

SYNOPSIS

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Packed columns are extensively used in the chemical industry for gas absorption. For designing these columns, apart from hydrodynamic conditions and physico chemical properties of system, one requires the knowledge of important parameters like hold up (h) pressure drop (ΔP), effective interfacial area available for mass transfer (a) and mass transfer coefficients ($k_L a$ and $k_G a$). When gas absorption is accompanied by chemical reaction, the knowledge of true mass transfer coefficients (k_L and k_G) and effective interfacial area (a) is also required separately.

Design parameters like capacity limits, holdup, pressure drop, effective interfacial areas and mass transfer coefficients have been studied by numerous investigators. Attempts have also been made to correlate experimental data on h , ΔP , a , $k_L a$ etc. by some investigators using semi empirical correlations. Predicting the values of capacity limits, holdup and pressure drop by these generalised correlations appear to be appropriate and sound. However there exists considerable amount of discrepancy regarding the values of effective interfacial area and wetted surface area. In particular the values of effective interfacial areas during physical absorption and chemical absorption (a_p and a_c respectively) are not at all comparable under otherwise similar conditions. Further the values of wetted surface area (a_w) have been mostly used by many investigators to obtain the values of the gas side and the liquid side mass

transfer coefficients (k_G and k_L respectively) from the corresponding values of volumetric mass transfer coefficients. Thus, the predicted values of k_G and k_L are expected to involve considerable amount of error.

Hence, the experimental data available in the literature on effective interfacial areas for gas absorption with and without chemical reaction and wetted surface area could be analysed critically and correlations could be developed for predicting the values of effective interfacial areas by mathematical modelling. Similarly, the volumetric mass transfer coefficients ($k_L a$ and $k_G a$) also the overall mass transfer coefficient ($K_G a$) for the cases of absorption with chemical reaction could also be analysed in systematic manner. The values of k_G and k_L could then be predicted by utilising the appropriate values of effective interfacial area. The values of k_G and k_L so obtained could then be utilised for developing generalised correlations by mathematical modelling. Further, a suitable mathematical model could also be proposed for predicting the values of volumetric liquid side mass transfer coefficient with chemical reaction ($k_L' a$). The generalised correlations so developed for different cases could be used conveniently to elucidate the mechanism of mass transfer between gas and liquid in irrigated packed columns.

The present work is thus addressed to the following :-

1. To formulate a mathematical model based on the concept of static area and dynamic area which is expected to represent the mechanism of mass transfer for the cases under consideration.

2. To obtain generalised correlations for predicting the values of effective interfacial area in terms of dimensionless numbers for the cases under consideration by mathematical modelling.
3. To obtain generalised correlations for predicting the values of static area (a_{st}) and dynamic area (a_{dy}) and to utilise these correlations to throw light on the mechanism of mass transfer.
4. To obtain generalised correlations for predicting the values of volumetric liquid side mass transfer coefficient, true liquid side and gas side mass transfer coefficients using appropriate values of effective interfacial area.
5. To extend the concept of static area and dynamic area to mass transfer coefficients and to formulate a suitable mass transfer coefficient model for predicting the values of volumetric liquid side mass transfer coefficients during chemical absorption ($k_L'a$). Hence also, to obtain generalised correlations for predicting the values of mass transfer coefficients (k_La , k_Ga and $k_L'a$) for the case of absorption with chemical reaction.
6. To formulate a suitable mathematical model to predict the height equivalent to a theoretical plate (HETP) for distillation operation by utilising the generalised correlations of k_L , k_G and ' a ' developed for gas absorption i.e. applicability of generalised correlations developed for gas absorption to distillation.

The thesis is presented in ten chapters. Chapter (1) is devoted to the introduction just described above.

Chapter (2) presents the literature survey with respect to effective interfacial areas and mass transfer coefficients in packed columns for cases of physical absorption and chemical absorption along with relevant wetted surface area data which has been used for preparing data banks for a_p , a_c , a_w , $k_L a$ and $k_G a$. This chapter also reviews liquid distribution in packed columns, pressure drop and relevant information on holdup in packed columns.

Further the generalised correlations available in the literature for predicting the values of pressure drop, holdup effective interfacial areas (a_w , a_p and a_c) and mass transfer coefficients ($k_L a$, k_G and k_L) have also been reviewed. Some mass transfer data on distillation has also been reviewed.

Chapter (3) : Numerical methods and optimization techniques describes the mathematical modelling methods utilised in the present investigation.

The methods include multiple linear regression using the numerical methods of Gauss Jordan and Gauss Seidel as well as unconstrained optimization techniques. In the second category, the direct search method developed by Davies, Swann and Campey is utilised in conjunction with Powell's algorithm. This optimization routine known as DSC - Powell algorithm is considered as the most efficient alternative variable optimization method. Further the versatile modified simplex method of Nelder and Mead which is also utilised in this investigation, has been presented in this chapter.

Chapter (4) : General Considerations, includes the relevant details about estimating the values of k_G from $k_G a$, $k_L' a$ from $K_G a$ (chemical) and calculating the values of HETP from k_L , k_G and ' a '. It also includes estimation of physical properties/parameters like surface tension (σ), Henry's law constant for electrolyte as well as non electrolyte solutions (H' and H respectively), diffusivities of liquid and gas (D_L and D_G respectively), also the reaction velocity constants (k_{OH^-} , k_{MEA} , k_3 and k_{NH_3} etc.) for various reactive systems used in this investigation.

Chapter (5) : Data Tables, presents the relevant experimental data tabulations (based on literature survey) along with the required physical properties for the cases of a_w , a_p , a_c , $k_L a$, k_L , $K_G a$, $k_G a$ HTU and $K_G a$ (chemical). Further, explanatory notes at the end of each table indicate the relevant information regarding systems inclusive of packing characteristics and references for the various data points.

The static area model and the mass transfer coefficient model have been outlined in Chapter (6) : Mathematical modelling for effective interfacial area and mass transfer coefficients.

- The effective interfacial area available for mass transfer during absorption in a packed column can be split^t in two parts as follows :

$$a_e = a_{st} + a_{dy}$$

In the case of physical absorption in a packed column the semi-stagnant pockets as well as the slow moving film over the packings tend to become very rapidly saturated with solute gas. However, the fast moving film/rivulets, where the liquid load is more and hence renewal is rapid, retain their capacity to absorb the gas. Hence, in this case, it is apparent that the static area (a_{st}) is likely to be ineffective for gas absorption. Therefore, the effective interfacial area during physical absorption is given by the following equation :-

$$a_p = a_{dy} = a_w - a_{st}$$

In the case of chemical absorption in a packed columns excluding the regimes of very slow reaction, also the regime wherein concentration of reactive species being very low and the regime of instantaneous reaction, the semistagnant pockets (a_{st} part) are expected to be as effective as moving liquid (a_{dy} part). Therefore, the effective interfacial area during chemical absorption is given by the following equation :-

$$a_c = a_{dy} + a_{st} = a_p + a_{st}.$$

Thus, the static area model proposed in this chapter is expected to elucidate the mechanism of mass transfer between gas and liquid in irrigated packed column.

This chapter also outlines the formulation of the mass transfer coefficient model which is based on the assumption that the interface consists of two parts, that is the moving part and the semistagnant static part. Then, the volumetric mass transfer

coefficient for chemical absorption can also be splitted in two parts as under :-

$$(k_L' a)_{\text{chem.}} = (k_L' a)_{\text{dy.}} + (k_L' a)_{\text{st.}}$$

Therefore, in the regime where the concentration of reactive species is not very low and also the reaction is not in the regime of instantaneous reaction, the model correlation for predicting the values of $k_L' a$ can be expressed as under :-

$$(k_L' a)_{\text{chem.}} = \beta \cdot (k_L a)_{\text{phy.}} + \sqrt{D_L k_2 [B]} \cdot (a_{\text{st}}).$$

where β is the reaction factor.

However, in the regime where the concentration of reaction species is very low and the reaction regime is a very slow reaction, the values of $k_L a$ can be predicted by the following correlation :-

$$(k_L' a)_{\text{chem}} = \beta \cdot (k_L a)_{\text{phy}}$$

In Chapter (7) : Results and discussion for effective interfacial areas, the different generalised correlations developed by mathematical modelling of the relevant data on a_w , a_p , a_c etc. are presented.

CASE (I) : Generalised correlations for a_w , a_p and a_c are the following :-

- (i) $a_w/a_t = 1.431 (\text{Re})^{0.0014} (\text{We})^{0.165} (\text{Fr})^{0.002} (\sigma / \sigma_c)^{-0.442}$
- (ii) $a_p/a_t = 1.08 (\text{Re})^{0.099} (\text{We})^{0.22} (\text{Fr})^{0.002} (\sigma / \sigma_c)^{-0.442}$
- (iii) $a_c/a_t = 0.455 (\text{Re})^{0.227} (\text{We})^{0.058} (\text{Fr})^{0.002} (\sigma / \sigma_c)^{-1.104}$

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All these correlations are shown to be more reliable and more general in nature than previously published correlations.

CASE (II) : Generalised correlation for a_{st} based on the static area model is as under :-

$$a_{st}/a_t = 0.1605 (Re)^{0.1726} (Fr/We)^{0.5} (\sigma / \sigma_c)^{-0.725}$$

This model correlation for a_{st} can be utilised conveniently, to predict the values of (a_p/a_t) and (a_c/a_t) during gas absorption in packed column. This model correlation for a_{st} can also be extended further for analysing the data on mass transfer coefficients during chemical absorption.

CASE (III) : Generalised correlations for (a_p/a_t) and (a_c/a_t) based on the static area model are the following :-

$$(a_p/a_t) = (a_w/a_t)_{pred.} - (a_{st}/a_t)_{pred.}$$

$$(a_c/a_t) = (a_p/a_t)_{pred.} + (a_{st}/a_t)_{pred.}$$

In Chapter (8) : Results and discussion for mass transfer coefficients, the different generalised correlations developed by mathematical modelling of the relevant data on $k_L a$, k_L , k_G and $k_L' a$ are presented.

Generalised correlations for $k_L a$, k_G and k_L are the following

$$(1) \quad k_L a = [0.0833 (Re)^{0.286} (We)^{0.22} (Fr)^{0.002} (\sigma / \sigma_c)^{-0.442}] \times \\ \dots \times [(Sc)^{-0.5} (\rho_L / \mu_L g)^{-1/3} a_t]$$

$$(ii) \quad k_G = 1.75 (Re_G)^{0.70} (Sc_G)^{0.4125} (a_t d_p)^{-0.9} (RT/a_t D_G)^{-1}$$

$$(iii) \quad k_L = 0.099 (Re)^{0.187} (Sc)^{-0.5} (\rho_L / \mu_L g)^{-1/3}$$

These three correlations are shown to be more reliable and more general in nature than previously published correlations. The generalised correlations for $k_L a$ takes into account the effect of parameter (σ / σ_c) on the values of $k_L a$. It is interesting to observe that the generalised correlations for k_L and k_G do correlate satisfactorily the k_L and k_G data obtained by chemical technique.

It is further interesting to observe that the values of $k_L a$ obtained from $k_L' a$, in the regime of very low concentration of reactive species and also the values of $k_L a$ obtained by chemical technique in the regime of instantaneous reaction can be predicted satisfactorily by the generalised correlation of $k_L a$ obtained for physical gas absorption.

Based on the mass transfer coefficient model developed in this investigation, knowing the values of mass transfer coefficient during physical absorption ($k_L a$) under otherwise identical conditions, the static area (a_{st}) from the static area model also under otherwise identical conditions and the factors $-\beta$ and $[\sqrt{D_L k_2 [B]}]$, the volumetric liquid side mass transfer coefficient with chemical reaction ($k_L' a$) can be predicted satisfactorily by the model correlations. These model correlations are not merely the empirical correlations but these correlations elucidate the mechanism of mass transfer during chemical absorption.

In Chapter (9) : Distillation in Packed columns, a suitable mathematical model for predicting the values of HETP has been formulated. The relevant model correlation which can be used satisfactorily for predicting the values of HETP during distillation is as follows :-

$$\text{HETP} = \frac{\ln \lambda}{\lambda - 1} [(G)/(k_V \cdot a_d \cdot P \cdot M_{\text{avg}}) + \lambda (L/(k_L a)_{\text{dist.}} \rho_L)]$$

The model parameters k_L , k_V , a_d and $(k_L a)_{\text{dist.}}$ required for predicting the values of HETP, can be estimated conveniently by utilising the relevant generalised correlations developed for k_L , k_G , a_p and $(k_L a)_{\text{phy.}}$ for the case of gas absorption in packed columns.

It is expected to be interesting to perform the mathematical modelling for the case of distillation with chemical reaction in packed columns after obtaining the relevant data on HETP.

Chapter (10) presents the conclusions of the present work and its summary is as follows :-

Mathematical modelling performed in this investigation has resulted in the development of a few important thumb - rules for determining the effectiveness of static area (a_{st}) during mass transfer under different sets of conditions. The different generalised correlations developed by mathematical modelling based on 'the static area model' and 'the mass transfer coefficient model' can be utilised conveniently during designing of packed columns. These generalised correlations have thus established a powerful frame work for rational design of packed absorption columns as well as distillation columns.