMETER
                                --------------

  PACKING FACTOR= 52
  DP/M(mm.H2O)   = 20
  The calculated diameter(m)= 2.531524

   Y              X               HOG           A.U.The curve
 -----          -----            -----          -------------
.11065         .1042412         4.833687          463.6691
.1066175       9.945405E-02     4.841392          441.1994
.102585        9.464914E-02     4.849072          420.282
.0985525       8.982631E-02     4.856763          400.782
.09452         .0849855         4.864438          382.5772
.0904875       8.012658E-02     4.872104          365.5585
.086455        7.524946E-02     4.879757          349.6281
.0824225       7.035404E-02     4.887402          334.6967
.07839         6.544022E-02     4.895043          320.6855
.0743575       6.050789E-02     4.902367          307.502
.070325        5.555694E-02     4.909962          295.1183
.0662925       5.058726E-02     4.917554          283.4567
.06226         4.559877E-02     4.925149          272.4642
.0582275       4.059134E-02     4.932734          262.0906
.054195        3.556487E-02     4.940326          252.2913
.0501625       3.051925E-02     4.947906          243.0253
.04613         2.545436E-02     4.955496          234.2554
.0420975       2.037011E-02     4.963092          225.9477
.038065        1.526637E-02     4.970686          218.0699
.0340325       1.014304E-02     4.978275          210.5938
.03            .005             4.985875          203.4928

The height of the packed material (m)= 7.562001
```

Table (8-7) The calculated design parameter of the stripper using 82 for configuration (1)

```
                    VAPOUR DATA                     LIQUID DATA
                    -----------                     -----------

FLOW(kg/hr)        = 11375.29665149432              416807.4462691563
DENSITY(kg/m^3)    = 1.488746                       965.9456
VISCOSITY(CP)      = .03122                         .4
MOL. WT.           = 38.38324                       111.3822
                         TOWER DIAMETER
                         --------------

PACKING FACTOR        = 52
DP/M(mm.H2O)          = 20
The calculated diameter (m)= 2.181088

       Y                  X              HOG       A.U.the curve
     -----              -----           -----     --------------
 .1579476          1.029015E-02      9.69267          14.73559
 .1500503          9.344809E-03      4.439045         15.87625
 .1421529          8.479572E-03      3.343755         17.24018
 .1342555          7.684671E-03      2.766616         18.8737
 .1263581          6.951864E-03      2.395166         20.84072
 .1184607          6.274146E-03      2.13149          23.22302
 .1105634          5.645534E-03      1.93295          26.13233
 .102666           5.060875E-03      1.777398         29.72267
 9.476858E-02      4.515717E-03      1.651949         34.20951
 .0868712          4.006186E-03      1.548545         39.9027
 7.897381E-02      .0035289          1.461828         47.25856
 7.107643E-02      3.080893E-03      1.387987         56.96672
 6.317905E-02      2.65955E-03       1.32445          70.12264
 5.528167E-02      2.26256E-03       1.269173         88.52009
 4.738428E-02      1.887871E-03      1.220699         115.2747
 .0394869          1.533655E-03      1.177863         156.124
 3.158952E-02      1.198279E-03      1.139779         222.4637
 2.369214E-02      8.802784E-04      1.105525         338.8665
 1.579476E-02      5.783369E-04      1.074837         563.2181
 7.89738E-03       2.912683E-04      1.047015         1029.396
-1.862645E-09      1.799994E-05      1.022012         1853.869

The height of the packed material (m) = 9.060417
```

Table (8-8) High pressure flash tank design parameters using B2 for configuration (1).

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.1051736	.1855349	9.760133E-02
2	1.128832E-02	2.531176E-03	1.211349E-02
3	.1028172	.8119376	.0359984
4	.7807209	4.27143E-06	.8542861

The feed flow rate (kmole/hr) = 4544.977385986748
The vapour flow rate (kmole/hr) = 391.3837434300946
The liquid flow rate (kmole/hr) = 4153.593614871573

Component (1) = CO2
Component (2) = H2S
Component (3) = CH4
Component (4) = Acetonyl acetone

The volume of the tank (M3) = 44.92921

Table (8-9) Low pressure flash tank design parameters
using B2 for configuration (1)

```
 Comp.          Feed comp.        Vapour comp.        Liquid comp.
 ------        ------------      --------------      -------------
   1           9.760133E-02      .6563521            2.777279E-02
   2           1.211349E-02      2.670342E-02        1.029015E-02
   3           .0359984          .3169391            8.885085E-04
   4           .8542861          4.805239E-06        .9610478


The feed   flow rate  (kmole/hr) = 4153.600259291054
The vapour flow rate  (kmole/hr) = 461.4212956805695
The liquid folw rate  (kmole/hr) = 3692.178991295566


Component (1) = CO2
Component (2) = H2S
Component (3) = CH4
Component (4) = Acetonyl acetone


The volume of the tank  (M3) = 44.07115
```

Table (8-10) The design variables of the cooler using acetonyl acetone for configuration (1)

Process variable		**Tube-side**	**Shell-side**
Type of fluid		Water	acetonyl acetone
Mass flow rate	(kg/hr)	604464	410181
Inlet temperature	(^{o}C)	15	71
Outlet temperature	(^{o}C)	30	27
Average viscosity	(cP)	.963	1.13
Average sp. heat	(kJ/kg K)	4.2	2.11
Average ther. Cond.	(W/m K)	.59	.114
Average density	(kg/m^3)	995	973
Fouling factor	(W/m^{2}K)	6000	5000
Inside diameter	(m)	.016	1.2
outside diameter	(m)	.02	1.4
Number of passes		2	1
Reynolds number		22898	6757
Heat transfer coeff.	(W/m^{2}K)	4979	1057
Pressure drop (bar)		0.866	0.43

Total heat transfer area = 762 m^2

Number of tubes = 1211

Overall heat transfer coefficient = 600 W/m^{2}K

Table (8-11) The design variables of the economizer using acetonyl acetone for configuration (1)

Process variable		**Tube-side**	**Shell-side**
Type of fluid		acetonyl acetone	acetonyl acetone
Mass flow rate	(kg/hr)	416741	410181
Inlet temperature	(^oC)	24	127
Outlet temperature	(^oC)	82	71
Average viscosity	(cP)	1.07	0.54
Average sp. heat	(kJ/kg K)	2.0	2.11
Average ther. Cond.	(W/m K)	.114	.114
Average density	(kg/m^3)	973	973
Fouling factor	(W/m^{2}K)	5000	5000
Inside diameter	(m)	.046	1.6
outside diameter	(m)	.05	2.0
Number of passes		6	1
Renoyld number		30054	54860
Heat transfer coeff.	(W/m^{2}K)	723	1004
Pressure drop (bar)		.18	0.89

Total heat transfer area = 939 m^2

Number of tubes = 597

Overall heat transfer coefficient = 329 W/m^{2}K

Table (8-12) The design variables of the heater using acetonyl acetone for configuration (1)

Process variable		**Tube-side**	**Shell-side**
Type of fluid		Steam	acetonyl acetone
Mass flow rate	(kg/hr)	19267	416741
Inlet temperature	(°C)	138	82
Outlet temperature	(°C)	138	126
Average viscosity	(cP)	.014	.5
Average sp. heat	(kJ/kg K)	1.9	2.26
Average ther. Cond.	(W/m K)	.027	.114
Average density	(kg/m^3)	1.88	973
Fouling factor	(W/m^2K)	6000	5000
Inside diameter	(m)	.016	0.8
outside diameter	(m)	.02	1.0
Number of passes		2	1
Renoyld number		74266	22309
Heat transfer coeff.	(W/m^2)	8000	1617
Pressure drop (bar)		0.4	0.8

Total heat transfer area = 515 m^2

Number of tubes = 819

Overall heat transfer coefficient = 809 W/m^2K

Table (8-13) The calculated design parameters of the absorber using Selexol for configuration (2).

```
          VAPOUR DATA                                          LIQUID DATA
          -----------                                          -----------

      FLOW(KG/HR)           = 368157.3                          1574639
      DENSITY(KG/M3)        = 93.99849                          1021.003
      VISCOSITY(CP)         = .011                              5.8
      MOL. WT.              = 27.2                              278.82

                                      TOWER DIAMETER
                                      --------------

      PACKING FACTOR= 52
      DP/M(mm.H2O)   = 20
      The calculated diameter(meter)= 5.079618

 I         Y                  X                  HOG        A.U.the curve
---       -----              -----              -----      -------------
 1        .4                 .4384772           5.641565    47.422
 2        .38175             .4193503           5.890824    51.51735
 3        .3635              .3999895           6.131937    55.92525
 4        .34525             .3803904           6.365575    60.69119
 5        .3270001           .3605488           6.592358    65.867
 6        .3087501           .3404599           6.812852    71.51208
 7        .2905001           .3201192           7.027584    77.69509
 8        .2722501           .2995219           7.237526    84.50163
 9        .2540001           .2786631           7.441966    92.01188
 10       .2357501           .2575378           7.642019    100.3437
 11       .2175001           .236141            7.83805     109.6273
 12       .1992501           .2144671           8.030378    120.0177
 13       .1810001           .1925109           8.21932     131.701
 14       .1627501           .1702669           8.40517     144.9021
 15       .1445001           .1477294           8.588183    159.8939
 16       .1262501           .1248924           8.76862     177.0106
 17       .1080001           .10175             8.946704    196.6635
 18       8.975007E-02       7.829593E-02       9.122658    219.3631
 19       7.150006E-02       5.452397E-02       9.29668     245.7474
 20       5.325006E-02       3.042759E-02       9.468699    276.6118
 21       3.500006E-02       6.000083E-03       9.63991     313.0047


    The height of the packed material (M)= 14.56766
```

Table (8-14) The calculated design parameters of the absorber using B2 for configuration (2).

```
               VAPOUR DATA                               LIQUID DATA
               -----------                               -----------

 FLOW(kg/hr)           = 368157.3                           1028298
 DENSITY(kg/m^3)        = 93.99849                          973.0004
 VISCOSITY(CP)         = .011                               1.75
 MOL. WT.              = 27.2                               113.8

                            TOWER DIAMETER
                            --------------

 PACKING FACTOR= 52
 DP/M(mm.H2O)   = 20
 The calculated diameter(m)= 4.458981

    Y                 X               HOG            A.U. The curve
  -----             -----            -----           --------------
 .4               .3470104          4.860641           77.80608
 .38175           .3287254          4.85617            78.31041
 .3635            .3105792          4.85115            78.98555
 .34525           .2925702          4.845644           79.84103
 .3270001         .274697           4.839704           80.88861
 .3087501         .2569579          4.833383           82.14349
 .2905001         .2393515          4.826724           83.62434
 .2722501         .2218763          4.81977            85.35439
 .2540001         .2045309          4.812552           87.36224
 .2357501         .1873136          4.805096           89.6829
 .2175001         .1702233          4.797423           92.3599
 .1992501         .1532584          4.789572           95.44775
 .1810001         .1364176          4.781553           99.0144
 .1627501         .1196996          4.773385           103.1464
 .1445001         .1031029          4.765091           107.955
 .1262501         8.662639E-02      4.75668            113.5851
 .1080001         7.026862E-02      4.748171           120.2289
 8.975007E-02     5.402834E-02      4.739565           128.1467
 7.150006E-02     3.790432E-02      4.730897           137.7002
 5.325006E-02     .0218953          4.722152           149.4041
 3.500006E-02     6.000055E-03      4.71334            164.0206

 The height of the packed material (m)= 11.19624
```

Table (8-15) High pressure flash tank design parameters using Selexol for configuration (2).

```
Comp.     Feed comp.         Vapour comp.          Liquid comp.
------    ----------         ------------          ------------
  1        .4384772            .6204147              .3980995
  2        .0873395            .3795777              2.248268E-02
  3        .4741833            7.524905E-06          .5794178


The feed   flow rate   (kmole/hr)  =  11838.51014090486
The vapour flow rate   (kmole/hr)  =  2150.150977041074
The liquid flow rate   (kmole/hr)  =  9688.35916386379


Component (1) = CO2
Component (2) = CH4
Component (3) = Selexol

The volume of the tank (M3) = 176.1954
```

Table (8-16) Intermediate pressure flash tank design parameters using Selexol for configuration (2).

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.3980995	.8868824	.2956274
2	.0224827	.1131209	3.480643E-03
3	.5794178	1.752219E-05	.7008876

The feed flow rate (kmole/hr) = 9688.35916386379
The vapour flow rate (kmole/hr) = 1679.116341457769
The liquid flow rate (kmole/hr) = 8009.242600925371

The volume of the tank (M3) = 169.2361

Table (8-17) low pressure flash tank design parameters
using Selexol for configuration (2).

```
 Comp.     Feed comp.         Vapour comp.         Liquid comp.
-------   -----------        -------------        --------------
   1       .2956274           .9952781             2.488195E-02
   2       .003481            1.240251E-02         2.862119E-05
   3       .708876            3.276882E-04         .9830647


The feed   flow rate   (kmole/hr)  =  8009.242600925371
The vapour flow rate   (kmole/hr)  =  2234.61904563396
The liquid flow rate   (kmole/hr)  =  5774.623333810762


The volume of the tank (M3) = 164.3233
```

Table (8-18) High pressure flash tank design parameters using B2 for configuration (2).

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.3470104	.7132378	.2860381
2	.0539661	.2867683	1.520741E-02
3	.5990238	9.074705E-06	.6987523

The feed flow rate (kmole/hr) = 14994.05746527692
The vapour flow rate (kmole/hr) = 2140.035955782334
The liquid flow rate (kmole/hr) = 12854.02106653328

Component (1) = CO2
Component (2) = CH4
Component (3) = Selexol

The volume of the tank (M3) = 122.8843

Table (8-19) Intermediate pressure flash tank design parameters using B2 for configuration (2).

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.2860381	.9048921	.1885192
2	.0152074	9.508972E-02	2.619551E-03
3	.6987523	2.022146E-05	.8088584

The feed flow rate (kmole/hr) = 12854.02461022367
The vapour flow rate (kmole/hr) = 1749.802112198916
The liquid flow rate (kmole/hr) = 11104.22294098606

Component (1) = CO2
Component (2) = CH4
Component (3) = Selexol

The volume of the tank (M3) = 115.4185

```
Table (8-20) Low pressure flash tank design parameters
      using B2 for configuration (2).


 Comp.     Feed comp.         Vapour comp.          Liquid comp.
----------
          -----------        -------------         --------------
   1       .1885192           .9851544              1.539304E-02
   2       2.61955E-03        1.453515E-02          3.00313E-05
   3       .8088584           3.281899E-04          .9845696


The feed   flow rate   (kmole/hr)  =  11104.22471283125
The vapour flow rate   (kmole/hr)  =  1982.375841419531
The liquid flow rate   (kmole/hr)  =  9121.848871411719


Component (1) = CO2
Component (2) = CH4
Component (3) = Selexol


The volume of the tank (M3) = 108.4032
```

CHAPTER NINE

Discussion, Conclusions and Suggestions for Future Work

9-1 Discussion

This work has demonstrated, in fair detail, how the physical properties of a solvent relate to the different cost items of a physical gas absorption process. The effect of every property on the cost items has been evaluated and presented in figures (4-2) to (4-9). Then the optimum relationships were formulated by using the optimisation programme GRG2. A good agreement between the derived equations and the optimum formulated ones has been found. The role and the importance of every property was investigated and it was found that the solubility played the most important role in determining the investment and running costs for most items. The effect of the other properties is limited to certain cost items, but their effect on the total process cost is very significant. Equations (5-1) to (5-10) have clarified the contribution of every property to every cost item. So, the evaluation of a new candidate solvent for a gas absorption process can be made by applying these equations. All the properties that were mentioned in table (5-2) have to be found either by measurement, estimation, or from the literature. It is obvious that the optimum solvent should have the optimum combination of all the effective physical properties.

The configuration of any physical gas absorption process depends mainly on the purpose which is required to be achieved by that process, in spite of the fact that the solvent plays some part in determining the shape of the process. For example, the commercial plant in West Texas is used to remove most but not all of the CO_2 from natural gas. This type of plant (as seen in configuration two) does not need the use of a stripper or heat exchangers. In other words, the major equipment items are the absorber and a number of flash tanks. This means the specific heat and the thermal conductivity of the solvent have no role in determining the cost of such processes and also the effect of the vapour pressure is less, because normally the major loss of the solvent occurs during the stripping process. This discussion suggests that the number of the effective physical properties and their optimum combination are related to the configuration of the process, so the setting up of the shape of the process comes before selecting the best solvent.

The type of process selected and the operating conditions have a direct effect on the cost items. This effect was clarified by the coefficients of the cost equations. This means that these equations could be used to optimise the operating conditions for a certain solvent. In Appendix 1, where the design of the absorber and the stripper have been carried out, the absorption and stripping factors which give the optimum height of the packed material have been chosen as shown in figures (A1-1) and (A1-3). This may be acceptable if the process does not include heat exchangers. When the process includes heat exchangers, these two factors have to be related to the total cost of the process, because they have a crucial role in determining the cost of every cost item as the flow of the circulated solvent is determined by their values (the values of stripping and absorption factors). There are some other possible uses of the cost equations. For example, for fixed solvent properties, the purity of the product can be related to the cost of the absorber. Another example, the pressure of the first flash tank can be related to the cost of the compressor and the cost of the compressing power.

Sitthiosoth has suggested that if acetonyl acetone (B2) was used instead of Selexol to separate carbon dioxide and hydrogen sulfide from methane, the capital cost will be lower, but the running cost would be more because of the low selectivity of the acetonyl acetone. Low selectivity means the required power to compress the recycle gases is more. His suggestion was made due to the following reasons:

1- The comparison between the two solvents was made just in terms of the cost of the absorber and stripper, despite the fact that the cost of these two items represents not more than 40% of the total capital cost.

2- A mathematical relationship which relates the cost of the required compressing power to the selectivity was not formulated. This type of equation is vital to calculate how the difference between the two selectivities affects the total running cost of the process.

3- The heating steam and the cooling water represent a high percentage of the running cost. If Selexol is replaced by B2, these two cost items will be reduced significantly due to two reasons. The first is that the mass solubility of CO_2 in B2 is higher than that in Selexol, and the second is the viscosity of Selexol is higher than that of B2. These points were not considered by Sitthiosoth.

4- The role and the contribution of all the physical properties to the total investment and running cost were not known.

Macchietto went one step further when he suggested that the objective function which has to be minimised, can be represented by maximising the ratio of the solubility to the viscosity. This ratio can not be a comprehensive representation of the total capital and operating costs, because maximising it does not mean minimum capital or running cost. If we go back to table (5-2) and apply Macchietto's ratio we will find that acetone represents the best solvent in the selected group, followed by methyl ethyl ketone in the second position. From table (5-4) the running cost of the acetone process comes in the third highest position, while methyl ethyl ketone is in the highest position. Also from tables (5-2) and (5-4) we can easily conclude that Macchietto's objective function could be used to minimise only the cost of the absorber.

It was mentioned that Sitthiosoth suggested that acetonyl acetone could be competitive with Selexol if its selectivity is improved. In Chapter 5 when all the effective physical properties of the two solvents were considered, it was found that by using B2 instead of Selexol the capital and the running costs will be reduced by 44% and 28% respectively without improving the selectivity of B2. Unfortunately, the calculations of Chapter 5 were based on estimated vapour pressure, and also the solubilities of CO_2 and CH_4 in B2 at high pressure were predicted. This study had to be finalized either by recommending this solvent for commercial application or by dismissing it. This led to a decision to measure the above mentioned three physical properties and also measure the effect of water on the solubility of CO_2 in B2, because it is unrealistic to propose a new solvent based only on estimated properties.

The instrument which was used to measure the vapour pressure of B2 was constructed by the Chemical Engineering and Applied Chemistry department at Aston University and was based on the Swietoslawski ebulliometer. The relationship of the measured vapour pressure with the temperature was compared with that of the one estimated by using Lee-Kesler and Gomez-Thodos methods. It was found that the two figures agreed with each other at high temperature, but there was a significant deviation at low temperatures.

The solubilities of CO_2, CH_4 and C_3H_8 in pure solvent and the solubility of CO_2 in a different percentage of water-acetonyl acetone mixtures were measured for a partial pressure range from 1 to 20 bar at 25° C.

The results of that measurement were presented in figures (7-5), (7-6), (7-7) and (7-8).

It was explained in section (7-3) that contamination of the solvent with water is inevitable, and that the water has negative effects on the solubility. Because of this, it was necessary to measure the effect of different percentages of water in B2 on the solubility of CO_2. From figure (7-8) it can be seen that the solubility of CO_2 in a mixture of B2 and water differs by more than one order of magnitude which means the CO_2 solubility in a H_2O-B2 mixture can not be predicted by simple interpolation. This conclusion is in full agreement with the conclusion of Knapp (1985) when he measured the solubilities of carbon dioxide, ethylene and methane in mixtures of water and n-methylpyrrolidone. Figure (7-8) also shows that a small percentage of water does not reduce the solubility of CO_2 in B2 significantly. This work suggested that the weight percentage of the water should be kept below 5% if this solvent is used as an absorbent.

Figures (7-5) and (7-6) demonstrate that the solubilities of CO_2 and CH_4 (measured in gm of gas per kg of solvent) in B2 is more than that of Selexol. These two figures also show that the predicted solubilities by using (GCEOS) theory were significantly higher than the reality and that the differences increase as the partial pressure of the gas increases. These results confirm the need to develop a reliable theory to predict the solubility of a gas in a solvent. Figure (7-7) shows that the solubility of C_3H_8 in B2 is more or less the same as that of Selexol.

The selectivities of the solvents (B2 and Selexol) to CO_2 from a mixtures of CO_2-CH_4 and CO_2-C_3H_8 were calculated from the solubilities of each gas in each solvent at different partial pressures and the results were presented in figures (7-9) and (7-10). These two figures show that the selectivity of Selexol for CO_2 from a mixture of CO_2-CH_4 is slightly more than that of B2 , while the opposite was shown to be true for the mixture of CO_2-C_3H_8.

According to the above experimental results B2 had to be re-evaluated. There are two methods which could be used to evaluate a solvent. The first is by using the cost equations. This method is quick and straight forward but includes a certain percentage of error. The second is by a complete design for the process. This method is more accurate but it is tedious. Both methods were used and the design programs shown in Appendix 3 were used to calculate the cost of the process for both configurations considered. Table (8-2) shows that replacing Selexol by B2 reduced the T.C.C, T.R.C and T.P.C by 36%, 21% and 25% respectively for Configuration 1. For Configuration 2, table (8-3) shows that B2 can not be a good competitor to Selexol. That means the same solvent can not be the best for any process configuration. In other words the nature of the required objective plays an important role in determining the best solvent.

At this stage, this work may be claimed to be a successful forward step in the strategy of selecting and evaluating physical solvents for gas absorption, because it provides engineers with a straight-forward strategy to evaluate any solvent or to compare any suggested candidates. It also provides researchers with a starting point of establishing an optimisation program to find the best combinations between the effective physical properties .

9-2 Conclusions

1- Acetonyl acetone is more economic than Selexol if it is used as a physical gas absorbent, for certain process configurations. This solvent can be recommended for a pilot plant study or for small scale commercial plant.

2- The solubilities of CO_2, CH_4, and C_3H_8 (measured in gm of gas/kg of solvent) in B2 were higher than those in Selexol.

3- The selectivity of Selexol for CO_2 from a mixture of CO_2-CH_4 was slightly higher than that of the B2, while the opposite was true for a mixture of CO_2-C_3H_8.

4- A new straight-forward strategy was developed in order to evaluate any solvent or to compare between some alternative solvents.

5- New objective functions have been formulated. These functions explain the real role and the contribution of every (effective) physical property in the determination of the costs of the major items. They also provide a starting point to establish an optimisation program which could be used to find the best combinations of the physical properties in order to minimise the total cost of a process.

6- If a physical gas absorption process has to include some heat exchangers, the specific heat and the thermal conductivity of the solvent have to be included in any suggested objective function.

7- The optimum values of the absorption and stripping factors have to be found by relating them to the total process costs rather than the costs of the absorber and the stripper.

9-3 Suggestions for Future Work

1- Perform experiments on a pilot plant scale to separate carbon dioxide from methane for different percentages and to study the effect of the presence of one gas on the solubility of the other.

2- In all gas absorption processes, the temperature of the circulated solvent fluctuates between low at the absorption column, medium at the flashing stages and high at the stripping column, so the effect of the temperature on the solubility of different gases in acetonyl acetone needs to be measured.

3- The experimental determination of the solubility of hydrogen sulfide in the new solvent at different conditions.

4- The experimental determination of the effect of the presence of one acid gas on the solubility of the other.

5- Determination of the thermal stability of the new solvent and its reactivity with the acid gases at elevated temperatures, and also the maximum operating temperature needs to be known.

6- An optimisation program to establish the best combination of the physical properties of a liquid which minimises the total cost of the process.

7- Developing the suggested equations by reducing the number of the constraints.

8- A theory is needed to be developed to predict the solubility of gases in liquids at high pressure.

9- A theory is required to be developed to predict the effect of the water on the solubility of physical solvents.

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APPENDIX ONE

Process and Equipment Design

Figure (4-1) shows the West Texas process which is used to separate CO_2 and H_2S from CH_4 by Selexol. This process consists mainly of an absorber, two flash tanks, stripper, heat exchangers and compressor. In this appendix the required calculations for the flow rates, compositions of the streams and the design of every piece of equipment will be carried out.

A1-1 The Absorber Design

The actual gas flow to the absorber is a mixture of the raw gas and the recycle stream from the first flash tank. The height of the packed material and the other design variables depend on the actual inlet flow to the absorber rather than the flow of the actual raw gas. The flow rate of the recycle stream depends on the composition and the flow of the outlet liquid from the absorber. So, trial and error calculations have to be made to find the recycle flow rate and it is composition.

Stream (10):- Raw feed gas

Total flow = 5000 kmole/hr

mol % CO_2 = 10

mol % H_2S = 1

mol % CH_4 = 89

Stream (20):-The assumed recycle flow

Total flow = 322 kmole/hr

mol % CO_2 = 22.6

mol %H_2S = 0.4

mol %CH_4 = 77

Stream (30) :- This stream is equal to the summation of stream (10) and stream (20).

Total flow = 5322 kmole/hr

mol % CO_2 = 10.8

mol % H_2S = 0.96

mol %CH_4 = 88.24

A1-1-1 First estimation of the solvent flow rate

K_{CO_2} = 0.6 at 68 atm and 27°C

$Y = 0.6X$ equation of equilibrium line (A1-1)

$G_m(Y_1 - Y_2) = L_m(X_1 - X_2)$ Eqn. of the operating line (A1-2)

At minimum solvent flow rate the operating line will intersect the equilibrium line at the inlet CO_2 concentration (Y_1 = 0.1124)

$$X_1 = \frac{Y_1}{0.6} = \frac{0.112}{0.6} = 0.187333$$

$$L_m = \frac{G_m(Y_1 - Y_2)}{X_1 - X_2} = 4765\left(\frac{0.1124 - 0.03}{0.18733 - 0.005}\right) = 2153.4 \text{ kmole/hr}$$

Y, X = Mole fraction of solute in the gas phase and liquid phase

Y_1,Y_2 = Mole fraction of solute in the gas phase at the concentrated end and dilute end of the packing material respectively

X_1, X_2 = Mole fraction of solute in the liquid phase at the concentrate end and dilute end of the packing material respectively

G_m, L_m = The average molar flows of the gas and the liquid (kmole/hr)

A1-1-2 Calculation of the diameter of the absorber

The capacity of a packed column depends on many factors, namely the flows of the gas and the liquid, liquid viscosity and density, gas density, size and type of the packed material. Normally the column should be designed to operate at the highest economical pressure drop, to ensure good liquid and gas distribution. A pressure drop of 20 mm of water per metre of packed height and 38 mm ceramic Intalox saddles were selected for the absorber and stripper in this work. Usually, the column cross-sectional area for the selected pressure drop can be determined from a generalised pressure-drop correlation, which is adapted in many different ways. In order to simplify the calculation of the diameter, (for the computer program) the equations given by Dennis (5) have been used in this work as shown below.

The Tower Diameter Calculation Steps

$$A = 0.02368\ DP^{0.65278} \qquad \text{----------(A1-3)}$$

$$B = -0.0241\ DP^{0.91939} \qquad \text{----------(A1-4)}$$

$$V = \left[\frac{(T + 460)\ P}{492\ \ 14.7}\right] 359 \qquad \text{----------(A1-5)}$$

$$DG = \frac{MW}{V} \qquad \text{----------(A1-6)}$$

$$G = G_m\ MW \qquad \text{----------(A1-7)}$$

$$L = L_m\ MW1 \qquad \text{----------(A1-8)}$$

$$X6 = \frac{L}{G}\sqrt{\frac{DG}{DL}} \qquad \text{----------(A1-9)}$$

$$Y5 = A + B\ \ln(X6) \qquad \text{----------(A1-10)}$$

$$X5 = \frac{Y5\ DL\ DG}{CF\ CP^{0.2}\left(\frac{DL}{62.3}\right)} \qquad \text{----------(A1-11)}$$

$$G5 = 3600\sqrt{X5} \qquad \text{----------(A1-12)}$$

$$A1 = \frac{G}{G5} \qquad \text{----------(A1-13)}$$

$$D1 = 24\sqrt{\frac{A1}{3.1416}} \qquad \text{----------(A1-14)}$$

where A,B = Correlation constants
DP = Tower pressure drop (mmH_2O/m)
V = molar volume (kmol/m^3)
T,P = Operating temperature (K) and pressure (atm)
DG,DL = Density of the feed gas and the liquid (kg/m^3)
MW = Molecular weight of the feed gas
MW1 = Molecular weight of the solvent
G,L = Mass flow rate of the gas and the liquid (kg/hr)
X6 = Temporary variable
X5 = Temporary variable
Y5 = Temporary variable
CF = Packing factor
CP = Liquid viscosity (CP)

G5 = Flooding rate (kg/s m^3)
A1 = Tower cross-sectional area (m^2)
D1 = Tower diameter (m)

A1-1-3 Calculation of the liquid and gas mass transfer coefficients

Absorbers and strippers are operated usually in a counter-current flow between gas and liquid to transfer one or more solutes from one fluid to another. The rate of transfer of any solute can be computed, if the concentration at the gas-liquid interface is known. It is quite difficult to measure the solute concentration at the gas-liquid interface. So the mass transfer coefficient is expressed as an overall coefficient, rather than as coefficients of the individual phases. This volumetric overall coefficient depends directly upon fluid properties, flow rates and the type of packing material. In this work Onda's (36) method has been used to calculate the gas-phase mass transfer coefficient (K_G) and liquid phase mass transfer coefficient (K_L). These two coefficients can be used to calculate the heights of the film transfer unit for the gas phase and liquid phase (H_G, H_L). Below are shown the equations and the steps sequence of the H_G, H_L calculations.

Mass Transfer Coefficients Calculation Steps

Input SL, SS, A2, G3, DL1, DP1, R, DV, CP1

$$L_W = \frac{(L/3600)}{[(\pi/4)(D1)^2]} \qquad \text{----------(A1-15)}$$

$$V_W = \frac{(G/3600)}{[(\pi/4)(D1)^2]} \qquad \text{----------(A1-16)}$$

$$C_T = \frac{DL}{MW1} \qquad \text{----------(A1-17)}$$

$$\frac{A_W}{A2} = 1 - EXP\left[-1.45 \left(\frac{SS}{SL}\right)^{.75} \left(\frac{1488.2\ L_W}{A2\ CP}\right)^{.1} \left(\frac{L_W^2\ A2}{DL^2\ G3}\right)^{-.05} \left(\frac{L_W^2}{32\ DL\ SL\ A2}\right)^{.2}\right] \qquad \text{(A1-18)}$$

$$K_L \left(\frac{1488.2\ DL}{CP\ G3}\right)^{1/3} = .0051 \left(\frac{1488.2\ L_W}{A_W\ CP}\right)^{2/3} \left(\frac{CP}{1488.2\ DL\ DL1}\right)^{-.5} (A2\ DP1)^{.4} \qquad \text{(A1-19)}$$

$$\frac{K_G\,R(T+460)}{A2\,DV} = 5.23\left(\frac{1488.2\,V_W}{A2\,CP1}\right)^{.7}\left(\frac{CP1}{1488.2\,DV\,DG}\right)^{1/3}(A2\,DP1)^{-2.0} \qquad \text{(A1-20)}$$

$$H_G = \frac{V_W}{MW\,K_G\,A_W\,P} \qquad \text{----------(A1-21)}$$

$$H_L = \frac{L_W}{MW1\,K_L\,A_W\,C_T} \qquad \text{----------(A1-22)}$$

where

SL = Surface tension of the solvent (N/m)
SS = Surface tension of the ceramic (N/m)
A_W = Effective interfacial area of the packing per unit volume (m^2/m^3)
A2 = Actual area of the packing per unit volume (m^2/m^3)
L_W = Liquid mass flow per unit cross-sectional area (kg/m^2s)
V_W = Gas mass flow per unit cross-sectional area (kg/m^2s)
G3 = Gravity constant (9.81 m/s^2)
DL1 = Diffusivity of the solute in the solvent (m^2/s)
DV = Diffusivity of the solute in the gas phase (m^2/s)
DP1 = Packing size (m)
R = Gas constant (.08206 atm m^3/kmol K)
CP1 = Viscosity of the gas phase (CP)
C_T = Total molar concentration ($kmol/m^3$)
K_G = Gas film mass transfer coefficient ($kmol/m^2s$ atm)
K_L = Liquid film mass transfer coefficient (m/s)
H_G = Height of the gas-phase transfer unit (m)
H_L = Height of the liquid-phase transfer unit (m)

A1-1-4 Diffusivity calculations

All the required physical properties of the Selexol were obtained by private communications except the diffusivities of carbon dioxide in methane and in Selexol, hydrogen sulfide in the steam and in Selexol. Treybal (52) has recommended the Wilke-Lee method to calculate diffusivity of a gas in another gas, so this method was used to calculate the diffusivity of CO_2 in CH_4 and H_2S in steam, while the Wilke-Chang (59) method has been used to calculate the diffusivity of CO_2 and H_2S in Selexol as shown below.

A- Calculation the diffusivity of CO_2 in CH_4

$$D_{AB} = \frac{10^{-4}\left(1.084-.249\sqrt{\frac{1}{MA}+\frac{1}{MB}}\right) T^{3/2}\sqrt{\frac{1}{MA}+\frac{1}{MB}}}{P\,(r_{AB})^2\, f\left(\frac{KT}{\varphi_{AB}}\right)} \qquad \text{-------------(A1-23)}$$

$f\left(\frac{KT}{\varphi_{AB}}\right)$ = 0.56 (Collision function given in Figure(2-5)/ 52/ page 32

For CO_2 $\frac{\varphi}{K} = 195.2$ $r = .3941$

For CH_4 $\frac{\varphi}{K} = 148.6$ $r = .3758$

The above data are given in Table (2-2)/ 52/ page 33

$$r_{AB} = \frac{.3941+.3758}{2} = .385$$

$$\varphi_{AB} = \sqrt{195.2 \times 148.6} = 170.316$$

$$\frac{TK}{\varphi_{AB}} = \frac{299.67}{170.316} = 1.76$$

$$\sqrt{\frac{1}{44}+\frac{1}{16}} = .292$$

$$D_{AB} = \frac{10^{-4}(1.084-.249\times.292)\,(299.67)^{1.5}\,(.292)}{6894800\,(.385)^2\,(.56)} = 2.8\times10^{-7}\ m^2/s \quad (3.014\times10^{-6}\ ft^2/s)$$

The same procedure was used to calculate the diffusivity of H_2S in steam. The result was (D_{AB} = 2.1734E-5 m^2/s or D_{AB} =2.34E-4 ft^2/s)

B- Calculation the diffusivity of CO_2 in Selexol

$$D_{AB} = \frac{(117.3\times10^{-18})\,(\phi\ MW1)^{.5}\,T}{CP\ V_A^{.6}} \qquad \text{----------(A1-24)}$$

$\phi_{\text{of sel.}} = 1$, $V_{CO_2} = .034$ Table (2-3)/ 52

$$D_{AB} = \frac{(117.3\times10^{-18})\,(280)^{.5}\ 299.67}{5.8\times10^{-3}\ (.034)^{.6}} = 7.7126\times10^{-10}\ m^2/s\ (8.3\times10^{-9}\ ft^2/s)$$

The same procedure was used to calculate the diffusivity of H_2S in the Selexol, the result was (D_{AB} = 56.34E-10 m^2/s or 6.06522E-8 ft2/s)

where

D_{AB} = Diffusivity of component A in component B ((m2/S)

MA,MB = Molecular weight of components A and B

r_{AB} = Molecular separation at collision $(r_A+r_B)/2$

A1-1-5 Height calculation of the absorber

There are various methods for estimation of the required tower height for absorption of one component or more from one fluid to another. In this work, it is necessary to consider the effect of simultaneous mass transfer of the other components and the volatile quantity of the solvent on the absorber design parameters. Sherwood (41) has recommended Wile's method as a good approximate treatment of multicomponent mass transfer. The height of a packed material can be calculate from the following equations.

$$h_T = \int_{Y2}^{Y1} H_{OG} \frac{Y_f^* \, dY}{(1+Y)(Y-Y^*)} \qquad \text{----------(A1-25)}$$

$$Y_f^* = \frac{(1-tY) - (1-tY^*)}{\ln\left[{(1-tY)}/{(1-tY^*)}\right]} \qquad \text{----------(A1-26)}$$

$$H_{OG} = \frac{Y_f}{Y_f^*} H_G + \frac{K\,G_m}{L_m} \frac{X_f}{Y_f^*} H_L \qquad \text{----------(A1-27)}$$

$$X_f = \frac{(1-tX) - (1-tX_i)}{\ln\left[(1-tX)/(1-tX_i)\right]} \qquad \text{----------(A1-28)}$$

$$Y_f = \frac{(1-tY) - (1-tY_i)}{\ln\left[{(1-tY)}/{(1-tY_i)}\right]} \qquad \text{----------(A1-29)}$$

$$t = 1/\theta_A \qquad \text{----------(A1-30)}$$

$$\theta_A = \frac{\Delta g_A}{\Delta g_A + \Delta g_I} \qquad \text{———(A1-31)}$$

From material balances on the gas and liquid streams around the dilute end and any point of compositions X, Y within the tower, it can be shown that:-

$$\frac{G_m}{L_m} = \frac{G2\,(1 - tY2)\,(1 - tX)}{L2\,(1 - tX2)\,(1 - tY)} \qquad \text{----------(A1-32)}$$

To evaluate Y_f and X_f it is necessary to calculate the interfacial composition X_i and Y_i at each Y value used in the calculation of H_{OG}. The following equations can be used for this purpose.

$$\frac{Y - Y_i}{X - X_i} = - \frac{L_m}{G_m} \frac{H_G}{H_L} \frac{Y_f}{X_f} \quad \text{----------(A1-33)}$$

The solute composition in the liquid phase and gas phase can be calculated at any point within the tower by the following equations.

$$Y = \frac{L2\,(1 - tX2)X + (G2Y2 - L2X2)\,(1 - tX)}{G2\,(1 - tX) + t\,L2\,(X - X2)} \quad \text{----------(A1-34)}$$

$$X = \frac{G2\,(1 - tY2)Y + (L2X2 - G2Y2)\,(1 - tY)}{L2\,(1 - tY) + t\,G2\,(Y - Y2)} \quad \text{----------(A1-35)}$$

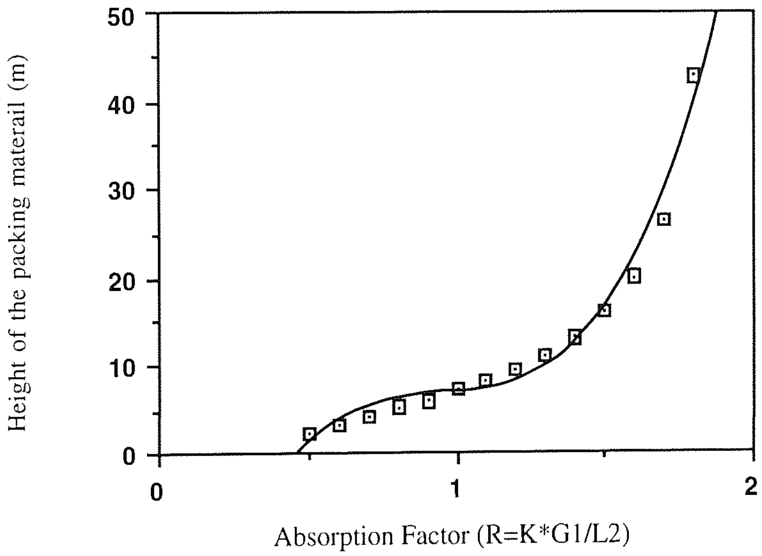
h_T = Height of the packed material (m).
H_{OG} = Height of overall transfer unit (m).
Y^* = Equilibrium concentration of the solute in the gas-phase.
K = Equilibrium constant.
X_i, Y_i = Interfacial solute concentration in the liquid and gas phases respectively.
G1,G2 = Inlet molar mass flow rate of the gas at the concentrated end and diluted end respectively.
L1,L2 = Inlet molar flow rate of the liquid at the concentrated end and diluted end respectively
Δg_A = Total moles of compound (A) absorbed over the tower (kmole/hrm^2)
Δg_I = Net total mole of all compounds other than (A) absorbed or desorbed over the tower (kmole/hrm^2
$= \Delta g_B + \Delta g_C + \Delta g_D + \ldots\ldots$

Using the above equations and others which have been given before, a comprehensive computer program to calculate the diameter of the packed tower, the overall height of the transfer unit and the height of the packed material has been designed. A computer listing of the program is shown in Appendix 3 (program A) and its output is shown in table (A1-1).

A1-2 Calculation of the Optimum Solvent Flow Rate

To calculate the optimum solvent flow rate, different values of the absorption factor (R) were applied in the comprehensive computer program, to predict how the absorption factor affects the height of the packed material. The relationship between the absorption factor (R) and the height of the packed material has been drawn in figure (A1-1). From this figure the optimum absorption factor has been chosen as R=1.4388.

Fig. (A1-1) The relationship of the absorber height to the absorption factor



A1-3 Flash Tank Design

The flash tank is considered the simplest equilibrium stage process. The flashing process includes three main steps. (a) The regulation of a binary (or multicomponent) stream to the desired temperature and pressure. (b) Sudden reduction in the pressure across a valve. (c) The separation of the resulting liquid and vapour. Figure (A1-3) is a schematic representation of the process. Normally, the feed must be maintained in the liquid state by controlling T_1 and P_1. When the pressure reduces from P_1 to P_2 across the valve, part of the feed is converted to a vapour phase. Usually the flash process occurs under adiabatic conditions, so the latent heat of vaporisation has to come from the sensible-heat content, and as a consequence the temperature of the outlet streams would be less than the inlet. If the change in the pressure across the valve is too high, this would cause an increase in the temperature of the resulting liquid and vapour. So, it is important to calculate the net change in the temperature. Usually the vapour and the liquid in the flash tank can be considered to be in equilibrium with each other owing to the intimate contact which prevails during the flash process. In designing the flash tank, three parameters have to be calculated. (1) The flow rates of the resulting liquid and vapour streams. (2) The compositions of those vapour and liquid streams. (3) The volume of the tank. Smith (45) has recommended the following method to calculate these three parameters.

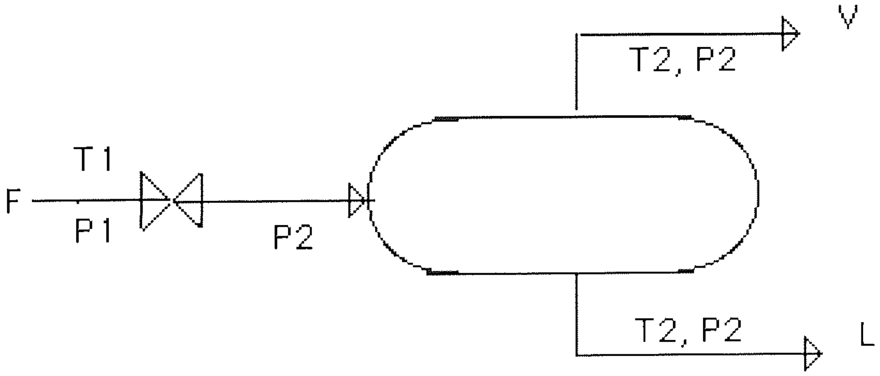


Figure (A1-3) Equilibrium flash separator

A1-3-1 Checking the presence of the two phases in the feed

A- Finding out if the feed is subcooled liquid, by applying the following equation:

$$F(\frac{V}{F}) = \sum_{i=1}^{N} Z_i (K_i - 1) \qquad \text{----------(A1-36)}$$

N = Number of compounds in the feed
V = Flow of the outlet vapour (kmole/hr)
Z_i = Mole fraction of each compound in the feed
K_i = Equilibrium constant of each compound
F = The molar flow rate of the feed (kmole/hr)

If F(V/F) is negative, that means the feed is subcooled liquid.

B- Finding out if the feed is superheated vapour by the following equation

$$F(\frac{V}{F}) = \sum_{i=1}^{N} \frac{Z_i\,(K_i - 1)}{(K_i - 1) - 1} \qquad \text{----------(A1-37)}$$

If F(V/F) is positive, that means the feed is superheated liquid

A2-7-2 Calculate the ratio of the vapour to the feed (V/F) from the following equations

$$F(\frac{V}{F}, T) = \sum_{i=1}^{N} \frac{Z_i\,(K_i - 1)}{(K_i - 1)\frac{V}{F} + 1)} \qquad \text{----------(A1-38)}$$

$$\bar{F}(\frac{V}{F}, T) = \sum_{i=1}^{N} \frac{Z_i\,(K_i - 1)^2}{((K_i - 1)\,\frac{V}{F} + 1)^2} \qquad \text{----------(A1-39)}$$

The above two equations have to be solved by trial and error calculations, after assuming the outlet liquid and vapour temperature.

A2-3-3 Calculation the outlet vapour and liquid compositions

This could be done by applying the following two equations.

$$Y_i = \frac{K_i\,Z_i}{(K_i - 1)\frac{V}{F} + 1} \qquad \text{----------(A1-40)}$$

$$X_i = \frac{K_i}{(K_i - 1)\frac{V}{F} + 1} \qquad \text{----------(A1-41)}$$

A1-3-4 Checking the assumed temperature

The assumed temperature should be checked, to see if it is correct or not, by enthalpy balance, as follows.

A-Calculate the cooling effect:- This effect due to the vaporization of some compound.

$$CE = \sum_{i}^{N} (Y_i\,L_i\,M_i)V \qquad \text{----------(A1-42)}$$

B-Calculate the heating effect:- This effect is due to the reduction of the pressure of the feed.

$$HE = \Delta P\, F1 \qquad \text{----------(A1-43)}$$

where

CE = Cooling effect (kJ/hr)
L_i = Heat vaporization of each compound (kJ/kg)
M_i = Molecular weight of each compound
HE = Heating effect (kJ/hr)
ΔP = Change in pressure (atm)
F1 = Mass flow rate of the feed (kg/hr)

C- Calculation the net temperature change:-

$$\Delta T = \frac{HE - CE}{CP_{sel}\ L_{sel}} \qquad \text{----------(A1-44)}$$

If ΔT is approximately equal to the difference between the assumed temperature and the feed temperature. This means the assumed temperature is correct, otherwise another assumption has to be made, and the calculations have to be repeated.

Normally the residence time of the solvent in the tanks is assumed to be three minutes and the tank is running half full to ensure complete disengagement of the gas from the liquid. According to the above equations a computer program has been made and applied to the high pressure and low pressure flash tanks. Tables (A1-2) and (A1-3) show the design parameters of those tanks. The list of that program is shown in Appendix 3 (program B).

A1-4 Calculation the Actual Recycle

As shown before, the flow and compositions of the vapour from the high pressure flash tank were arbitrary assumed, so the actual values have to be calculated, and all design parameters must be recalculated according to the actual recycle value. Trial and error calculations have been made after merging the design programs of the absorber and the high pressure flash tank. The output of that calculation is shown in table (4-3)

A1-5 Stripper Design

The stripper, which is used to regenerate the solvent for reuse, is a similar column to the absorber. The design procedure of this column is the same as for absorber which includes the following steps.

A- First estimation of the steam flow rate

B- Calculation of the required diameter

C- Calculation of the mass transfer coefficients (H_G, H_L)

D- Finding out the optimum stripping factor ($S=L_1/mG_2$)

E- Repeat the steps A, B and C using the calculated optimum (S)

Program A was adapted and used to calculate the design parameter of the stripper. Table (A1-4) shows the output of that program and figure (A1-2) shows the relationship between the stripping factor and the height of the packed material. From this figure the optimum stripping factor has been chosen as (S = 0.8)

Fig. (A1-2) The relationship of the stripper height to the stripping factor

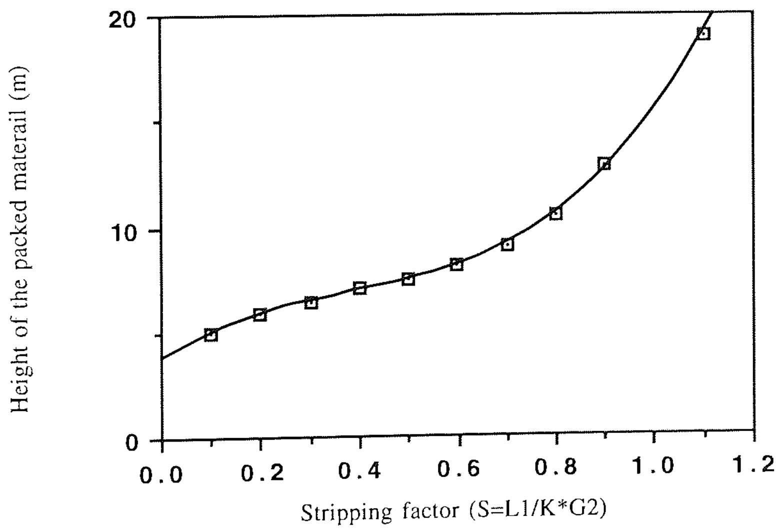


Table (A1.1) The calculated design parameters of the absorber by using Selexol for Configuration (1)

```
           VAPOUR DATA                                      LIQUID DATA
           -----------                                      -----------

   FLOW(kg/hr)        = 102944.6                             621104.8
   DENSITY(kg/m3)     = 66.59867                             1021.003
   VISCOSITY(cP)      = .011                                 5.8
   MOL. WT.           = 19.27142                             278.82

                              TOWER DIAMETER
                              --------------

   PACKING FACTOR= 52
   DP/M(mm.H2O)  = 20
   The calculated diameter(m)= 2.980944

 I          Y              X               HOG           A.U.the curve
 --       -----          -----           -----          -------------
 1        .11065         .1516714        11.18348          582.3365
 2        .1066175       .1453179        11.33309          596.5487
 3        .102585        .1388745        11.48397          609.476
 4        .0985525       .1323391        11.6362           620.9424
 5        .09452         .1257098        11.78983          630.7885
 6        .0904875       .1189845        11.94485          638.8729
 7        .086455        .1121611        12.10134          645.0862
 8        .0824225       .1052375        12.25935          649.3511
 9        .07839         9.821152E-02    12.41891          651.6214
 10       .0743575       9.108076E-02    12.58011          651.8922
 11       .070325        8.384291E-02    12.74295          650.1915
 12       .0662925       7.649552E-02    12.90751          646.5831
 13       .06226         6.903609E-02    13.07384          641.163
 14       .0582275       6.146206E-02    13.242            634.0534
 15       .054195        5.377075E-02    13.41202          625.3965
 16       .0501625       4.595941E-02    13.58399          615.3544
 17       .04613         .0380252        13.75795          604.0956
 18       .0420975       2.996523E-02    13.9331           591.7584
 19       .038065        2.177646E-02    14.11163          578.6074
 20       .0340325       1.345579E-02    14.29237          564.7585
 21       .03            5.000002E-03    14.47534          550.371

   The height of the packed material (m)= 15.25977
```

Table (A1-2) High pressure flash tank design parameters
using Selexol for Configuration (1)

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.151671	.2614112	.1375163
2	1.663262E-02	3.820774E-03	1.828514E-02
3	.1128	.7347647	3.257683E-02
4	.7188962	4.058107E-06	.8116214

The feed flow rate (Kmol/hr) = 3083.172542198472
The vapour flow rate (Kmol/hr) = 352.2446243584015
The liquid flow rate (Kmol/hr) = 2730.927945525152

Component (1) = CO2
Component (2) = H2S
Component (3) = CH4
Component (4) = Selexol

The Volume of the tank (m3) = 62.8939

Table (A1-3) Low pressure flash tank design parameters using Selexol for Configuration (1)

Comp.	Feed comp.	Vapour comp.	Liquid comp.
1	.1375163	.7466059	2.907411E-02
2	1.828514E-02	4.121056E-02	.0142035
3	3.257683E-02	.2122036	5.961197E-04
4	.8116214	4.780607E-06	.9561215

The feed flow rate (Kmol/hr) = 2730.999926736211
The vapour flow rate (Kmol/hr) = 412.7421468010962
The liquid folw rate (Kmol/hr) = 2318.25789067544

Component (1) = CO2
Component (2) = H2S
Component (3) = CH4
Component (4) = Selexol

The volume of the tank (m3) = 62.0965

Table (A1-4) The calculated design parameter of the stripper by using Selexol for Configuration (1)

```
          VAPOUR DATA                        LIQUID DATA
          -----------                        -----------

 FLOW(KG/HR)       = 8143.824874580528       624753.59512964
 DENSITY(LB/FT3)   = 1.06437                 1021
 VISCOSITY(CP)     = .03122                  1.07
 MOL. WT.          = 27.44187                276.8642

                              TOWER DIAMETER
                              --------------

 PACKING FACTOR          = 52
 DP/M(mm.H2O)            = 20
 The calculated diameter (meter)= 2.514659

I          Y              X              HOG          A.U.the curve
---      -----          -----           -----         -------------

1        .1106445       1.418106E-02    4.883725         34.67828
2        .1051123       1.316557E-02    4.469179         36.83654
3        9.958009E-02   1.219544E-02    4.130196         39.29166
4        9.404787E-02   1.126769E-02    3.846682         42.09762
5        8.851564E-02   1.037961E-02    3.605363         45.32233
6        8.298341E-02   9.528697E-03    3.397062         49.05256
7        7.745118E-02   8.712676E-03    3.215202         53.40054
8        7.191896E-02   7.92944E-03     3.05478          58.51111
9        6.638673E-02   7.177052E-03    2.912137         64.58086
10       .0608545       6.453726E-03    2.784422         71.87778
11       5.532227E-02   5.757808E-03    2.669374         80.77695
12       4.979005E-02   5.087772E-03    2.565148         91.81798
13       4.425782E-02   4.442198E-03    2.470244         105.8083
14       3.872559E-02   3.819773E-03    2.383517         124.0145
15       3.319336E-02   3.21927E-03     2.303867         148.522
16       2.766114E-02   2.639554E-03    2.230528         183.0526
17       2.212891E-02   2.079564E-03    2.162763         234.9101
18       1.659668E-02   1.538308E-03    2.099977         320.6663
19       1.106445E-02   1.014863E-03    2.041644         487.6118
20       5.532227E-03   5.083636E-04    1.987228         946.1619
21       0              .000018         1.936751         7169.684

 The height of the packed material (m) = 9.791991
```

A1-6 Heat Transfer Equipment Design

The process of separating carbon dioxide and hydrogen sulfide from methane is one of the processes that needs a large quantity of energy to cool (or heat) the solvent to the temperatures of the absorption and desorption processes. It was seen in figure (4-1) that there were four different types of heat exchangers. The first one is a cooler to reduce the temperature of the solvent to the required absorption temperature, the second one is an economizer to save some energy by transfer of heat from the hot stream to the cooled one, the duty of the third one is to heat the solvent to the stripping temperature by using saturated steam at (3.4) atm, the final one is the condenser which is used to separate the stripped gases from the steam that is used as a stripper to recycle it to the process.

A1-6-1 Cooler Design

The duty of the cooler is to cool the solvent from 71°C to 21°C by using cooling water.

The flow rate of Selexol = 621094 kg/hr

Its average viscosity (μ_{sel}) = 15.2868 - 0.4059t + .0032t^2 (CP)

Its average density (P_{sel}) = 1021 kg/m^3

Its average specific heat (CP_{sel}) = 2.47 kJ/kg K

Its average thermal cond. (K_{sel}) = 0.17307 w/m K

The chosen water temperature rise is 15°C

The chosen pipe dimensions are 20 mm OD , 16 mm ID and 10 m long

Fouling factor for the Selexol is 5000 w/m^2K

Fouling factor for the water is 6000 w/m^2K

Carbon steel is sufficient for this heat exchanger, Its thermal conductivity (K_m = 45 w/m K)

The water viscosity (μ_W) = 1.7651 - .0475t + 5.846E-4t^2 - 2.6E-6t^3

Its average density (P_w) = 995 kg/m^3

Its average sp. heat (CP_w) = 4.2 kJ/kg K

Its average thermal cond. (K_w) = .59 w/m K

A1-6-1-1 Fluid allocation

If no phase change occurs either in the tube- or shell-side, the following factors determine the allocation of each stream.

(a) Corrosion: The most corrosive fluid should be allocated in the tube side.

(b) Fouling: The fluid that has the greatest tendency to foul should be in the tubes.

(c) Fluid temperature : Generally the higher temperature preferable to be placed in the tubes.

(d) Operating pressure :The higher pressure preferably to be placed inside the tube.

According to these factors, the water has been placed in the tubeside.

A1-6-1-2 First estimation of the number of tubes and inside shell diameter

(a) Calculation of the heat load:-

$$Q = m_s \ CP_s \ \Delta t_s \qquad \text{----------(A1-45)}$$

where Q = Heat transfer per unit time (W)

m_s = Mass flow rate of the solvent (kg/s)

CP_s = Specific heat of the solvent (kJ/kg K)

Δt_s = Solvent temperature difference (K)

(b) Calculation of the flow of the cooled water:-

$$m_W = Q/CP_W \ \Delta t_W \qquad \text{----------(A1-46)}$$

m_W = water flow rate (kg/s)

Δt_W = water temperature difference (K)

(c) Calculation the true temperature difference:-

$$\Delta t_{LM} = (\Delta t_S - \Delta t_W)/\ln(\Delta t_s / \Delta t_W) \qquad \text{-----(A1-47)}$$

$$R = \frac{THi - THo}{TCo - TCi} \ , \quad S = \frac{TCo - TCi}{THi - TCi} \qquad \text{----------(A1-48)}$$

R, S = Dimensionless ratios

Δt_{LM} = Log mean temperature (K)

Δt_m = FT Δt_{LM} ------(A1-49)

FT = Correction factor which can be found from figure (12-19)/43/page 531

Δt_m = True temperature difference

(D) First estimation of the number of the tubes:-

A = Q/ Δt_m U -------(A1-50)

A = Total heat transfer area (m^2)

U = Assumed overall heat transfer coefficient (w/m^2 K)

N = A/A1 -------(A1-51)

N = Number of tubes

A1 = Heat transfer area for one tube (m^2)

(E) Ist estimation of the inside shell diameter:-

$$BD = OD \left(\frac{N}{k1}\right)^{1/n1}$$ ----------(A1-52)

k1, n1 = Constants depending on the tube sheet layout

BD = Tube bandle diameter (m)

From figure (12-10)/43/552 and after choosing the type of the shell head, the clearance between the tube bandle and the inside shell diameter can be found.

SID = DCL + BD --------(A1-53)

SID = Inside-shell diameter (m)

DCL = Clearance between the tube-bandle and the shell (m)

A1-6-1-3 Calculation of the tubeside heat transfer coefficient

(a) For turbulent flow:- (when Re > 6000)

$$Nu = .023\ Re^{.8}\ Pr^{.3} \left(\frac{\mu}{\mu_w}\right)^{.14}$$ ----------(A1-54)

(b) For laminar flow:- (when Re < 2000)

$$Nu = 1.86\,(Re\,Pr)^{.33}\left(\frac{d_e}{L}\right)^{.3}\left(\frac{\mu}{\mu_w}\right)^{.14} \qquad \text{----------(A1-55)}$$

L = Length of the tube (m)
d_e = Equivalent diameter (m)
μ = Viscosity of the solvent at the bulk temperature (cP)
μ_w = Viscosity of the solvent at the wall temperature (cP)

(c) For transition region:- (2000 < Re > 6000)

This should be avoided, if this is not practicable the coefficients should be evaluated using both equations (turbulent and laminar) then the lesser value should be used.

(d) Viscosity correction factor:-

$$H_i\,(t_w - t) = U\,(T - t) \qquad \text{----------(A1-56)}$$

t = Tube side bulk temperature (°C)
T = Shell side bulk temperature (°C)
t_w = Wall temperature (°C)
H_i = Tube side heat transfer coefficient (w/m^2K)

Trial and error calculations can be made to calculate the exact value of the tube side heat transfer coefficient (H_i)

A1-6-1-4 Calculation of the shellside heat transfer coefficient

(a) Calculation of the area for cross flow:-

$$A_s = \frac{(P_t - OD)\,SID\,L_B}{P_t} \qquad \text{----------(A1-57)}$$

A_s = Cross-flow area (m^2)
P_t = Tube pitch (m)
L_B = Baffle spacing (m)

(b) Calculation of the shellside mass velocity and linear velocity:-

$$G_S = \frac{W_S}{A_S}\ , \qquad U_S = \frac{G_S}{DL} \qquad \text{----------(A1-58)}$$

W_s = Fluid flow rate on the shell side (kg/s)
U_s = Linear fluid velocity (m/s)

(c) Calculation of the shell equivalent diameter:-

$$d_e = \frac{1.1}{OD}(P_t^2 - .917\,OD^2) \qquad \text{----------(A1-59)}$$

(d) Calculation of the shell side Reynolds number:-

$$Re = G_s\, d_e/\mu = U_s\, d_e\, D_L/\mu \qquad \text{-------(A1-60)}$$

Then find out the value of heat transfer coefficient (J_h) from figure (12-29)/43/page 546 after choosing the baffle cut (commonly 25%)

(e) Calculation of the outside heat transfer coefficient (H_O):-

$$Nu = Jh\, Re\, Pr^{1/3}\left(\frac{\mu}{\mu_w}\right)^{.14} \qquad \text{----------(A1-61)}$$

At the first trial H_O is calculated without correction the wall temperature. Then trial and error can be made after calculation the wall temperature, by the following equation

$$t_w = T - \frac{U}{H_O}(T - t) \qquad \text{----------(A1-62)}$$

A1-6-1-5 Calculation of the overall heat transfer coefficient

$$\frac{1}{CU} = \frac{1}{H_O} + \frac{1}{HOD} + \frac{OD\, Lin(\frac{OD}{ID})}{2\, K_w} + \frac{OD}{ID} \times \frac{1}{HID} + \frac{OD}{ID} \times \frac{1}{H_i} \qquad \text{----------(A1-63)}$$

The calculated (CU) must approximately equal the assumed (U) otherwise another trial should be made after assuming U = CU

A1-6-1-6 Calculation of the pressure drop in the tubeside

$$\Delta P_t = N_p\left[8\, Jf\left(\frac{L}{ID}\right)\left(\frac{\mu}{\mu_w}\right)^{.14}\right]\frac{P\, U_S^2}{2} \qquad \text{----------(A1-64)}$$

ΔP_t = Tube side pressure drop (N/m^2)
N_p = number of passes
Jf can be found from figure (12-24)/43/page 541

A1-6-1-7 Calculation of the pressure drop in the shellside

$$\Delta P_S = 8\ Jfs\ (\frac{SID}{d_e})\ (\frac{L}{L_B})\ \frac{DL\ U_S^2}{2}\ (\frac{\mu}{\mu_w})^{-.14} \qquad \text{----------(A1-65)}$$

Jfs can be found from figure (12-30)/43/page 547

According to the above procedure, a computer program has been written, to calculate the design variables of the required cooler. The outcome of that program is shown in Table (A1-5).

Table (A1-5) The design variables of the cooler

Process variable		**Tubeside**	**Shellside**
Type of fluid		Water	Selexol
Mass flow rate	(kg/hr)	996828	620555
Inlet temperature	(°C)	15	71
Outlet temperature	(°C)	30	27
Average viscosity	(cP)	.963	3.2
Average sp. heat	(kJ/kg K)	4.2	2.3
Average therm. cond.	(W/m K)	.59	.1731
Average density	(kg/m^3)	995	1021
Fouling factor	(W/m^{2}K)	6000	5000
Inside diameter	(m)	.016	1.2
Outside diameter	(m)	.02	1.4
Number of passes		2	1
Reynolds number		24664	2375
Heat transfer coeff.	(W/m K)	5285	1189
Pressure drop (bar)		1.0	0.5

Total heat transfer area = 1166 m^2
Number of tubes = 1853
Overall heat transfer coefficient = 647 W/m K

A1-6-2 Economizer Design

The duty of this equipment is to transfer the heat from the hot stream (which comes out from the stripper) to the cooled stream (which comes out from the low pressure flash tank). The procedure of design is, more or less, similar to that of the cooler. The design dimensions and the other parameters are shown in Table (A1-6)

Table (A1-6) The design variables of the economizer

Process variable		**Tubeside**	**Shellside**
Type of fluid		Selexol	Selexol
Mass flow rate	(kg/hr)	624740	620555
Inlet temperature	(°C)	24	127
Outlet temperature	(°C)	82	71
Average viscosity	(cP)	3.31	0.94
Average sp. heat	(kJ/kg K)	2.2	2.3
Average ther. Cond.	(W/m K)	.17307	.17307
Average density	(kg/m^3)	1021	1021
Fouling factor	(W/m^{2}K)	5000	5000
Inside diameter	(m)	.046	2.6
Outside diameter	(m)	.05	2.8
Number of passes		8	1
Renoyld number		8761	33610
Heat transfer coeff.	(W/m K)	406	1261
Pressure drop (bar)		.17	1.18

Total heat transfer area = 2082 m^2
Number of tubes = 1323
Overall heat transfer coefficient = 244 W/m K

A1-6-3 Heater Design

The duty of this exchanger is to heat the Selexol to the stripping temperature, before it goes inside the stripper. Saturated steam has been used as heating fluid. The typical value of the condensation film heat transfer coefficient which is used for this design was 8000 W/m^{2}K (1500 Btu/hr ft^2 F). The design dimensions and the other parameters are shown in Table (A1-7)

Table (A1-7) The design variables of the heater

Process variable		**Tubeside**	**Shellside**
Type of fluid		Steam	Selexol
Mass flow rate	(kg/hr)	33890	624740
Inlet temperature	(°C)	138	82
Outlet temperature	(°C)	138	126
Average viscosity	(cP)	.014	.81
Average sp. heat	(kJ/kg K)	1.9	2.61
Average therm. cond.	(W/m K)	.027	.17307
Average density	(kg/m^3)	1.88	1021
Fouling factor	(w/m^{2}K)	6000	5000
Inside diameter	(m)	.016	1.0
Outside diameter	(m)	.02	1.2
Number of passes		2	1
Renoyld number		83996	14310
Heat transfer coeff.	(W/m K)	8000	2102
Pressure drop (bar)		0.5	0.98

Total heat transfer area = 801 m^2
Number of tubes = 1274
Overall heat transfer coefficient = 915 W/m K

A1-6-4 Condenser Design

This condenser condenses the stripping steam that comes out from the stripper and separates it from the uncondensable gases (CO_2, H_2S and CH_4) by using cooling water. The rules that have been suggested by Frank were recommended by Sinnott (43). These rules suggested ignoring of the presence of the uncondensable gases if their proportion is less than 50%. The design dimensions and the other parameters are shown in Table (A1-8)

Table (A1-8) The design variables of the condenser

Process variable		**Tubeside**	**Shellside**
Type of fluid		Water	Gases mixture
Mass flow rate	(kg/hr)	3285	7660
Inlet temperature	(°C)	20	127
Outlet temperature	(°C)	35	50
Average viscosity	(cP)	.96	.0144
Average sp. heat	(kJ/kg K)	4.2	.9
Average therm. cond.	(W/m K)	.59	.0173
Average density	(kg/m^3)	995	1.1
Fouling factor	(W/m^{2}K)	6000	6000
Inside diameter	(m)	.016	.5
Outside diameter	(m)	.02	.7
Number of passes		2	1
Renoyld number		114	30973
Heat transfer coeff.	(W/m K)	453	154
Pressure drop (bar)		.02	.01

Total heat transfer area = 10.4 m^2
Number of tubes = 165
Overall heat transfer coefficient = 103 W/m K

A1-7 Cost Estimation

Simple costing methods, which can be used to make a preliminary estimate of the cost at the flow sheet stage, have been used for this work. The emphasis here has been made on the cost of the major equipment and just the items of the operating cost that are affected by changing of the solvent. As seen in figure (4-1), the main equipment were absorber, stripper, flash tanks, heat exchangers and compressor. The main operating items that were considered in this work are the electricity power consumption by the compressor, the steam consumption for stripping and heating, cooling water and the cost of the solvent loss.

A1-7-1 Capital Cost Estimation

This cost includes the cost of the vessels (absorber, stripper and flash tanks), heat exchangers and compressor. The vessels are usually designed in accordance with the current ASME pressure vessel codes. They are usually cylindrical shells capped by two elliptical heads. The methods given by Garrett (12) were used to estimate their cost. Figure A1/12/page 268 relates vessel diameter to the cost of the unit length of the column. Wall thickness is included in the pressure factor. The base cost represents pressure vessel fabricated in carbon steel to resist 3.4 atm (50 psia) internal pressure with average nozzles, manways and supports. Factors can be used to adjust for other shell materials, and pressure up to 340 atm. Packed beds are priced separately and added to the shell cost by using figure A2/12/page 270.

The cost of the field materials (piping, concrete, instrumentation, insulation, etc.), field labour and other indirect cost (taxes, insurance, temporary facilities, importing duties, etc.) will not be considered in these calculations because they may be represented by a factor (called the Lang factor) from the cost of the major equipment. Usually a factor of 4.5 times the fob. cost is used for preliminary cost estimation.

The time-base of the figures given by Garrett (12) is based on mid 1987, so these costs have to be converted to mid 1993, this can be done by the following equation.

$$\text{Cost in year A} = \text{cost in year B} = \frac{\text{cost index in year A}}{\text{cost index in year B}} \qquad \text{(A1-66)}$$

or $\quad$ Cost in 1993 = Cost in 1987* IR

where $\quad$ $\text{IR} = \frac{\text{cost index in 1993}}{\text{cost index in 1987}}$

A1-7-1-1 Absorber/Stripper Cost

The cost of the column includes the cost of the vessel and the cost of the packed material.

(a) Vessel cost:-

Diameter	= 3 m	≈ 10 ft
Packing height	= 15.26 m	≈ 50 ft
Total height	= 50 + 0.2 * 50	= 60 ft

The following equation represents the best fitting equation for the cost graph given by Garrett/pp-268.

The cost ($) per foot $= 139.4 + 195.09D - 25.731D^2 + 1.8775D^3$

$= 1394.7$ at mid 1987

Total basic cost $= 1394.7 * 60 =$ $ 83682

Adjust for material, pressure and escalation

Correction factor for carbon steel = 1

Correction factor for 68 atm pressure = 4.2

Expected cost at mid 1993 = 83682 * 1 * 4.2 * IR

= $ 351464 * IR

(b) Packing cost :-

The cost of the packing material = 17.5 $\$/ft^3$ (figure A2/12/page 270)

The volume of the packed materia = $(\pi/4) * 100 * 50 = 3927\ ft^3$

The total cost of the absorber = \$351464.4 * IR + 17.5 * 3927 *IR

= \$420187 * IR at mid 1993

The same procedure has been used to calculate the cost of the stripper

The total cost of the stripper = \$70325 * IR

A1-7-1-2 Flash Tanks Cost

This includes the cost of the high pressure and the low pressure tanks.

(a) High pressure tank:-

The volume = 63 m^3

Assume (L/D) = 4

So, D = 2.717 m ≈ 9 ft

L = 10.867m ≈ 35.6 ft

The minimum acceptable thickness = 10 mm for this size of tank, Sinnott, (43)

The volume of the metal = $\pi * 9 * (10 /(25.4*12)) * 35.6$

= 33.024 ft^3

The weight of the vessel = 33.024 * (7700/16.1) =15804 Lb

From cost figure, the cost = \$ 32000 (figure A3/12/page 298)

Adjust for material, pressure and escalation

Correction factor for carbon steel =1

Correction factor for the pressure = 2

Expected cost at mid 19993 = 32000 * 2 * IR = 64000 * IR

(b) The same procedure has been used for the low pressure flash tank and the result = 32000 * IR

A1-7-1-3 Heat Exchangers Cost

Figure A3/12/page 286 is based on a floating-head construction with carbon steel shell and tubes. The cost is related directly to the heat transfer area. Some corrections have to be made to adjust for design type, material of construction and design pressure

(A) Cooler cost estimation:-
Heat transfer area = 1166 m^2 = 126551 ft^2
From figure A3/12/ page 286 the cost = \$125000 at mid 1987

Adjust for the type, material and escalation
Correction factor for the type = 1
Correction factor for the material = 1
Expected cost at mid. 1993 = \$125000 * IR

The same procedure has been used to calculate the cost of the other heat exchangers.

The cost of the economizer = \$190414 * IR
The cost of the heater = \$99450 * IR
The cost of the condenser = \$5000 * IR

A1-7-1-4 Compressor Cost

Figure A5/12/page-272 is based on field-assembled cost for centrifugal machines with motor drive range from 200-5000 hp. Factors are included to adjust for other compressor/driver combinations; carbon steel is assumed in all applications.

Flow of the recycle gases (RC) = 204 ft^3/min before compression
HP = $0.0044 * P_1 * Q_1 * \ln(P_2/P_1)$
= 324
HP = horse power
P_1 = inlet pressure (300 psi)
Q_1 = inlet flow rate (204 ft^3/min)
P_2 = outlet pressure (1000 psi)

From figure A4/12/page 272 the cost = \$105000 at mid 1987
Adjust for design type and escalation
Correction factor for type = 1
Expected cost at mid 1993 = \$105000 * IR

A1-7-2 Operating Cost Estimation

Estimation of the operating cost is needed to judge the viability of a project and to make choices between possible alternatives process schemes. The operating cost can be estimated approximately, at the flow-sheet stage. Generally, the operating cost can be divided into two groups.

1- Fixed group:- This group includes the cost of the items that are not affected by the rate of production, such as maintenance, operating labour, laboratory costs, etc.

2- Variable group:- This includes the cost of the items that vary with the product rate, such as raw material, miscellaneous operating material, utilities, etc.

The carbon dioxide separation unit is only a part of a larger plant, this means the items of the fixed groups are almost the same for different physical properties of the solvent. But some of the items of the variable group are depended upon the physical properties; such as (a) the steam which is used for the stripping and heating processes, (b) the cooling water which is used to cool Selexol before it goes in the absorber and to condense the stripping steam, (c) the electrical power required for running the compressor and the pumps, and (d) the solvent loss.

In this work, the cost which is required to circulate the solvent within the unit (pumping cost) will not be considered as a major cost item. We will consider only the effects of the varying the required quantity of steam, cooling water, solvent loss and electricity for the compressor, on the operating cost, because the other items would not make a significant difference on the operating cost.

We assume that the operating cost of the process can be represented by the annual cost of the steam consumed for stripping and heating, cooling water, solvent loss and energy for compression.

A1-7-2-1 Compressing Power Cost

Horse power = 324

Electricity cost = 0.08 $ /kW hp

Annual power cost = (0.08 $ /kW hp)(0.7457 kW/hp)(24 * 300) * 324
= 139166 $/year

A1-7-2-2 Stripping Steam Cost

Steam cost = 0.0221 $/kg
Consumed steam = 3478 kg/hr
Annual stripping steam cost = 553419 $/year

A1-7-2-3 Heating Steam Cost

Consumed steam = 33890 kg/hr
Annual heating steam cost = 5392577 $/year

A1-7-2-4 Cooling Water Cost

Cooling water cost = 0.044 $/1000 kg
Consumed cooling water = 996828 kg/hr
Annual cooling water cost = 315795 $/year

A1-7-2-5 Solvent Loss Cost

Solvent loss cost = 9.65 $/ kg
Consumed solvent = 0.5 kg/hr (from material balance
around the condenser)
Annual solvent loss cost = 34740 $/year

A1-7-3 Total Process Cost Calculation

In this work, the calculation of the total process cost was based on amortisation of the total capital cost. The capital cost can be estimated from the cost of the major equipment which are required for the process. Lang (43) suggested the following simple equation to calculate the capital cost ones the preliminary flow-sheet has been drawn up and the main items of the equipment have been sized.

$$C_f = f_L C_e \qquad \text{............ (A1-66)}$$

where C_f = Fixed capital cost
C_e = The total cost of the equipment
f_L = the "Lang factor" which is depends on the type of the process,
= 3.1 for predominated solid processing plant
= 4.7 for predominated fluids processing plant
= 3.6 for a mixed fluid-solid processing plant

The values of f_L were suggested by Sinnott (43) and could be used as a guide, but it is best to derive these values from an organisation's own cost files. The Lang factor is a rough estimation of the cost of following items.

- Equipment erection, which includes foundations and any related structural work.
- The site and its preparation, which includes ancillary buildings, offices, laboratory buildings, workshops, stores, process buildings and structures.
- Piping together with their insulation and paint.
- Electrical power and process control instrumentation.

Physical gas absorption processes are predominated liquid processes, so f_L=4.7 will be used in this work. To amortize the capital cost, the pay-back time for the process considered has to be set. The pay-back time is the time required after the start of the project to pay off the initial investment from income. Typically, a pay-back time of 2 to 5 years would be expected for this type of project. In this work, a pay-back time of 3 years was considered.

$$\text{Amortized total capital cost} = \text{T. E. C.} * f_L \ / \ \text{PBT} \qquad \text{......(A1-67)}$$

where T. E. C. = Total equipment cost ($)
PBT = Pay-back time (year)

The operating cost of a chemical process plant is the summation of many cost items, such as raw material, utility services, maintenance, operating labour, laboratory operation, taxes, insurance, etc. In physical gas absorption processes most of these items are not related to the type of the solvent used. Only the running cost items which are affected by the type of the solvent were considered.

Normally, the economic evaluation of any chemical plant project can be made by estimating the net profit, which represents the difference between the earnings and expenditure. The earnings depend on the quantity and the quality of the product. In physical gas absorption processes, the rate and the quality of the gas product can be kept constant, when different solvents are used, by changing the rate of the circulated solvent and the size of the compressor. This means that the earnings are the same by using different solvents, but the expenditure will vary. So, if the purpose is just to compare between two solvents, the total cost of a physical gas absorption process can be represented by the expenditure.

The above discussion suggests that the total process cost can be calculated from the following equation.

$$\text{T. P. C.} = \text{T. E. C.} * f_L / \text{PBT} + \text{T. R. C.} \qquad \text{................(A1-68)}$$

where T. P. C. = Total process cost (£/y)

T. R. C. = Total running cost (£/y)

APPENDIX TWO

Estimation of the Physical Properties

A2-1 Thermal Conductivity Estimation

The following three methods of estimation were recommended by Reid et al. (40) .

1- Latini et al. method.

2- Sato- Riedel method.

3- Missenard method.

The techniques of these methods were illustrated by Reid et al. (40) in details. The first method has been chosen for this work, as there is no limitation and the percentage of error is lower compared with the other two methods. Latini and his co-worker's formulated the following correlation to calculate the thermal conductivity of any liquid.

$$KL = \frac{A(1 - T_r)^{.38}}{T_r^{1/6}} \qquad \text{(A2 - 1)}$$

$$A = \frac{A^* T_b^\alpha}{M^\beta T_c^\gamma}$$

where KL = The thermal conductivity of the solvent, W/m K

T_b = The normal boiling point K,

T_c = Critical temperature K

M = Molecular weight.

$A^* = 0.00383$, $\alpha = 1.2$, $\beta = 0.5$, $\gamma = 0.167$

These parameters are given in Table (10-6)/40/page 550

So, the thermal conductivity of B2 (KL) = 0.114 eqn. (A2-1)

A2-2 Heat Capacity Estimation

Two group-contribution techniques have been recommended by Reid el at. (40) to estimate the specific heat of a liquids. The first one is Chueh-Swanson's method which is used to estimate the specific heat at room temperature, while Missenard's method is valid for a range of temperatures between -25°C and 100°C . Those two methods assumed that the contribution of various groups in a molecule to the total heat capacity is independent of other groups present. The heat capacities of most chemical groups are shown in Tables (5-10) and (5-11) page 138 Reid el at. (40).

The specific heat of B2 at 50°C can be estimated by using the data of the above mentioned tables.

$$CP = 2(CH_3-) + 2(CH_2-) + 2(CO-)$$

$$= 2(43.5) + 2(29.1) + 2(44.4) = 234 \text{ J/m K} = 2.11 \text{ kJ/kg K} \quad \text{at } 50^{o}C$$

A2-3 Estimation of the Equilibrium Constants

The solubilities of CO_2, CH_4 and H_2S in all the selected solvents (except B2 and Selexol) at desorption conditions have been predicted by using Sitthiosoth's program (44), while the solubilities of these gases at absorption conditions were given by Zawacki (60) as an experimental data. The solubilities of the gases in the Selexol at absorption and desorption conditions were obtained by private communications and for B2 were given by Sitthiosoth (44).

A2-4 Viscosity Estimation

The Andrade equation is considered the simplest method to predict the viscosity at any temperature below the boiling point of a liquid.

$$\ln \mu_L = A + \frac{B}{T} \qquad \text{(A2-2)}$$

The equation requires at least two viscosity-temperature data points to determine the two constants. If only one data point is available, one of the few ways to extrapolate this value is to employ the approximate Lewis-Squires Chart, Figure (9-14)/44/page 440, which is based on the empirical fact that the sensitivity of the viscosity to the temperature variations appears to depend primarily upon the value of the viscosity. That chart has been expressed in an equation form as,

$$\mu_L^{-.2661} = \mu_K^{-.2661} + \frac{T - T_K}{233} \qquad \text{(A2-3)}$$

where μ_L = Liquid viscosity at T, cP

μ_K = Known value of the liquid viscosity at T_K, cP

APPENDIX THREE

The Computer Program Lists

PROGRAM (A)

PROGRAM LIST FOR ABSORBER DESIGN

```
LPRINT "Table (A1-1) The calculated Design parameters of the"
LPRINT " absorber by using Selexol for configuration (1)"
LPRINT
DIM Y(100), N(100)
INPUT "HOW MANY INTEGRATION INTERVALS"; IN
READ Y1, Y2, X2, G1
READ S, Z1
GOSUB 1000
GOSUB 2000
GOSUB 3000
G2 = (1 - Y1 * RPHI) * G1 / (1 - Y2 * RPHI)
X1 = ((G2 * (1 - Y2 * RPHI) * Y1) + (L2 * X2 - G2 * Y2) *
(1 - Y1 * RPHI)) / (L2 * (1 - Y1 * RPHI) + RPHI * G2 *
(Y1 - Y2))
LPRINT TAB(11); "I"; TAB(21); "Y"; TAB(36); "X"; TAB(49);
"HOG"; TAB(60); "A.U.the curve"
LPRINT TAB(10); "---"; TAB(19); "-----"; TAB(34); "------";
TAB(48); "------"; TAB(60); "-------------"
DY = (Y1 - Y2) / IN
Y = Y1
FOR I = 1 TO IN + 1
GOSUB 340
YE = S * X
YEF = ((1 - Y * RPHI) - (1 - YE * RPHI)) / (LOG((1 - Y * RPHI)
/ (1 - YE * RPHI)))
HOG = YF * HG / YEF + S * GM * XF * HL / (LM * YEF)
INV = HOG * YEF / ((1 - Y * RPHI) * (Y - YE))
LPRINT TAB(10); I, TAB(16); Y; TAB(31); X; TAB(46); HOG;
TAB(62); INV
Y(I) = Y
N(I) = INV
Y = Y - DY
NEXT I
A = 0
FOR I = 1 TO IN + 1
IF I = 1 GOTO 310
IF I = IN + 1 GOTO 310
R = I / 2: R1 = INT(R)
IF R1 = R GOTO 300
A = A + 2 * N(I)
GOTO 310
A = A + 4 * N(I)
NEXT I (310)
A = DY * (A + N(1) + N(IN + 1)) / 3
LPRINT : LPRINT
LPRINT "The height of the packed material (M)="; A * .3048
L1 = L2 * (1 - X2) + MCH4 + MCO2 + MH2S - G2 * YSEL
XCO2 = MCO2 / L1: XH2S = MH2S / L1: XCH4 = MCH4 / L1: XSEL
= (L2 * (1 - X2) - KG2 * YSEL) / L1
END
X = (G2 * (1 - Y2 * RPHI) * Y + (L2 * X2 - G2 * Y2) * (1 -
```

```
Y * RPHI)) / (L2 * (1 - Y * RPHI) + RPHI * G2 * (Y - Y2)) (340)
GM = G2 * (1 - Y2 * RPHI) / (1 - Y * RPHI)
LM = L2 * (1 - X2 * RPHI) / (1 - X * RPHI)
C = -LM * HG / (GM * HL)
CHEK = O: CKF = C
XI = (Y - C * X) / (S - C) (490)
YI = XI * S
IF CHEK = O GOTO 530
IF ABS(YIC - YI) <= .00005 GOTO 590
YIC = YI
YF = ((1 - Y * RPHI) - (1 - YI * RPHI)) / LOG((1 - Y *
RPHI) / (1 - YI * RPHI))
XF = ((1 - X * RPHI) - (1 - XI * RPHI)) / LOG((1 - X *
RPHI) / (1 - XI * RPHI))
C = CKE: C = C * YF / XF
CHEK = 1
GOTO 490
RETURN
DATA .11065,.03,.005,11776.72
DATA .6,0
YCH4 = .8797563: YH2S = .0095924: XH2S = .000018:
VPS = .00088: P = 1000 (1000)
L2 = 4911.059: PRINT "L2="; L2
X1 = Y1 * .85 / S
KCH4 = 7.2748 - 4.645 * X1 - 2.445 * (X1 ^ 2)
XCH4 = YCH4 / KCH4: PRINT "XCH4="; XCH4
MCH4 = (XCH4 * L2 * (1 - X2)) / (1 - XCH4)
MH2S = YH2S * G1 + L2 * XH2S: PRINT "MH2S="; MH2S
PCH4 = G1 * YCH4 - MCH4: PRINT "PCH4="; PCH4
PCO2 = PCH4 * (.03 / .97): PRINT "PCO2="; PCO2
ACO2 = Y1 * G1 - PCO2: PRINT "ACO2="; ACO2
MCO2 = ACO2 + L2 * X2
YSEL = (VPS * 14.7) / (P * 760): PRINT "YSEL="; YSEL
G2 = (PCH4 + PCO2) / (1 - YSEL): PRINT "G2="; G2
PYCO2 = PCO2 / G2: PYCH4 = PCH4 / G2: PSEL = YSEL
PRINT "PYCO2="; PYCO2; "PYCH4="; PYCH4
RPHI = (ACO2 + MCH4 + G1 * YH2S - G2 * YSEL) / ACO2
PRINT "RPHI="; RPHI
L1 = L2 + ACO2 + YH2S * G1 + MCH4 - G2 * YSEL
MW1 = 16 * MCH4 / L1 + 44 * MCO2 / L1 + 34.06 * MH2S /
L1 + 280 * L2 * (1 - X2) / L1
PRINT "MW1="; MW1; "SELEC="; X1 / XCH4
X123 = ACO2 * 44 / (L2 * 280): PRINT "X123="; X123
X234 = MCH4 * 16 / (280 * L2): PRINT "X234="; X234
INPUT "STOP="; STO
RETURN
READ T, P, MW, DL, CP, CF, DP(2000)
A = .02368 * (DP ^ .65278)
B = -.0241 * (DP ^ .91939)
V = (T + 460) * 10.73 * .8 / P
DG = MW / V: G = G1 * MW: L = L1 * MW1
X6 = L / G * SQR(DG / DL)
Y5 = A + B * LOG(X6)
X5 = Y5 * DG * 32.2 / ((CP ^ .2) * CF * (1 / 62.3))
G5 = SQR(X5) * 3600: A1 = G / G5
```

```
D1 = SQR(A1 / 3.14126) * 24
LPRINT TAB(20); "VAPOUR DATA"; TAB(60); "LIQUID DATA"
LPRINT TAB(20); "-----------"; TAB(60); "-----------"
LPRINT
LPRINT "              FLOW(KG/HR)        ="; G * .4535924;
TAB(61); L2 * .4535924 * 278.82
LPRINT "              DENSITY(KG/M3)     ="; DG * 16.019; TAB(61);
DL * 16.019
LPRINT "              VISCOSITY(CP)      = .011"; TAB(61); CP
LPRINT "              MOL. WT.           ="; MW; TAB(61); 278.82
LPRINT
LPRINT TAB(38); "TOWER DIAMETER"
LPRINT TAB(37); "--------------"
LPRINT
LPRINT "              PACKING FACTOR="; CF
LPRINT "              DP/M(mm.H2O)  = 20"
LPRINT "       The calculated diameter(meter)="; D1 * .0254
LPRINT
RETURN
DATA 80,1000,19.271418,63.737,5.8,52,.24
 READ SL, SS, A2, G3, DL1, DP1, R, DV, CP1(3000)
 LW = (L / 3600) / ((22 / 28) * (D1 / 12) ^ 2)
 VW = (G / 3600) / ((22 / 28) * (D1 / 12) ^ 2)
 CT = DL / MW1
 AW = A2 * (1 - EXP(-1.45 * ((SS / SL) ^ .75) * ((LW *
 1488.2 / (A2 * CP)) ^ .1) * ((LW * LW * A2 / (DL * DL
 * G3)) ^ -.05) * ((LW * LW / (DL * SL * A2 * 32.2)) ^ .2)))
 KL = .0051 * ((LW * 1488.2 / (AW * CP)) ^ .6666667) *
 ((CP / (DL * DL1 * 1488.2)) ^ -.5) * ((A2 * DP1) ^ .4)
 KL1 = ((DL * 1488.2 / (CP * G3)) ^ (1 / 3))
 KL = KL / KL1
 KG = (5.23 * ((VW * 1488.2 / (A2 * CP1)) ^ .7) * ((CP1 /
 (1488.2 * DG * DV)) ^ (1 / 3)) * ((A2 * DP1) ^ -2)) /
 ((R * (T + 460)) / (A2 * DV))
 HG = VW / (MW * KG * AW * P)
 HL = LW / (MW1 * KL * AW * CT)
 PRINT "HG="; HG; "HL="; HL
RETURN
DATA .00235,.0041796,59.128,32.187,8.3E-9,.125,10.734,
3.014E-6,.011
```

PROGRAM (B)

```
REM           PROGRAM LIST FOR THE FLASH TANK DESIGN

LPRINT : LPRINT : LPRINT : LPRINT : LPRINT : LPRINT : LPRINT
LPRINT TAB(10); "Table (A1-2) High pressure flash tank design"
parameters ""
LPRINT TAB(16); "using Selexol for configuration (1)"
LPRINT : LPRINT
REM flash calculation & flash tank design
F = 6797.232: N = 4: PF = 1000: PT = 300: R(1) = .5: CP = .49:
TF = 80: TS = TF
PRINT "F="; F; "PF="; PF; "PT="; PT; "TF="; TF; "N="; N
FOR I = 1 TO N: READ Z(I), V(I), M(I)
PRINT "Z("; I; ")="; Z(I); "V("; I; ")="; V(1); "M("; I; ")="; M(1)
NEXT I

DATA .151671,160,44,.01663262,190,34.06,.1128,75,16,.7188962,0,280
PRINT "Input the first estimation for the CO2 & H2S conc. in the"
liquid outlet"
INPUT XC, XH
GOSUB 560
FR = 0: FOR I = 1 TO N: FR = FR + Z(I) * (K(I) - 1): NEXT I
IF FR > 0 GOTO 110
PRINT "The feed is subcooled liquid": END
FR = 0: FOR I = 1 TO N: FR = FR + (Z(I) * (K(I) - 1)) / ((K(I) -
1) + 1): NEXT I
IF FR < 0 GOTO 140
PRINT "The feed is superheated vapour"
PRINT TAB(1); "K"; TAB(5); "R(K)"; TAB(20); "FR(K)"; TAB(35);
"FR1(K)"; TAB(50); "R(K+1)"; TAB(65); "B"
PRINT TAB(1); "_"; TAB(5); "____"; TAB(20); "______"; TAB(35);
"________"; TAB(50); "________"; TAB(65); "_"
FOR K = 1 TO 50
FR(K) = 0: FR1(K) = 0
FOR I = 1 TO N
FR(K) = FR(K) + (Z(I) * (K(I) - 1)) / ((K(I) - 1) * R(K) + 1)
FR1(K) = FR1(K) - (Z(I) * ((K(I) - 1) ^ 2)) / (((K(I) - 1) * R(K)
+ 1) ^ 2)
NEXT I
R(K + 1) = R(K) - FR(K) / FR1(K)
IF R(K + 1) < 0 GOTO 280
IF R(K + 1) > 1 GOTO 290
B = ABS((R(K + 1) - R(K)) / R(K))
IF B < .0001 GOTO 340
GOTO 320
T1 = R(K) / 2: GOTO 300
T1 = (1 - R(K)) / 2
PRINT "R(;"; K + 1; ")="; R(K + 1)
R(K + 1) = T1
PRINT TAB(1); K; TAB(5); R(K); TAB(20); FR(K); TAB(35); FR1(K);
TAB(50); R(K + 1); TAB(65); B
IF B < .0001 GOTO 340
NEXT K
LPRINT : LPRINT TAB(11); "Comp."; TAB(22); "Feed comp."; TAB(39);
"Vapour comp."; TAB(59); "Liquid comp."
```

```
LPRINT TAB(10); "-------"; TAB(21); "-------------"; TAB(38); "------
---------"; TAB(58); "----------------"
FOR I = 1 TO N
Y(I) = (K(I) * Z(I)) / ((K(I) - 1) * R(K) + 1): X(I) = Y(I) / K(I)
LPRINT TAB(14); I; TAB(23); Z(I); TAB(40); Y(I); TAB(61); X(I)
NEXT I
LPRINT
V = R(K) * F: L = F - V
PRINT "R("; K; ")="; R(K); "F="; F; "V="; V; "L="; L
REM Calculation of cooling effec
CE = 0: FOR I = 1 TO N: CE = CE + V * Y(I) * V(I) * M(I): NEXT I
PRINT "CE="; CE
REM Calculation of heating effect
DP = (PF - PT) * 2.2154: PRINT "DP="; DP
V1 = 0: FOR I = 1 TO N: V1 = V1 + F * Z(I) * M(I): NEXT I
HE = V1 * DP * .001286: PRINT "HE="; HE
DT = (HE - CE) / (F * Z(4) * M(4) * CP)
PRINT "DT="; DT; "TS="; TS; "XC="; XC; "XH="; XH
Z1 = ABS(ABS(TS - TF) - ABS(DT))
TS = TS + DT
XC = X(1): XH = X(2)
PRINT "TS="; TS; "Z1="; Z1; "X(1)="; X(1); "X(2)="; X(2)
IF Z1 <= 2 GOTO 534
GOTO 70
REM Calculation the volume of flash tank
V1 = 0: FOR I = 1 TO N: V1 = V1 + F * Z(I) * M(I): NEXT I
V2 = V1 * 3 / (64.36 * 60 * 35.32)
LPRINT : LPRINT : LPRINT
LPRINT TAB(10); "The feed   flow rate   (Kg-mole/hr)  = "; F
* .45359237£
LPRINT TAB(10); "The vapour flow rate   (Kg-mole/hr)  = "; V
* .45359237£
LPRINT TAB(10); "The liquid flow rate   (Kg-mole/hr)  = "; L
* .45359237£
LPRINT : LPRINT : LPRINT
LPRINT TAB(10); "Component (1) = C02"
LPRINT TAB(10); "Component (2) = H2S"
LPRINT TAB(10); "Component (3) = CH4"
LPRINT TAB(10); "Component (4) = Selexol"
LPRINT : LPRINT : LPRINT
LPRINT TAB(10); "The Volume of the tank (m3) ="; V2 * 2
END
PCC = 1000: PCH = 1000: PCM = 1000
X(1) = 0: X(2) = .1: X(3) = .2: X(4) = .3: X(5) = .4: X(6) = .5:
X(7) = .6
FOR I = 1 TO 7
IF XC > X(I) GOTO 730
IF X(I) = 0 THEN K(I) = .2077 + .0028 * TS + 1.676E-05 * (TS ^ 2)
IF X(I) = .1 THEN K(I) = .2195 + .0031 * TS + 1.606E-05 * (TS ^ 2)
IF X(I) = .2 THEN K(I) = .2307 + .0033 * TS + 1.743E-05 * (TS ^ 2)
IF X(I) = .3 THEN K(I) = .245 + .0036 * TS + 1.801E-05 * (TS ^ 2)
IF X(I) = .5 THEN K(I) = .2871 + .004 * TS + 2.313E-05 * (TS ^ 2)
IF X(I) = .6 THEN K(I) = .3049 + .0049 * TS + 2.143E-05 * (TS ^ 2)
IF XC = X(I) GOTO 700
IF XC > X(I) GOTO 710
```

```
I = I - 1: GOTO 610
K(1) = K(I): GOTO 720
K(1) = K(I + 1) - ((X(I + 1) - XC) / (X(I + 1) - X(I))) * (K(I + 1)
- K(I))
K1 = K(1) * (PCC / PT): GOTO 750
NEXT I
X(1) = 0: X(2) = .1: X(3) = .2: X(4) = .3: X(5) = .4: X(6) = .5:
X(7) = .6
X(8) = .7: X(9) = .8
FOR I = 1 TO 9
IF XH > X(I) GOTO 914
IF X(I) = 0 THEN K(I) = .0221 + .000173 * TS + 4.02E-06 * (TS ^ 2)
IF X(I) = .1 THEN K(I) = .024 + .000261 * TS + 4.17E-06 * (TS ^ 2)
IF X(I) = .2 THEN K(I) = .026 + .000354 * TS + 4.94E-06 * (TS ^ 2)
IF X(I) = .3 THEN K(I) = .033 + .000361 * TS + 6.55E-06 * (TS ^ 2)
IF X(I) = .4 THEN K(I) = .0391 + .000496 * TS + .000007 * (TS ^ 2)
IF X(I) = .5 THEN K(I) = .043 + .000636 * TS + 8.33E-06 * (TS ^ 2)
IF X(I) = .6 THEN K(I) = .069 + .000096 * TS + 1.43E-06 * (TS ^ 2)
IF X(I) = .7 THEN K(I) = .0711 + .000561 * TS + .000015 * (TS ^ 2)
IF X(I) = .8 THEN K(I) = .0819 + .0011 * TS + 1.488E-05 * (TS ^ 2)
IF XH = X(I) GOTO 900
IF XH > X(I) GOTO 910
I = I - 1: GOTO 780
K(2) = K(I): GOTO 920
K(2) = K(I + 1) - ((X(I + 1) - XH) / (X(I + 1) - X(I))) * (K(I +
1) - K(I))
K2 = K(2) * (PCH / PT): GOTO 920
NEXT I
K(3) = 7.2474 - 4.575 * XC - 2.3452 * (XC ^ 2)
K(3) = K(3) * (PCM / PT)
K(4) = .000005: K(1) = K1: K(2) = K2
PRINT "K(1)="; K(1); "K(2)="; K(2); "K(3)="; K(3); "K(4)="; K(4)
RETURN
```

PROGRAM (C)

```
REM                  Program List for cooler design

READ CPH, TH1, TH2, CPC, TC1, TC2, AU, OD, ID, LT, K1, N1, CKF, CD
READ HKF, HD, HOD, HID, MKF
MH = 620555: HVS = 3.4
CVS1 = 1.7651 - .0475 * ((TC1 + TC2) / 2) + .0005846 * (((TC1 +
TC2) / 2) ^ 2) - 2.599E-06 * (((TC1 + TC2) / 2) ^ 3)
PRINT "CPH="; CPH; "MH="; MH; "TH1="; TH1; "TH2="; TH2; "CPC=";
CPC; "TC1="; TC1; "TC2="; TC2; "AU="; AU; "CVS1="; CVS1; "CKF=";
CKF; "CD="; CD; "HVS="; HVS
PRINT "HKF="; HKF; "HD="; HD; "HOD="; HOD; "HID="; HID; "MKF=";
MKF; "hvs="; HVS
Q = (MH / 3600) * CPH * (TH1 - TH2)
MC = Q / (CPC * (TC2 - TC1))
DTM = ((TH1 - TC2) - (TH2 - TC1)) / (LOG((TH1 - TC2) / (TH2 - TC1)))
R = (TH1 - TH2) / (TC2 - TC1): S = (TC2 - TC1) / (TH1 - TC1)
INPUT "from fig. 12.20 (.97)  FT="; FT
PRINT "Q="; Q; "FT="; FT; "DTM="; DTM
A = Q * 1000 / (DTM * FT * AU): TES = 0: TEST = 0: CHI = 0: CHO = 0
A1 = LT * OD * 3.146: PRINT "A="; A; "A1="; A1
N = A / A1: PRINT "N="; N
BD = OD * (N / K1) ^ (1 / N1): PRINT "BD="; BD
DCL = (45.4 + 26.75 * BD) / 1000
SID = BD + DCL
REM Calculation of tube side coefficient
GT = MC / ((N / 2) * (3.146 * ID ^ 2 / 4))
CLV = GT / CD: PRINT "GT="; GT
REI = (CD * CLV * ID) * 1000 / CVS1: PRI = CPC * CVS1 / CKF
R = LT / ID
PRINT "REI="; REI; "R="; R; "CD="; CD; "CLV="; CLV; "ID=", ID
PRINT "HI="; HI, "CVS1="; CVS1
IF TES = 0 GOTO 200
CVSCF = (CVS1 / CVSW) ^ .14
GOTO 201
CVSCF = 1
IF REI < 6000 AND REI > 200 GOTO 220
IF REI > 600 GOTO 208
HI = (1.86 * ((REI * PRI) ^ .33) * ((ID / LT) * .33) * CVSCF *
CKF) / ID
GOTO 210
HI = (.023 * (REI ^ .8) * (PRI ^ .33) * CVSCF * CKF) / ID
IF ABS(CHI - HI) < 10 GOTO 230
CHI = HI
THA = (TH1 + TH2) / 2: TCA = (TC1 + TC2) / 2
TWC = (AU * (THA - TCA) + TCA * HI) / HI
CVSW = 1.7651 - .0475 * TWC + .0005846 * (TWC ^ 2) - 2.599E-06 *
(TWC ^ 3)
TES = 1: GOTO 194
HI1 = (1.86 * ((REI * PRI) ^ .33) * ((ID / LT) ^ .33) * CVSCF *
CKF) / ID
HI2 = (.023 * (REI ^ .8) * (PRI ^ .33) * CVSCF * CKF) / ID
IF (HI1 - HI2) < 0 GOTO 228
HI = HI2: GOTO 210
HI = HI1: GOTO 210
```

```
REM Calculation of shell side coefficient
LB = SID: PT = 1.25 * OD
AS1 = ((PT - OD) * SID * LB) / PT
GS = MH / (3600 * AS1)
ED = (1.1 * (PT ^ 2 - .917 * (OD ^ 2))) / OD
REO = GS * ED * 1000 / HVS: PRO = CPH * HVS / HKF
PRINT "REO="; REO
JHO = .4503 * (REO ^ -.4679)
IF TEST = 0 GOTO 330
VSCF = (HVS / HVSW) ^ .14
GOTO 340
VSCF = 1
HO = (JHO * REO * (PRO ^ (1 / 3)) * VSCF * HKF) / ED
IF ABS(CHO - HO) < 10 GOTO 410
CHO = HO
THA = (TH1 + TH2) / 2: TCA = (TC1 + TC2) / 2
TW = (HO * THA - AU * (THA - TC2)) / HO
PRINT "TW="; TW; "HVS="; HVS; "HO="; HO
HVSW = LOG((5.8 ^ -.2661) + ((TW - 25) / 233))
HVSW = EXP(HVSW / -.2661): PRINT "TW="; TW; "HVSW="; HVSW
TEST = 1: GOTO 270
REM Calculation of the over all heat transfer coefficient
CU = 1 / HO + 1 / HOD + OD * LOG(OD / ID) / (2 * MKF) + OD /
(ID * HID) + OD / (ID * HI)
CU = 1 / CU
IF ABS(AU - CU) < 10 GOTO 460
AU = CU: GOTO 100
PRINT "A="; A; "HI="; HI; "HO="; HO; "AU="; AU; "N="; N; "MC="; MC
PRINT "REI="; REI; "CLV="; CLV; "REO="; REO; "SID="; SID
DATA 2.3,71,27,4.2,15,30,600,.02,.016,10,.175,2.285, 59,995
DATA .17307,1021,5000,6000,45
COOL = 110000 * (((A / .092903) / 10000) ^ .68)
PRINT "COOL="; COOL
C.WTER = (MC / .45359237E) * 517.24: PRINT "C.WTER="; C.WTER
INPUT "from fig. 12.24 TJFC=(.0039) "; JF
TPD = 4 * (8 * JF * (LT / ID) * CVSCF + 2.5) * (CD * (CLV ^ 2)
/ 2): PRINT "TPD="; TPD
TPD = TPD / 100000: PRINT "TPD(bar)="; TPD
INPUT "from fig. 12.30 SJFC=(.06)"; JF1
GS1 = GS / HD: PRINT "GS="; GS; "GS1="; GS1
SPD = 8 * JF1 * (SID / ED) * (LT / LB) * (HD * (GS1 ^ 2) / 2) *
(VSCF): PRINT "SPD="; SPD
SPD = SPD / 100000: PRINT "SPD(bar)="; SPD
END
```

PROGRAM (D)

PROGRAM LIST FOR CALCULATION OF THE COEFFICIENTS OF COST EQUATIONS

```
REM DATA OF THE SELEXOL
GOTO 10
REM DATA OF THE SELEXOL
MW1 = 280: CP = 5.8: S = .6: S11 = 6.5: DL = 62.43: CPS = 1.07
SP = 2.3: KS = .17307: CPCC = 3.2: CPE = 3.2: CPH = 3.2: SS = 15
VP = .0008: C = 9.65
GOTO 200
REM ESTIMATED DATA OF THE B2
MW1 = 114: CP = 1.75: S = .6: S11 = 3: DL = 62.43: CPS = .4
SP = 2.11: KS = .114: CPCC = 1.13: CPE = 1.13: CPH = 1.13
SS = 30.6: VP = .26: C = 16
GOTO 200
REM EXPERIMENTAL DATA OF THE B2
MW1 = 114: CP = 1.75: S = .96: S11 = 7.26: DL = 62.43: CPS = .4
SP = 2.11: KS = .114: CPCC = 1.13: CPE = 1.13: CPH = 1.13
SS = 30.6: VP = .0203: C = 16
GOTO 200
REM DATA OF THE ATHYL ACETATE
MW1 = 88.11: CP = .42: S = .97: S11 = 2.57: DL = 62.43: CPS = .14
SP = 2.17: KS = .1463: CPCC = .31: CPE = .31: CPH = .31: SS = 31.1
VP = 87: C = 8.86
GOTO 200
REM DATA OF THE N-FORMYL MORPHOLINE
MW1 = 115.13: CP = 6.79: S = 1.42: S11 = 24.84: DL = 62.43
CPS = .94: SP = 1.73: KS = .06152: CPCC = 4.11: CPE = 4.11
CPH = 4.11: SS = 31.9: VP = .009: C = 47.5
GOTO 200
REM DATA OF THE ACETONE
MW1 = 58.1: CP = .3: S = 1.29: S11 = 9.65: DL = 62.43
CPS = .11: SP = 2.7: KS = .138: CPCC = .23: CPE = .23
CPH = .23: SS = 31.8: VP = 222: C = 2.96
GOTO 200
REM DATA OF THE DIMETHYL ACETAMIDE
MW1 = 87.12: CP = 1.95: S = 1.17: S11 = 9.84: DL = 62.43
CPS = .4: SP = 2.104: KS = .179: CPCC = 1.24: CPE = 1.24
CPH = 1.24: SS = 27.4: VP = 1.7: C = 8.32
GOTO 200
REM DATA OF THE DIMETHYL FORMAMIDE
MW1 = 73.1: CP = .85: S = 1.17: S11 = 13.572: DL = 62.43
CPS = .23: SP = 1.913: KS = .188: CPCC = .59: CPE = .59
CPH = .59: SS = 37.7: VP = 3: C = 7.84
GOTO 200
REM DATA OF THE METHANOL
MW1 = 32.04: CP = .514: S = 2.64: S11 = 15.6552: DL = 62.43
CPS = .16: SP = 2.99: KS = .169: CPCC = .372: CPE = .372
CPH = .372: SS = 38.9: VP = 121: C = 3.2
GOTO 200
REM DATA OF THE METHYL ETHEL KETONE
MW1 = 72.1: CP = .37: S = 1.05: S11 = 6.5625: DL = 62.43
CPS = .125: SP = 2.23: KS = .138: CPCC = .275: CPE = .275
CPH = .275: SS = 28.9: VP = 83.2: C = 10.1
GOTO 200
REM DATA OF THE METHYL PYRROLIDONE
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MW1 = 29.13: CP = 1.67: S = 1.24: S11 = 14.632: DL = 62.43
CPS = .36: SP = 1.85: KS = .188: CPCC = 1.08: CPE = 1.08
CPH = 1.08: SS = 26.2: VP = .971: C = 6.84
T = 80: P = 1000: MW = 27.2: CF = 52: DP = .24: ABSCP = CP
G1 = 8.289: G3 = 32.187: CP1 = .011: VAC = .034: A2 = 59.128
DP1 = .1235: R = 10.734: Y1 = .4: Y2 = .035: X2 = .005
RAT = 1.4388: SF = .8: PF = 4.2: DV = 3.014E-06

REM Calculation of the coefficients of the absorber cost equation
and the cost of the absorber
L1 = S * G1 / RAT
V = (T + 460) / 460 * 14.7 / P * 359
DG = MW / V: G = G1 * MW: L = L1 * MW1
C13 = (3.1416 / 4) * (D ^ 2) * 17.5
C12 = 139.4 + 195.09 * D - 25.731 * (D ^ 2) + 1.8775 * (D ^ 3)
C12 = 1800
L2 = L1
TK = (T - 32) / 1.8 + 273
C2 = (1.173E-16 * (MW1 ^ .5) * TK * 9300) / (VAC ^ .6)
A1 = G1 / RAT * (MW1) * (1 / ((22 / 28) * (D ^ 2)))
C3 = .0051 * ((1488.2 * A1) ^ (2 / 3)) * (A2 ^ (-2 / 3)) * ((1 /
(1488.2 * DL * C2)) ^ -.5) * ((A2 * DP1) ^ .4) * ((1488.2 * DL /
G3) ^ (-1 / 3))
VW = (G1 * MW) / (22 * (D ^ 2) / 28)
C6 = (5.23 * ((1488.2 * VW / (A2 * CP1)) ^ .7) * ((CP1 / (1488.2
* DV * DG)) ^ (1 / 3)) * ((A2 * DP1) ^ -2)) / ((R * (T + 460)) /
(A2 * DV))
C5 = (G1 / RAT) * (1 / ((22 / 28) * (D ^ 2)))
RAT1 = (G1 - (G1 * Y1 / 2)) * S / (L1 + (G1 * Y1 / 2))
NOG1 = (1 / (1 - RAT1)) * LOG((1 - RAT1) * (Y1 / Y2) + RAT1)
NOG = 3.36
C15 = (1.2 * PF * C12 + C13) * (VW * NOG / (MW * C6 * A2 * P))
CT = DL / MW1
C16 = (1.2 * PF * C12 + C13) * ((C5 / C3) * (1 / (A2 * CT))) *
(RAT * NOG)
ABS. = C15 + C16 * (S ^ .962) * (CP ^ 1.43)
PRINT "Absorber Cost ="; ABS.; "a1="; C15; "a2="; C16;

FA1 = (G1 * 60 / RAT) * (3 * 2 / DL)
FA2 = (FA1 / 3.14126) ^ (1 / 3)
FA3 = 4 * 3.14126 * (FA2 ^ 2) * (10 / (25.4 * 12)) * (7700 / 16.09)
FA4 = 8971.2
FA5 = FA3 * 1.4992
COST = (FA4 + FA5 * (MW1 ^ .66667) * (S ^ .66667))
PRINT "Flash tanks cost = "; 3 * COST; "a5="; FA4; "a6="; FA5

CP1 = .01322: DV = .000234
MW = 18: D = 8: VAC = .0329: T = 260
P = 20: PF = 1: SF = .8: S1 = SS: X1 = 1.420392E-02
TK = (T - 32) / 1.8 + 273
C2 = (1.173E-16 * (MW1 ^ .5) * TK * 9300) / (VAC ^ .6)
A1 = (G1 / RAT) * MW1 * (1 / ((22 / 28) * (D ^ 2)))
C3 = .0051 * ((1488.2 * A1) ^ (2 / 3)) * (A2 ^ (-2 / 3)) * ((1 /
(1488.2 * DL * C2)) ^ -.5) * ((A2 * DP1) ^ .4) * ((1488.2 * DL /
G3) ^ (-1 / 3))
V = (T + 460) / 460 * 14.7 / P * 359
DG = MW / V
```

```
VW = ((S * G1 / (RAT * SF * S1)) * (18)) / (22 * (D ^ 2) / 28)
C6 = (5.23 * ((1488.2 * VW / (A2 * CP1)) ^ .7) * ((CP1 / (1488.2 *
DV * DG)) ^ (1 / 3)) * ((A2 * DP1) ^ -2)) / ((R * (T + 460)) /
(A2 * DV))
C5 = (G1 / RAT) * (1 / ((22 / 28) * (D ^ 2)))
C13 = (3.1416 / 4) * (D ^ 2) * 17.5
C12 = 139.4 + 195.09 * D - 25.731 * (D ^ 2) + 1.8775 * (D ^ 3)
NOG = (1 / (1 - SF)) * LOG((1 - SF) * (X1 / .000018) + SF)
C15 = (1.2 * PF * C12 + C13) * (VW * NOG * SF / (MW * C6 * A2 * P))
CT = DL / MW1
C16 = (1.2 * PF * C12 + C13) * ((C5 / C3) * (1 / (A2 * CT))) * (NOG)
STR. = C15 + C16 * (S ^ .81) * (CPS ^ 1.143)
PRINT "Stripper cost ="; STR.; "a3="; C15; "a4="; C16
THI = 71: THO = 27: TCI = 15: TCO = 30
DTS = TH1 - THO: DTM = ((TH1 - TCO) - (THO - TCI)) / LOG((TH1 - TCO)
/ (THO - TCI))
PRINT "DTS="; DTS; "DTM="; DTM
OD = .02: DTS = 44: DTM = 23: CF = 1
CA1 = G1 * .4535923 / RAT
CA2 = .01 * ((1 / 3000) ^ -.5)
CA3 = CA2 * ((DL * 16.019 * .6 * OD * 1000) ^ -.5) * (.6 * DL *
16.019 * 1000)
CA4 = DTS * 1000 / (DTM * CF)
CA5 = CA1 * CA4 / CA3
CA6 = 110000 * ((CA5 / 929.03) ^ .68)
PRINT "CA1="; CA1; "CA2="; CA2; "CA3="; CA3; "CA4=";
CA4; "CA5="; CA5; "CA6="; CA6
COOL = CA6 * ((MW1 ^ .68) * (S ^ .624) * (CPCC ^ .2) * ((SP / KS)
^ .45333))
OFH = ((MW1 ^ .68) * (S ^ .624) * (CPCC ^ .2) * ((SP / KS) ^ .45333))
PRINT "cost of the cooler="; 4 * COOL; "a7="; CA6
P1 = 300: P2 = 1000: YP = .9: YCO2 = .1: T = 80: Z = 1
PA1 = .0044 * .9 * 60 * (T + 460) * R * Z * (YP * G1 / RAT) *
LOG(P2 / P1)
PA2 = .0044 * .1 * 60 * (T + 460) * R * Z * (YCO2 * G1 / RAT) *
LOG(P2 / P1)
SL = S11 / S
OFC = (1 / SL) ^ .8
COMP = 750000 * OFC
PRINT "a8="; PA1; "a9="; PA2; "Cost of the compressor ="; COMP

TCC = COMP + 4 * COOL + STR. + 3 * COST + ABS.: PRINT "TCC="; TCC
T.OF = OFA + OFT + OFS + OFH + OFC
PRINT "OFA="; OFA; "OFS = "; OFS; "OFH = "; OFH; " OFT = ";
OFT; " OFC = "; OFC
PRINT "ABS.="; ABS.; "STR.="; STR.; "H.E="; 4 * COOL;
"F.T="; 3 * cost; "COMP="; COMP

OFE = 1 / SL
AEC = 1500000 * OFE
PRINT "AEC="; AEC; "OFE="; OFE; "FAC= 1500000"

SA1 = G1 * 18 / (RAT * SF)
SA1 = SA1 * 259200
OFSS = (S / SS)
CSA1 = SA1 * OFSS
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```
PRINT "SA1="; SA1; "SS="; SS; "CSA1="; CSA1; "OFSS="; OFSS
T1 = 126.67: T2 = 77: LMD = 2149.224
HA1 = G1 * (T1 - T2) / (RAT * LMD) * (259200)
OFHS = MW1 * SP * S
CHA1 = OFHS * HA1
PRINT "HA1="; HA1; "CHA1="; CHA1; "OFHS="; OFHS

T1 = 71: T2 = 27: T11 = 30: T22 = 15: SPW = 4.2
WA1 = (G1 * .4535924 / RAT) * (1 / SPW) * ((T1 - T2) / (T11 - T22))
WA2 = (.2 * 3600 * 24 * 300 / 4546.1) * WA1
CWA1 = WA2 * MW1 * SP * S: LPRINT "WA2="; WA2; "CWA1="; CWA1,
"RCOW="; S * SP * MW1

p = 20
VA1 = G1 * .4535924 * 14.7 * 3600 * 24 * 300 / (RAT * SF * p * 760)
F.LOS = G1 * .4535924 * S * VP * 14.7 * MW1 * 3600 / (RAT * SF *
SS * p * 760)
OFVL = (S / SS) * C * VP * MW1
L.C = VA1 * OFVL
PRINT "VA1="; VA1; "L.C="; L.C; "OFVL="; OFVL; "RCOSL="; (S / SS)
* C * VP * MW1

TOP = AEC + CSA1 + CHA1 + CWA1 + L.C: PRINT "TOP="; TOP
T.OF = OFE + OFSS + 2 * OFHS + OFVL: LPRINT "T.OF="; T.OF;
LPRINT "AEC="; AEC; "CSA1="; CSA1; "CHA1="; CHA1, "CWA1=";
CWA1; "L.C="; L.C
LPRINT "OFE="; OFE; "OFSS="; OFSS; "OFHS="; OFHS; "OFVL="; OFVL
LPRINT
END
```