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RIGOROUS AND SHORT-CUT DESIGN CALCULATIONS FOR GAS ABSORPTION INVOLVING LARGE HEAT EFFECTS PART I. A NEW COMPUTATIONAL METHOD FOR PACKED GAS ABSORBERS

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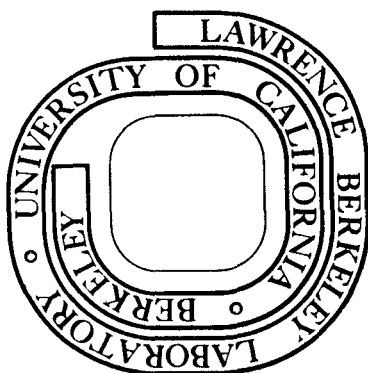
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RIGOROUS AND SHORT-CUT DESIGN CALCULATIONS  
FOR GAS ABSORPTION INVOLVING LARGE HEAT EFFECTS

PART I. A NEW COMPUTATIONAL METHOD FOR  
PACKED GAS ABSORBERS \*

by

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## ABSTRACT

Gas absorption in packed columns has been modelled taking into account all heat effects for physical gas absorption. Multicomponent diffusion effects were incorporated in terms of the film factor concept. An algorithm of very stable convergence behavior was obtained by simulating the start-up procedure of the column dynamically in order to evaluate the steady state operation. The importance of rigorous design calculations was assessed by comparing the rigorous solution with simplified hand-calculations for a large number of cases. If the solvent is volatile, it appears impossible to estimate the highly irregular temperature profiles by hand and to design the column approximately by simplified calculations based on neglecting one or more of the heat effects. Simplifying assumptions are also unsuitable to obtain a limiting conservative design.

## I. INTRODUCTION

Whenever a gas absorption process is to be designed, one of the most important considerations should concern the temperature distribution within the column because the solubility of the solute gas generally depends strongly on temperature. This profile must either be calculated by modelling the system rigorously or estimated by introducing simplifying assumptions. The classical assumption consisted of treating the process as isothermal. This made the design calculations extremely simple; e.g. on a McCabe-Thiele diagram.

An alternative classical simplification allowed for the heat of solution and rested on the assumption that the heat of solution will manifest itself entirely as sensible heat in the liquid stream. On the basis of this simple adiabatic model it becomes possible to relate the temperature increase experienced by the liquid flowing through the tower to the concentration increase through a simple enthalpy balance and thus to correct the equilibrium line in a Y-X diagram for the heat of solution.

But both these models represent oversimplifications, since the real situation implies a multitude of heat effects:

- 1) The heat of solution tends to increase the temperature and thus to reduce the solubility.
- 2) In case of a volatile solvent, partial solvent evaporation will absorb some of the sensible heat. This effect is particularly important with the cheapest of all solvents, namely, water.
- 3) Sensible heat will be transferred from the liquid to the gas phase and vice versa.

4) Sensible heat will be transferred from both phase streams to the shell of the column and from there to the outside, or to cooling coils.

These heat effects may only be neglected in very special circumstances, which are not normally fulfilled (1). If cooling coils are absent, it is often possible to neglect heat effect No. 4, since large scale absorption towers can be shown to operate predominantly adiabatically (1),(2). Although the temperature increases in gas absorption towers may alter solubilities very drastically, they often are not sufficiently large to cause an appreciable heat transfer to the surrounding air.

In the general case the temperature profile is determined by all four heat effects simultaneously. The temperature in turn influences the transfer of mass and heat to a large extent by changing the solubilities. This turns the simple process of gas absorption into a very complex process, with all factors exhibiting a high degree of interaction, which is essentially impossible to calculate without the aid of a digital computer.

In this paper, a rigorous model of the system will be presented along with a novel computing technique of superior convergence properties, which may serve to design gas absorption processes in packed towers rigorously on the computer while accounting for all possible heat effects. It is the goal of the second paper, Part II to present a new short-cut design procedure which also takes into account the heat effects and thus yields much better results than the two classical models mentioned at the beginning, while requiring rather less computation.

## II. FUNDAMENTAL EQUATIONS

If one interprets the process in terms of the two film theory, the application of the classical rate equations for mass transfer is inappropriate, because the gas phase mass transfer coefficient,  $k_G$ , is a function of concentration, since one is dealing with a situation involving diffusional transfer of several components simultaneously:

$$N_A = k_G P (Y - Y_i) \quad (1)$$

In principle, the mass transfer coefficient may only be regarded as constant in the special case of no net molar transport through the film, i.e. with equimolar counterdiffusion, which is obviously not necessarily true here. A possible choice in such situations are Colburn-Drew type rate equations (3), which operate with constant transfer coefficients, but are of very different form than the ordinary rate equation (1).

In order to preserve the normal concept of a linear driving force we based our model on the so called film factor concept developed by Wilke (4) which assumes that the flux through the stagnant film adjacent to the interface is given by expressions such as the following:

$$N_A = - \frac{D_{Am} P}{RT} \frac{dY_A}{dx} + t_A N_A Y_A \quad (2)$$

The last term in Eq. 2 represents the bulk flow of gas through the film, as  $t_A$  is defined as



$$t_A = \frac{\sum_j N_j}{N_A} \quad (3)$$

Equation 2 can be rearranged and integrated over the diffusion path to yield the following rate equation:

$$N_A = k'_{G,A} P (Y_A - Y_{Ai}) \cdot \frac{1}{(Y_f)_A} \quad (4)$$

where

$$(Y_f)_A = \frac{(1 - t_A Y_A) - (1 - t_A Y_{Ai})}{\ln \frac{1 - t_A Y_A}{1 - t_A Y_{Ai}}} \quad (5)$$

and

$$k'_{G,A} = \frac{D_{Am} P}{RT} = k_{G,A} \cdot (Y_f)_A \quad (6)$$

The gas phase mass transfer constant  $k'_G$  in the modified rate equation (4) has thus been made independent of the effect of net molar transport through the film. In situations involving a pair of ideal gases and in multicomponent mixtures where constant effective mean diffusivities  $D_{Am}$  may be used,  $k'_G$  is independent of concentration and constant. (For mixtures with a stagnant component the values of  $D_{Am}$  may be calculated according to the procedure suggested by Wilke (4). Formulas for  $D_{Am}$  in tertiary mixtures with a stagnant component are given by Treybal (5).) The concentration dependence due to the net molar transport in the rate equation (4) is separated from the transfer coefficient and reflected by a special function called the "film factor,"  $Y_f$ .

In situations with no net molar transport through the film, i.e. with equimolar counterdiffusion, the factor termed "t" becomes zero and the film factor equals unity irrespective of the concentrations. The modified rate equation (4) reduces, therefore, to the classical rate equation (1) with a constant gas phase mass

transfer coefficient, If, on the other hand, only one substance diffuses as in the common situation of unidirectional diffusion through a stagnant gas,  $t$  becomes unity and the film factor,  $Y_f$ , reduces to the familiar logarithmic mean of stagnant gas concentration between bulk and interface conditions, normally termed  $Y_{BM}$ :

$$Y_{BM} = \frac{(1 - Y) - (1 - Y_i)}{\ln \frac{1 - Y}{1 - Y_i}} \quad (7)$$

The film factor,  $Y_f$ , may therefore be interpreted as a  $Y_{BM}$ -factor generalized for more than one diffusing component which corrects the rate equations for the effect of net molar transport of material through the film. For strong counterdiffusion, giving rise to a net molar movement of mass which is opposed to the diffusion of the species under consideration, the film factor becomes larger than unity and therefore decreases the flux of this species. For weak or negative counterdiffusion, producing a bulk movement in the same direction of the diffusion of the component under consideration,  $Y_f$  is smaller than one and increases its flux. In special situations the counterdiffusion may become large enough to reverse the direction of transport of a given component and thus to force it to diffuse against its own driving force. These situations are characterized by negative film factors.

For integration purposes it is often preferable to work with heights of a transfer unit rather than with mass transfer coefficients, as the former may be considered constant in a wider range. The rate equation for the model then becomes:

$$N_j^a = \frac{G_M}{H_{G,j}} (Y_j - Y_{ji}) \cdot \frac{1}{(Y_f)_j} \quad (8)$$

with

$$H_{G,j} = \frac{G_M}{k'_{G,j} P} = \text{gas phase height of a transfer unit} \quad (9)$$

$j = A$  for solute,  $j = B$  for solvent

Since the "film factor concept" preserves the familiar form of a linear driving force, the interfacial concentrations may be found in the usual way as the intersection of the equilibrium curve and a tie line whose slope is given by:

$$\frac{Y_j - Y_{ji}}{X_j - X_{ji}} = - \frac{k'_L \bar{\rho} (Y_f)_j}{k'_{G,j} P (X_f)_j} = - \frac{H_{G,j} L_M (Y_f)_j}{H_L G_M (X_f)_j} \quad (10)$$

This expression is found by combining Eq. 4 with a similar one for the liquid side. In solving the equations advantage can be taken of the fact that the film factors, and especially their ratio, are in many cases not far from unity.

The interfacial temperature is found by a similar procedure applying rate equations for the sensible heat:

$$q = h_G (T_G - T_i) \cdot \frac{1}{T_f} = h_L (T_i - T_L) \quad (11)$$

In an analogous form to Eq. 4, in Eq. 11 the gas phase heat transfer coefficient has been made independent of mass transfer effects, which are reflected in a special function,  $T_f$ :

$$T_f = \frac{1 - e^{c_0}}{c_0} \quad (12)$$

$$c_0 = \frac{1}{h_G} (c_{pA} N_A + c_{pB} N_B) \quad (13)$$

## 2. The Dynamic Model

The convergence problems associated with the two point boundary value problem can be avoided and a certain convergence insured by simulating the start-up procedure of the column. If the model of the column is realistic enough, the computation must converge irrespective of the starting values--just as the physical column does.

This method has been developed and its effectiveness demonstrated only for plate absorber calculations (10) (11) (12). To apply it to packed columns, the differential unsteady state mass and enthalpy balances must be formulated for the packing and integrated with respect to time up to the steady state:

$$\frac{\partial (L_M X_A)}{\partial z} - \frac{\partial (G_M Y_A)}{\partial z} = \frac{\partial X_A}{\partial t} b \quad (14)$$

$$\frac{\partial (L_M \bar{h}_L)}{\partial z} - \frac{\partial (G_M \bar{h}_G)}{\partial z} - H_{ex} = \frac{\partial \bar{h}_L}{\partial t} b \quad (15)$$

### a. General Procedure

Convenient algorithms for the above procedure are shown in Figs. 1 and 2. Since the dynamic model closely simulates a real column, the computations should be done at a fixed tower height. If, in the design calculation, the steady state does not yield the specified recovery, the tower height is adjusted iteratively as shown in Fig. 1 to match the specification. Very fast convergence is obtained using a Newton-Raphson scheme based on a logarithmic function of the recovery, because the solute content of the exit gas roughly decreases exponentially with the tower height.

$1/T_f$  is equivalent to the Ackermann correction for large mass transfer fluxes (6).

### III. COMPUTATIONAL METHOD

#### 1. General Considerations

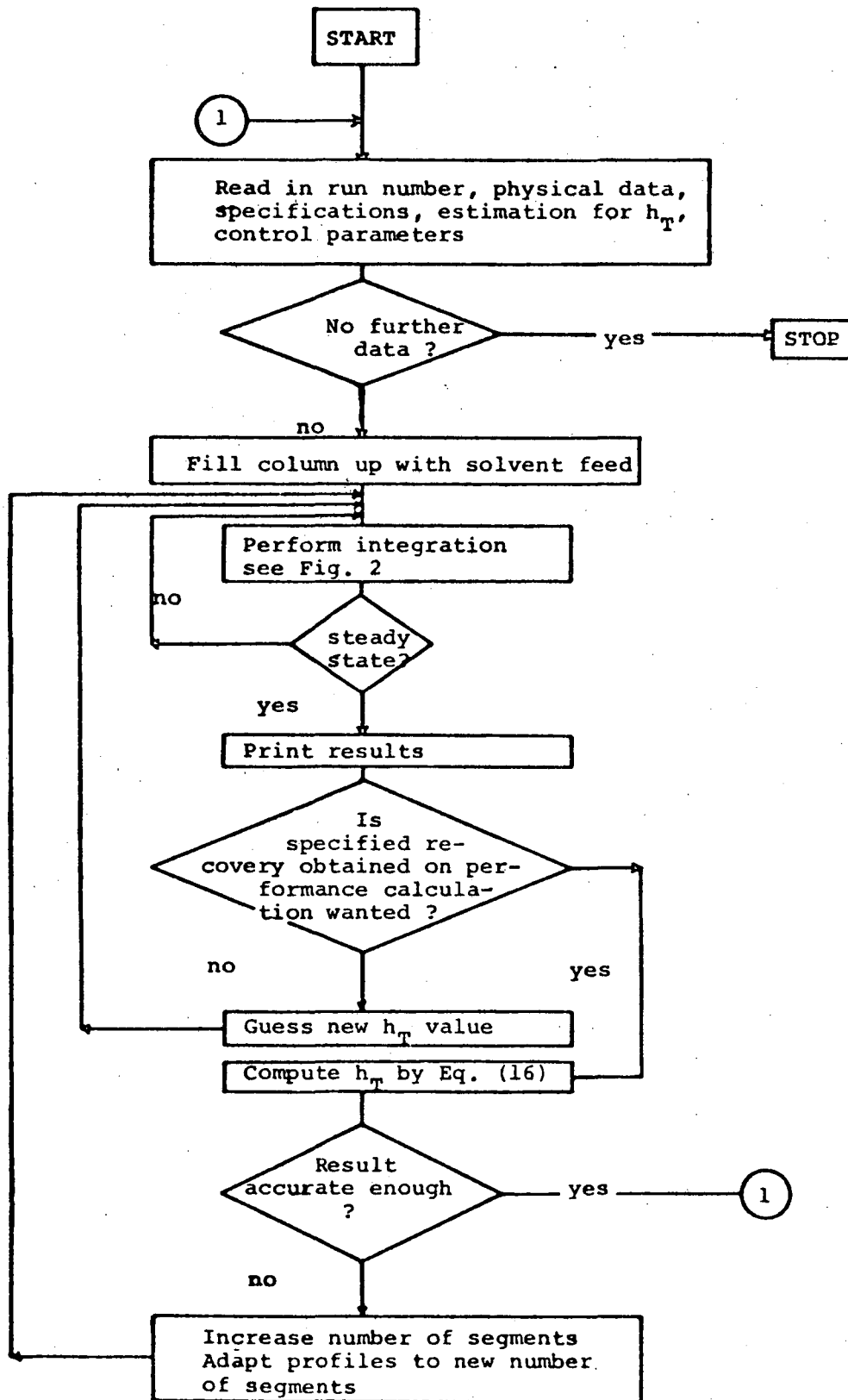
It can be shown that the degrees of freedom available in gas absorber calculations never suffice to specify all the variables in one of the exit streams if the feed streams are specified. Therefore, the state of neither end of the column is known completely in advance, which leads to a two point boundary value problem when integrating the profiles through the tower. This integration is usually started at one end of the tower by assigning trial values to the unknown variables in the exit stream which must be checked and improved iteratively. In gas absorption calculations, this may present extremely difficult convergence problems requiring a great deal of experienced judgment in choosing the trial values (7)(8). Among the more important reasons which have been discussed in detail by Bourne et al. (1), is that most gas solutions involved in gas absorption processes are strongly non-ideal in behavior and thus give rise to a highly coupled and non-linear system of equations and to irregular, unpredictable concentration and temperature profiles.

A computational method based on such iterations was suggested by Treybal (5) and tested by Raal and Khurana (9). Although it worked well for the absorption of ammonia in water at molar L/G ratios of higher than 6, it is not known whether it would converge in cases with lower L/G ratios and with highly irregular temperature profiles exhibiting sharper maxima.

To simulate the accumulation rates at various locations in the column in a digital computer, it is necessary to divide the packing up arbitrarily into segments of finite length. Our model approximates the absorber by a number of segments of uniform average liquid concentrations and driving forces. The accuracy of the approximation is, of course, increased if more of those segments are introduced, but the number of segments required for a certain degree of accuracy depends on the nature of the problem under consideration. On the other hand, it was found that the computations reached the steady state much faster with a small number of segments. It was, therefore, possible to economize a substantial amount of computing time by first calculating the profiles roughly using a small number of segments, e.g. 25. The subsequent refinement of the profiles with a larger number can be done in a comparatively short time because it requires only minor adjustments to already existing profiles. To take full advantage of this strategy, our program was equipped with a special subroutine capable of adapting the profiles to any new number of segments by estimating the values in the new subdivisions through interpolation.

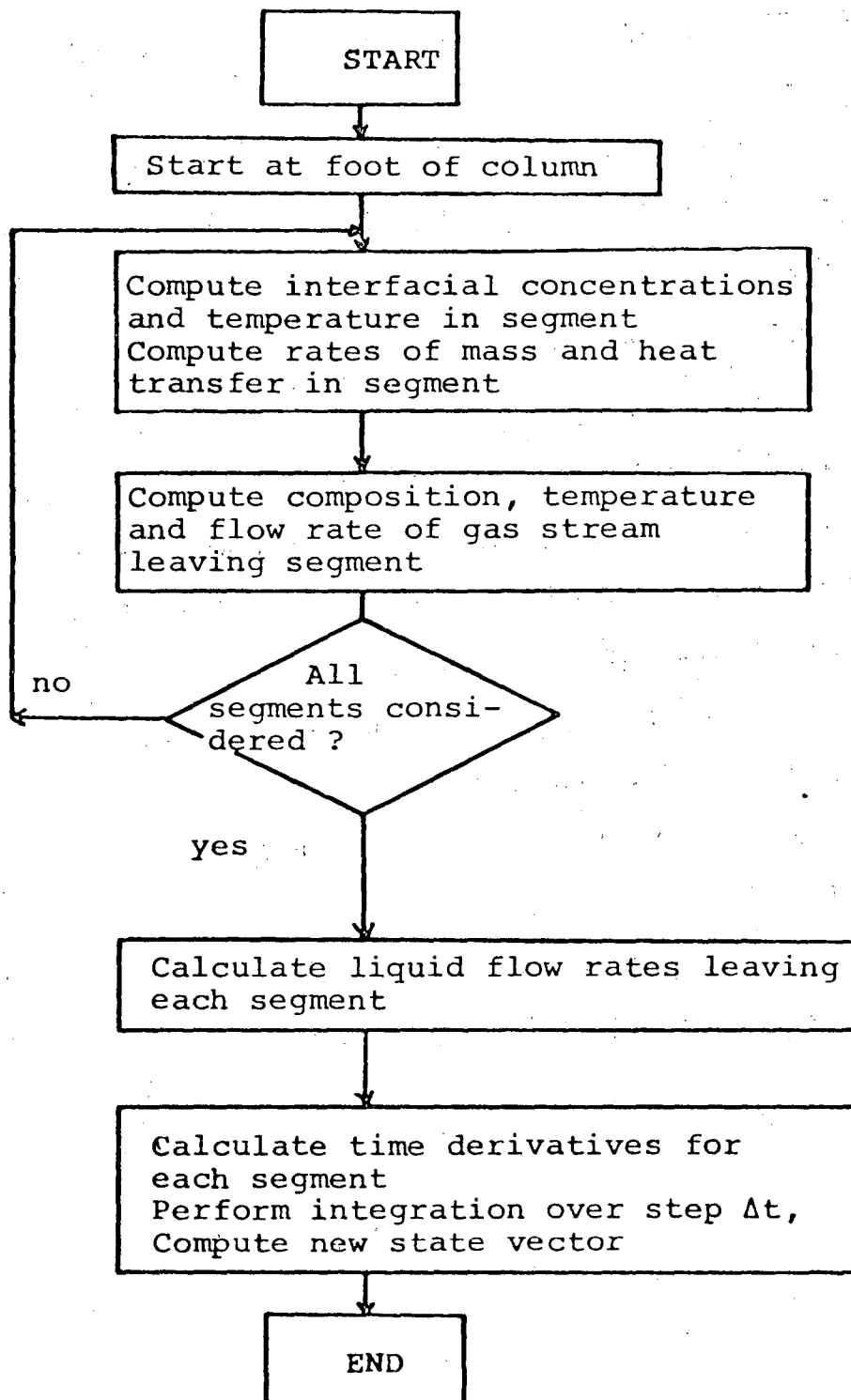
As shown in Fig. 1, the accuracy of the approximation by a given number of segments was checked by integrating numerically on the basis of the established profiles the following equation, which represents a rigorous expression for the tower height in terms of the film factor theory:

$$h_T = \int_{Y_2}^{Y_1} H_G \frac{(Y_f)_A}{(1 - t_A Y_A)} \frac{dY_A}{Y_A - Y_{Ai}} \quad (16)$$



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Fig. 1. Flow diagram for computing packed gas absorption columns.



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Fig. 2. Algorithm for integrating unsteady state mass and enthalpy balances.



The value computed by Eq. 16 and the current value used to integrate Eqs. 14 and 15 to the steady state normally embrace the true solution and converge to it as the number of segments is increased. The computations done for this study were normally carried out with an accuracy of 1-2% which never required more than 100 segments.

#### b. Integration

The algorithm integrating Eqs. 14 and 15 is shown in Fig. 2 and its general organization is similar to corresponding algorithms published for tray columns (1)(10). The computations start by setting the liquid compositions and mean molar liquid enthalpies in all the segments, an array of numbers called the "state vector," equal to the corresponding values in the entering solvent stream, i.e. the column is filled up with the solvent feed.

Starting from the known gas feed at the foot of the tower and working upwards, the states of the gas streams leaving each segment or slice may be computed by mass and heat balances neglecting the gas hold-up in the segments:

$$G_{M, k+1} Y_{j, k+1} = G_{M, k} Y_{j, k} - N_{j, k} a \Delta z \quad (17)$$

$$G_{M, k+1} \bar{h}_{G, k+1} = G_{M, k} \bar{h}_{G, k} - q_k a \Delta z \quad (18)$$

$$G_{M, k+1} = G_{M, k} - (N_A + N_B) a \Delta z \quad (19)$$

Use of Eqs. 17 and 18 requires evaluation of the fluxes  $N_j$  and  $q_k$  via Eqs 8 and 11, for which the interfacial compositions and the interfacial temperature must be known. They are evaluated

first on the basis of the known states of the bulk liquid and gas phases using Eqs. 10 and 11.

To compute the interfacial conditions the following additional information is required:

Physiochemical data:

1) Equilibrium partial pressures of solute and solvent as functions of temperature and composition, allowing for non-idealities as accurately as possible:

$$Y_{ji} = f_{ji}(T_i, P) \quad (20)$$

2) Heat of solution  $H_{OS}$  for the solute and latent heat of evaporation  $H_V$  for the solvent. A single constant typical for the concentration and temperature range of interest is often sufficient.

3) Specific heat capacities of all the substances in the states in which they are present.

Mass, heat and momentum transfer data:

1) Gas and liquid heights of a transfer unit for the transferring substances,  $H_{G,j}$  and  $H_{L,j}$ . At high concentrations, their variation with the mass velocities should be accounted for;  $H_L$  should be given as a function of temperature.

2) Pressure drop as a function of the mass velocities.

This data is supplied to the program either as constants or in the form of regression models fitted to experimental values and organized as independent subroutines.

The algorithm used to solve for the interfacial conditions determines  $t_A$  and  $T_f$  iteratively in an outer loop applying Eqs. 3, 12 and 13. In a nested loop, the interfacial concentrations and temperature are found by means of Eqs. 10, 20 and 11, and

Eq. 8 is used to compute the fluxes. When the film factors are still unknown at the first time they are evaluated for each segment, their ratio may be assumed unity as a good approximation in the first trial. Iterations were normally carried out following a modified Wegstein method.

After determining the states of the gas streams leaving the slices for the whole column, the liquid flow profile ( $L_M$ ) is completed from

$$\frac{\partial L_M}{\partial z} = \frac{\partial G_M}{\partial z} \quad (b = \text{const.}) \quad (21)$$

leading to:

$$L_{M,k-1} = L_{M,k} + G_{M,k-1} - G_{M,k} \quad (22)$$

The time derivative of the state vector is then calculated applying a finite difference form of Eqs. 14 and 15. New values for liquid concentrations and mean molar enthalpies are found by integrating over  $\Delta t$ , e.g. employing a simple linearization or a Runge-Kutta procedure. The new liquid temperatures in the segments are found from the new values for the mean molar enthalpy and the composition of the liquid.

The integration is discontinued and steady state assumed when the accumulation rates of the column, based on the segment showing the largest accumulation rate, have fallen below a certain fraction of the liquid flow rate, e.g. 1%:

$$\left[ N_p \max \left\{ \frac{\Delta X_A}{\Delta t} \frac{\tau_k}{X_{A,k}} \right\} < 0.001 \right] \wedge \left[ N_p \max \left\{ \frac{\Delta \bar{h}_L}{\Delta t} \frac{\tau_k}{\bar{h}_{L,k}} \right\} < 0.001 \right] \quad (23)$$

The algorithm just described is given in full detail and further

explained elsewhere (15).

c. Convergence behavior

The computing time requirement to reach the steady state decreases as  $\Delta t$  is increased, but no convergence is obtained if the time step exceeds a certain value. When a linearization was used for the integration, the critical value of  $\Delta t$ , giving the fastest possible convergence, was found to be in an almost constant relation to the residence time of the liquid phase in each segment, irrespective of the problem under consideration:

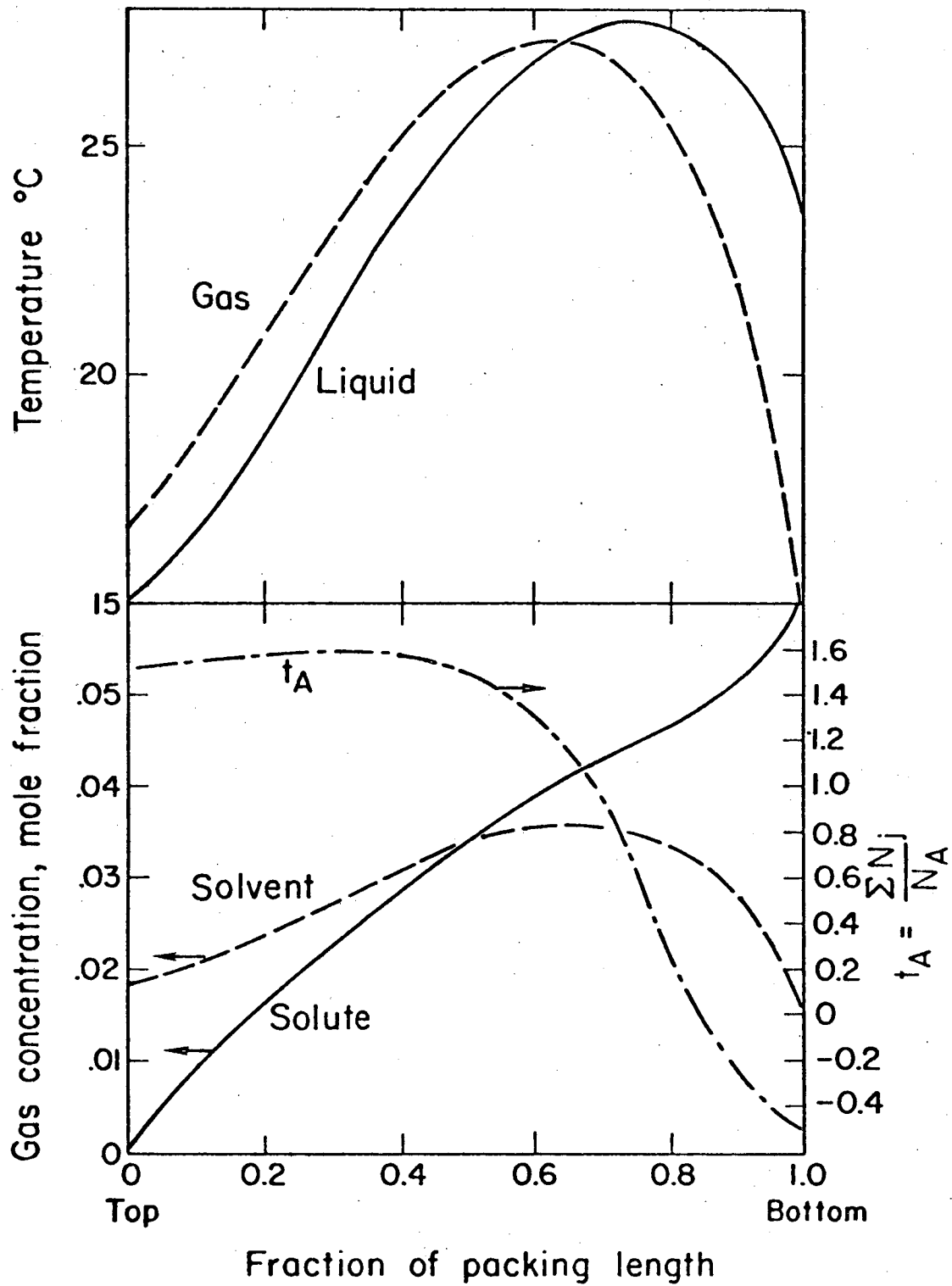
$$0.77 \leq \frac{\Delta t_{\text{crit}}}{\tau} \leq 0.9$$

Computing at a  $\Delta t$  near the critical value, a CDC 7600 digital computer needed less than 2 seconds to reach a steady state with 50 segments.

#### IV. RESULTS

##### 1. Calculated Profiles

The consequences of large heat effects are illustrated in Figures 3 and 5 using a typical design example. The example was selected from the textbook "Mass Transfer" by Sherwood, Pigford and Wilke (13) and is specified as follows: 4000 ft<sup>3</sup> of air per hour containing 6 mole-% of acetone are to be scrubbed countercurrently with water in order to recover 90% of the acetone. The water flow rate is 20% greater than the theoretical minimum and the temperature is 15°C. The gas is also at 15°C and saturated with water vapor. The problem calls for the determination of the required height of packing. (Details of the problem and of the solutions are given in the appendix of Part II of this work.)



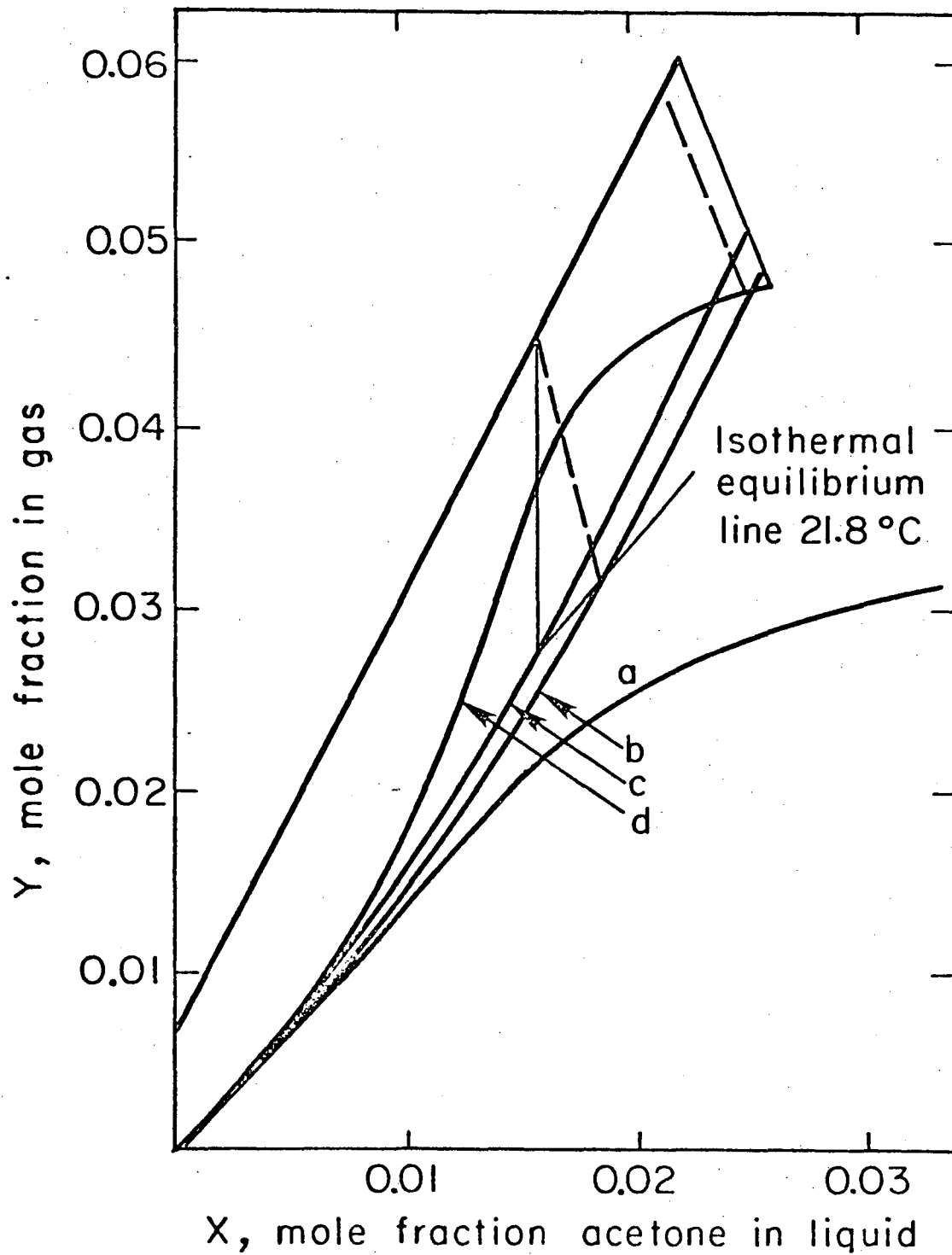
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Fig. 3. Computed rigorous profiles through column for design example.

Figure 3 shows the rigorously computed temperature and gas concentration profiles for this example. It is a typical feature of such calculations that the shapes of the temperature profiles are highly irregular and often exhibit maxima within the column. Such internal temperature maxima have been observed experimentally in plate and packed absorbers (9) (16) (14) and shown to agree closely with rigorous computations.

The temperature maximum occurs in part because the heat of solution causes the entering liquid stream to be heated up considerably. In the lower part of the tower, however, the heat of absorption is smaller than the opposite heat effects of solvent evaporation and heat transfer to the cold entering gas so that the net effect is a cooling of the liquid phase. As is obvious from Fig. 3, these transfers are reversed in the upper part of the column where the gas gives up sensible heat to the liquid and some of the solvent condenses from the gas stream into the liquid stream, which is therefore heated up much faster than would be the case with the absorption alone.

Because of solvent evaporation and condensation, the degree of counterdiffusion varies widely over the tower, as illustrated in Fig. 3 by the profile of the factor  $t_A$ , which is used in Eq. 5 to compute the film factor along the packing.  $t_A$  assumes negative values near the bottom of the tower, where solvent evaporation causes strong counterdiffusion, and varies to positive values higher than unity in the upper part, where solvent condensation causes parallel diffusion. The two conventional simplifying assumptions, namely, equimolar counterdiffusion ( $t_A = 0$ ) and



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Fig. 4. Y-X diagram for absorption of acetone in water (see Part II).

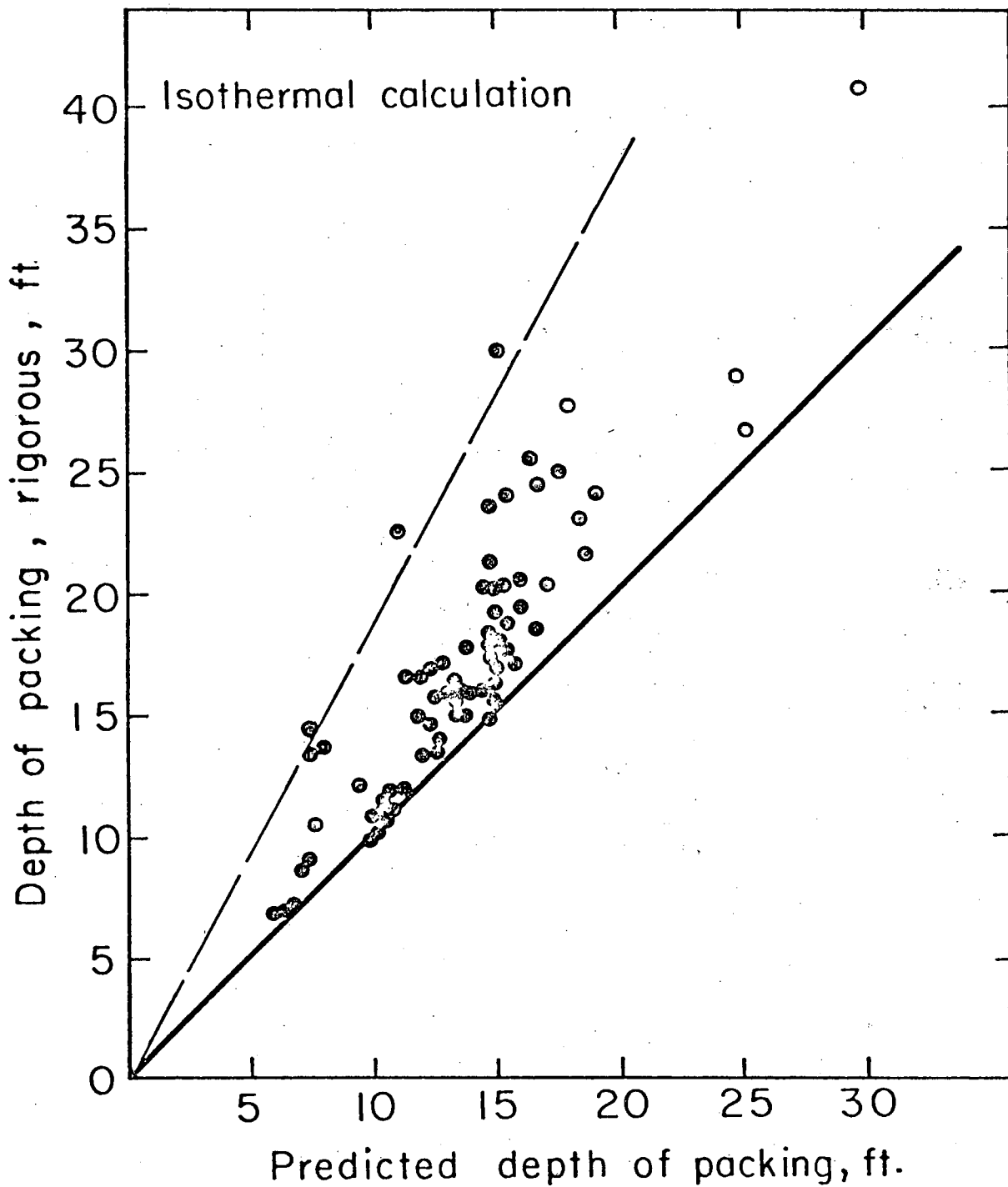
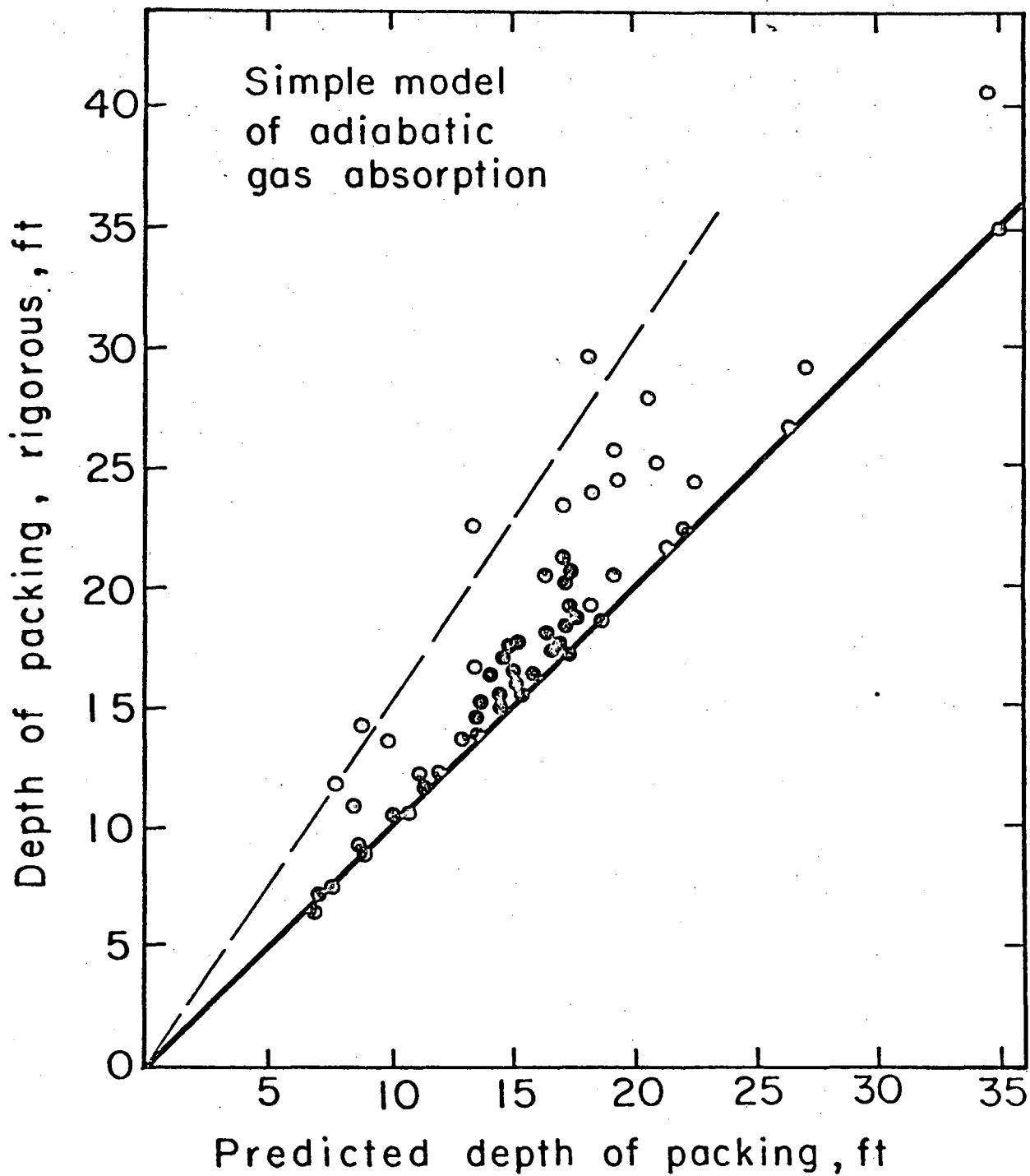


Fig. 5. Comparison of rigorous calculation and isothermal approximation.

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Fig. 6. Comparison of rigorous calculation and simple adiabatic model.

unidirectional diffusion through a stagnant gas ( $t_A = 1$ ) are valid approximations only in very short segments of the packing.

Figure 4 depicts the rigorously computed Y-X diagram for example shown in Fig. 3. The temperature maximum within the column produces a region of reduced solubility reflecting itself in the typical bulge in the middle of the equilibrium line (d). Since less acetone is absorbed in this part of the equipment, the gas concentration curve exhibits a slight plateau (Fig. 3).

## 2. Comparison of Rigorous Solution and Approximations

The example may also serve to demonstrate how difficult it is to estimate the required depth of packing approximately using simplifying assumptions. The isothermal approximation fails completely in this case yielding 6.4 ft of required packing as opposed to the rigorous answer of 11.90 ft. Neglecting the temperature increase completely, this model assumes a solute solubility much too large, reflected by equilibrium line (a) and thus underestimates the rigorous result by 90%.

The standard way to correct approximately for the heat of solution is to employ the simple adiabatic model mentioned in the introduction, which yields equilibrium line (b) if the gas phase driving force is used and line (c) on the basis of the overall driving force. (These two equilibrium lines coincide in non-isothermal gas absorption diagrams only in cases with no liquid mass transfer resistance. Because the interfacial temperature  $T_i$  and the bulk liquid temperature are virtually equal, the equilibrium concentration,  $Y_A^*$ , i.e. the gas concentration which would be in equilibrium with the bulk liquid ( $X_A, T_L$ ) is connected on the diagram with the actual interfacial concentration  $Y_i$  by an

isotherm.)

The simple adiabatic model is obviously a poor representation of the conditions prevailing in the absorber, as demonstrated by the deviation of its equilibrium line (b) from the rigorous line (d). The approximation underestimates the true value of 11.9 ft. by more than a third and yields 7.8 ft.

The rigorous design procedure is compared with the isothermal and the simple adiabatic approximations in Figs. 5 and 6 by plotting the results over 90 hypothetical rigorous design calculations versus the approximation estimations. Most of the cases involve volatile solvents. The design examples, which cover a wide range of system properties and operating conditions are described further in Part II, Table 1 where they are employed as a basis for development of a short-cut design procedure. With the isothermal approximation (Fig. 5), the points are scattered over a wide range and indicate that the rigorously computed tower heights often exceed the estimations by almost a factor of two. A much larger fraction of cases fall on the ideal 45 degree line if the simple model of adiabatic gas absorption is used as an approximation. Many cases, however, are still underestimated by as much as 30%.

One might argue that the simple adiabatic model should at least be of value in obtaining a conservative result or an upper limit, as the two heat effects neglected by this model, namely solvent evaporation and heat transfer to the gas phase, can both be expected to "cool" the liquid phase. Bourne et al. (14) indeed found that the model often yielded more conservative results than both the rigorous calculations and the experimental

measurements in a study on plate absorbers. In the calculations depicted in Figs. 4 and 6, however, this is obviously not the case: the simple model underestimates the true value in most cases by up to 30%. This condition is typical for high solute recoveries, where the exit gas cannot deviate far in temperature from the cold solvent feed. The amount of enthalpy which can be removed by the gas phase, and therefore its overall cooling effect, is very limited in such cases. Although a large amount of sensible heat is absorbed in the lower part of the tower by the gas phase due to solvent evaporation, most of it must be returned to the liquid near the top and merely serves to heat it up. Therefore, the temperature maximum becomes more pronounced, the average temperature higher and the amount of required packing larger than without solvent evaporation and liquid/gas heat transfer.

## V. CONCLUSIONS

The results of this study show that nothing short of the rigorous calculation on the computer will yield a sufficiently certain solution for design purposes if the solvent is volatile. Although the conventional short-cut techniques, the isothermal approximation and the simple adiabatic model may give good estimations in certain cases, their accuracy is no better than mere rough guesses in other instances, and, more important, it is not normally possible to recognize the cases in which the simple computation suffice beforehand without a rigorous treatment on the digital computer.

The rigorous solution is readily available through the

algorithm employed above. The dynamic model, based on the film factor concept, guarantees a stable and certain convergence in all cases irrespective of the starting values.

Despite the reliability of the present rigorous method an approximate, reasonably accurate, short-cut method would be very desirable. For even if computer access is available and appropriate models known through the literature, it still takes a considerable amount of time and effort to set up a program of this complexity and to insure its trouble-free operation. This is often too time consuming and cumbersome a procedure to follow for a first approximate assessment of a design problem. Therefore, the development of a suitable short-cut design procedure will be described in Part II of this study.

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Symbols

$a$	Specific interfacial surface, $\text{ft}^{-1}$
$b$	Specific liquid holdup, $\text{lb moles}/\text{ft}^3$
$c_p$	Specific heat of a gas, $\text{cal}/(\text{mole})^\circ\text{C}$
$c_q$	Specific heat of a liquid, $\text{cal}/(\text{mole})^\circ\text{C}$
$D_{jm}$	Effective diffusivity of component $j$ in a mixture, $\text{ft}^2/\text{hr}$
$G_M$	Molar gas flow rate, $\text{lb mole}/(\text{hr})$ or $\text{lb mole}/(\text{hr})(\text{ft}^2)$
$H_{\text{ex}}$	Enthalpy loss transferred through shell and cooling coils, $\text{cal}/(\text{hr}\text{-ft}^2)$
$H_G$	Gas phase height of a mass or heat transfer unit, $\text{ft}$
$H_L$	Liquid phase height of a transfer unit, $\text{ft}$
$H_{\text{OG}}$	Overall gas phase height of a transfer unit, $\text{ft}$
$H_{\text{OS}}$	Integral heat of solution for solute, $\text{cal}/\text{mole}$
$H_V$	Heat of vaporization for solvent, $\text{cal}/\text{mole}$
$h_G$	Heat transfer coefficient for gas film, $\text{cal}/(\text{hr})(\text{ft}^2)^\circ\text{C}$
$\bar{h}_G$	Mean enthalpy of the gas, $\text{cal}/\text{lb mole}$
$\bar{h}_L$	Mean enthalpy of the solution, $\text{cal}/\text{lb mole}$
$h_T$	Required tower height, $\text{ft}$
$k_G$	Gas phase mass transfer coefficient, $\text{lb mole}/(\text{hr})(\text{ft}^2)(\text{atm})$
$k'_G$	Modified gas phase mass transfer coefficient, independent of concentration, $\text{lb mole}/(\text{hr})(\text{ft}^2)(\text{atm})$
$k'_L$	Modified liquid phase mass transfer coefficient, independent of concentration, $\text{lb mole}/(\text{hr})(\text{ft}^2)$
$L_M$	Molar liquid flow rate, $\text{lb mole}/\text{hr}$ or $\text{lb mole}/(\text{hr})(\text{ft}^2)$
$m_j$	Slope of equilibrium line of component $j$ , if without subscript, for solute

$N_p$	Number of segments in column
$N_j$	Flux of component $j$ through interface, lb mole/(hr)(ft <sup>2</sup> )
$p$	Pressure, atm
$p_j^o$	Vapor pressure of pure component $j$ , atm
$q$	Heat flux through interface, cal/(hr)(ft <sup>2</sup> )
$T$	Temperature, °K or °C
$t$	Net molar bulk flux per flux of solute, Eq. 3
$t$	Time, hr
$t_j$	Net molar bulk flux per flux of component $j$ , Eq. 3, Absorption is counted positively
$x_j$	Mole fraction of component $j$ ; if $j$ not specified, of solute
$(x_f)_j$	$= \frac{(1-t_j x_j) - (1-t_j x_{ji})}{\ln \frac{1-t_j x_j}{1-t_j x_{ji}}}$ , liquid film factor for component $j$ ; if $j$ not specified for solute
$Y_j$	Mole fraction of component of component $j$ ; or of solute if $j$ not specified
$Y_j^*$	Equilibrium concentration of component $j$ , or of solute if $j$ not specified
$(Y_f)_j$	Gas film factor of component $j$ , Eq. 5; or of solute if $j$ no specified
$Y_{BM}$	$= \frac{(1-Y) - (1-Y_i)}{\ln \frac{1-Y}{1-Y_i}}$ , logarithmic mean of stagnant gas concentration
$Y_f^*$	$= \frac{(1-tY) - (1-tY^*)}{\ln \frac{1-tY}{1-tY^*}}$ , film factor, overall driving-force basis (for solute)
$z$	Packed height, ft
$\Delta z$	Height of one segment
$\bar{\rho}$	Mean density of liquid, lb mole/ft <sup>3</sup>



Subscripts

A	Component A = solute
B	Component B = solvent
C	Component C = inert gas
G	Gas
Av	Average
i	Interphase
j	Component j
L	Liquid
k	Segment k, Segments are numbered from bottom to top; values refer to cross section <u>below</u> segment with corresponding numbers
1	Foot of absorber
2	Top of absorber

Captions

- Figure 1                    Flow diagram for computing packed gas absorption columns
- Figure 2                    Algorithm for integrating unsteady state mass and enthalpy balances
- Figure 3                    Computed rigorous profiles through column for design example
- Figure 4                    Liquid temperature profiles at different operating conditions
- Figure 5.                    Y-X diagram for absorption of acetone in water (see Part II)
- Figure 6                    Comparison of rigorous calculation and isothermal approximation
- Figure 7                    Comparison of rigorous calculation and simple adiabatic model

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