CHAPTER 10

CONCLUSIONS

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10.1 SOME OBSERVATIONS/CONCLUDING REMARKS FOR NUMERICAL METHODS AND OPTIMIZATION TECHNIQUES :

The following three methodologies were utilised in this investigation for performing the mathematical modelling of the data on effective interfacial areas and mass transfer coefficients :-

(i) Multiple linear regression using numerical methods of Gauss Jordan and Gauss Seidel.

(ii) Optimization by DSC-Powell algorithm.

(iii) Optimiation by modified simplex algorithm of Nelder and Mead.

Coventional routines avaliable in the literature were adopted for methodologies :- (i) and (iii). However for methodology (ii) Optimization by DSC-Powell algorithm - a suitable software package was developed in this investigation which can optimise any nonlinear function upto six variables. While performing mathematical modelling of the data by using these methodologies, many evidences were available to conclude the following :-

(i) While attempting mathematical modelling of a large data bank involving many variations, one has to exercise caution regarding the selection of the methodology for optimization of different

variables/parameters and subsequently developing a final generalised correlation. Otherwise, sometimes misleading results can be obtained/inconsistent results can be obtained. The correlation having inferior statistical analysis are likely to be developed. Further, in some instances data fit can be improved considerably by changing the direction of search sequence etc.

(ii) While using the DSC Powell algorithm unless and untill the parametric space has been explored from maximum possible directions of search sequences, one can not confidently say that the correlation obtained by mathematical modelling is the best correlation. It is likely that a better correlation may be in store some other direction not yet explored.

(iii) For objective functions with implicit constraints, while using the modified simplex algorithm of Nelder and Mead it is preferrable to adopt the Box Criteria regarding generation of the initial simplex.

10.2 CONCLUSIONS FOR EFFECTIVE INTERFACIAL AREAS :-

The information available in literature on the values of wetted surface area (a_w), effective interfacial area during physical absorption (a_p) and effective interfacial area during chemical absorption (a_c) was utilised to prepare the relevant data banks for a_w, a_p and a_c. These data banks have provided all of the model validation material for obtaining the generalised correlations for interfacial areas. The mathematical modelling of the data has resulted in the following generalised correlations for a_w, a_p and a_c

(I) Generalised correlation for wetted surface area (a_w) :-

An improved generalised correlation for predicting the values of wetted surface area (a_w) has been developed. The correlation is shown to be more reliable and more general than previously published correlations with 92 % of the predicted values falling within ± 15 % of the experimental - data bank values.

$$a_w/a_t = 1.431\ (Re)^{0.0014}\ (We)^{0.165}\ (Fr)^{0.002}\ (\sigma / \sigma_c)^{-0.442}$$

The statistical analysis of the correlation can be described as follows :- % E_{avg} = 0.45, % E_{abs} = 7.04 and % S_{dev} = 3.29.

(II) Generalised correlation for effective interfacial area during physical absorption (a_p) :-

The following generalised correlation can be used satisfactorily for predicting the values of effective interfacial area during physical absorption :-

$$a_p/a_t = 1.08\ (Re)^{0.099}\ (We)^{0.22}\ (Fr)^{0.002}\ (\sigma / \sigma_c)^{-0.442}$$

The statistical analysis of the correlation can be described as follows :- % E_{avg} = 3.45, % E_{abs} = 15.66 and % S_{dev} = 5.97.

The following generalised correlation can also be used for predicting the values of (a_w/a_t) or (a_p/a_t) satisfactorily :-

$$a_w/a_t \text{ or } a_p/a_t = 1.431\ (Re)^{0.0014}\ (We)^{\beta}\ (Fr)^{0.002}\ (\sigma / \sigma_c)^{-0.442}$$

where β = 0.165 for wetted surface area and β = 0.237 for physical absorption. The statistical analysis of this correlation for

predicting the values of (a_p/a_t) is as follows :- % E_{avg} = 5.14, % E_{a_bs} = 17.36 , % S_{dev} = 6.73. It is interesting to observe that the indices of different numbers and groups in this equation and that in the equation for (a_w/a_t) are identical except the index of Weber number.

(III) Generalised correlation for effective interfacial area during chemical absorption (a_c) :-

An improved generalised correlation for predicting the values of effective interfacial area during chemical absorption is as under

$$a_p/a_t = 0.455\,(Re)^{0.227}\,(We)^{0.058}\,(Fr)^{0.002}\,(\sigma/\sigma_c)^{-1.104}$$

The statistical analysis of the correlation can be described as follows :- % E_{avg} = 1.38, % E_{a_bs} = 8.25, % S_{dev} = 4.84. The correlation is shown to be more general [as it correlates the data of (a_c/a_t) for plastic packings quite satisfactorily] than previously published correlation of Puranik and Vogelpohl with 94 % of the predicted values falling within ± 20 % of the experimental data bank values.

(IV) The static area model and the generalised correlation for static area (a_{st}) :-

The effective interfacial area available for mass transfer during absorption in a packed column can be splited 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 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 equations :-

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

The values of a_{st} get affected by the liquid flow rate (L), the packing size (d_p) and its wettability (σ_c), and the physical properties of liquid or absorption media like density, viscosity, surface tension etc. The values of d_p (hence a_t) and (σ / σ_c) appear to have substantial effect on the values of a_{st}. Therefore the model parameters in terms of dimensionless numbers which should be included in the static area correlation are Re, Fr, We and (σ / σ_c). The observed values of a_{st} can be correlated satisfactorily by the following generalised correlation :

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

The statistical analysis of this correlation can be described as follows :- % E_{avg} = 0.4, % E_{abs} = 12.34, % S_{dev} = 2.42.

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

(V) Generalised correlation for effective interfacial area during gas absorption (a_p and a_c) based on the model :-

The static area model developed in this investigation can be used successfully to predict the values of (a_p/a_t) by using the following correlation :-

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

The detailed statistical analysis of the correlation is as under :- % E_{avg} = 4.76, % E_{abs} = 18.23 and % S_{dev} = 5.04. The generalised correlations developed in this investigation for wetted surface area and static area can be used to obtain the values of $(a_w/a_t)_{pred}$ and $(a_{st}/a_t)_{pred}$ under otherwise identical conditions. Accordingly (a_p/a_t) can be predicted.

The static area model can also be used successfully to predict the values of (a_c/a_t) by using the following correlation :-

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

The detailed statistical analysis of the correlation is as under :-

% E_{avg} = 2.29, % E_{abs} = 20.28 and % S_{dev} = 0.95. The generalised correlations developed in this investigation for effective interfacial area during physical absorption and static area can be used to obtain the values of $(a_p/a_t)_{pred}$ and $(a_{st}/a_t)_{pred}$ under otherwise identical conditions. Accordingly (a_c/a_t) can be predicted.

Thus, the static area model developed in this investigation can be utilised for predicting the values of effective interfacial area during physical absorption as well as during chemical absorption. These generalised correlations developed are not merely empirical correlations but these correlations elucidate the mechanism of mass transfer during physical and chemical absorption.

10.3 CONCLUSIONS FOR MASS TRANSFER COEFFICIENTS :-

(I) Generalised correlation for volumetric liquid side mass transfer coefficient ($k_L a$) :-

The information available in the literature on the values of volumetric liquid side mass transfer coefficient ($k_L a$) was analysed in a systematic manner and a generalised correlation has been developed which takes into account the effect of the wettability of the packing material on the values of $k_L a$.

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

The statistical analysis of the correlation can be described as follows :- % E_{avg} = 2.48, % E_{abs} = 11.48 and % S_{dev} = 0.20. This

correlation is shown to be more reliable and more general than previously published correlations. The unusually high error in most of the existing correlations stems from the fact that none of these correlations incorporate the effect of parameter (σ / σ_c) on the values of $k_L a$. Further most of the existing correlations are able to predict the values of $k_L a$ only under the conditions where the values of μ_L are not significantly greater than those of water.

(II) True gas side and liquid side mass transfer coefficients (k_G and k_L) :-

The values of true gas side and liquid side mass transfer coefficients for physical absorption have been obtained by many investigators from the corresponding values of volumetric mass transfer coefficient - $k_G a$ or $k_L a$ by dividing them with the values of a_t or a_w. Both these approaches appear to be inappropriate.

It has been established in this investigation that the values of a_t, a_v, a_p, a_c and a_w differ considerably from each other. Hence, while obtaining the values of k_L and k_G from $k_L a$ and $k_G a$, one must use the appropriate values of 'a'.

Generalised correlation for k_G :-

The generalised correlation obtained in this investigation for predicting the value of k_G is as follows :-

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

The statistical analysis of this correlation can be described as follows :- % E_{avg} = 0.76, % E_{abs} = 12.17 and % S_{dev} = 0.30. The

values of k_G obtained from k_Ga (physical) data and k_Ga (chemical) data, also k_Ga during vaporization can be correlated satisfactorily by this generalised correlation within ± 20 % error. The existing generalised correlation of Onda et al. wherein the statistical analysis was % E_{avg} = 47.11, % E_{abs} = 47.11 and % S_{dev} = 0.048 failed to correlate satsifacorily the observed values of k_G. In particular the values of k_G obtained by chemical technique resulted in very high error in prediction by Onda's correlation. Hence the generalised correlation developed in this investigation appears to be more appropriate and sound than the correlation of Onda and such other correlations.

Generalised correlation for k_L :-

The generalised correlation developed in this investigation for predicting the values of k_L is as follows :-

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

The statistical analysis of this correlation can be described as follows :- % E_{avg} = 3.39, % E_{abs} = 11.32 and % S_{dev} = 0.002. The values of k_L obtained by chemical technique can be considered as real values of k_L and that obtained from k_La data can be considered as apparent values of k_L. As could be seen from the statistical analysis the values of k_L obtained from both the approaches can be correlated satisfactorily by the generalised correlation developed in this investigation. However, none of the existing correlations (of Onda, Mersmann and Billet) can correlate the k_L data satisfactorily.

(III) The mass transfer coefficient model and the generalised correlation for $k_L'a$:-

No study has been reported in the literature which established relationship between $(k_La)_{phy}$ and $(k_L'a)_{chem}$.

The mass transfer coefficient model proposed in this investigation is based on the assumption that the interface consists of two parts, that is the moving part and the semi-stagnant part. The the volumetric mass transfer coefficient for chemical absorption can also be splitted in two parts as under :-

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

Therefore, the model correlation for predicting the values of mass transfer coefficient with chemical reaction can be as under :-

$$(k_L'a)_{chem.} = \beta \cdot (k_La)_{phy.} + \sqrt{D_Lk_2[B]}\ (a_{st}).$$

The model parameters k_La and a_{st} can be evaluated from the generalised correlationsdeveloped for k_La and a_{st}.

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 values of $k_L'a$ can be predicted satisfactorily by the above model correlation. The statistical analysis of this correlation can be described as follows :

$\%\ E_{avg} = -4.2$, $\%\ E_{abs} = 15.5$ and $\%\ S_{dev} = 9.6$. The satisfactory data fit by the model correlation clearly indicates that the contribution due to the static/semi stagnantpart/film in $k_L'a$ correlation is fully effective during the regimes under consideration.

However, when the concentration of reactive species is very low and the regime is a slow reaction regime the model correlation to be utilised for predicting the values of $k_L'a$ is as under :-

$$[k_L'a]_{chem} = \beta \ (k_La)_{phy}.$$

Here, in this regime the static/semi-stagnant part of the film becomes saturated very quickly. Therefore, the part of the film becomes ineffective for mass transfer in the region of very low concentration of reactive species in the absorption media. The values of $k_L'a$ can be predicted satisfactorily by the above model correlation having statistical analysis as under :- $\% E_{avg} = 8.66$, $\% E_{abs} = 17.87$ and $\% S_{dev} = 1.93$.

(IV) k_La by chemical technique :-

The observed values of k_La obtained from $k_L'a$ in the regime of very low concentration of reactive species and also the k_La obtained by chemical technique using an instantaneous reaction can be predicted satisfactorily by the generalised correlation of k_La developed in this investigation for physical gas absorption. The statistical analysis of the data predicted is as follows :-

$\% E_{avg} = 6.40$, $\% E_{abs} = 12.84$ and $\% S_{dev} = 0.17$.

Thus, the mass transfer coefficient model proposed in this investgation can be conveniently used to predict the values of $k_L'a$ and k_La under different sets of conditions. These generalised correlations developed in this investigation for mass transfer coefficients are not merely empirical correlations but these

correlations elucidate the mechansim of mass transfer during chemical and physical absorption.

10.4 CONCLUSIONS FOR DISTILLATION IN PACKED COLUMNS :-

The static area model proposed for effective interfacial areas during gas absorption can be extended to distillation in packed columns. The static area is also likely to be ineffective for mass transfer during distillation. Hence, the values of effective interfacial areas during distillation and that during physical absorption are expected to be comparable. The true liquid side and gas/vapour side mass transfer coefficients during physical absorption and that during distillationa are also expected to be comparable.

The following model correlation can be used satsifactorily for predicting the values of HETP during distillation :-

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

The statistical analysis of the model correlation can be described as follows :- % E_{avg} = 6.28, % E_{abs} = 14.7 and % S_{dev} = 3.27. Hence the model parameters k_L, k_V, a_d and $(k_L a)_{dist.}$ 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 $(k_L a)_{phy.}$ 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.

SUMMARY

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.