

THE ANALYTICAL CALCULATION OF THE NUMBER OF THEORETICAL PLATES

By

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I. Historical review

Besides the theoretically exact graphical determination and several approximative solutions, the *Lewis' integral* [2, 3, 4], — taking into account some restrictions enumerated below — is known for the determination of the number of theoretical plates.

1) Equal molal flow is assumed in the entire column (i.e. the operation line is linear, $R = \text{const}$).

2) Concentration change from plate to plate is low enough and constant; i.e. as shown in a former publication [1] on the general mathematical treatment of the problem the operation line and the equilibrium line are linear and nearly parallel. (Linear operation line is supposed implicate in Lewis' calculations as well.) The approaching integral of LEWIS [2] derived on the above-mentioned conditions is the following, using the symbols introduced in [1]:

$$(N_L)_{\text{rect}} = \int_{x_T}^{x_D} \frac{g'(x)}{f(x) - g(x)} dx \quad \text{and} \quad (N_L)_{\text{exh}} = \int_{x_M}^{x_T} \frac{g'(x)}{f(x) - g(x)} dx \quad (1)$$

where $y = f(x)$ is the equilibrium line function and

$y = g(x)$ is the operation line function in the x — y co-ordinate system.

LEWIS made no attempts at the explicit solutions of the integral but treated a non-ideal mixture, viz. alcohol and water by using graphical integration.

An explicit solution of the Lewis-integral was found by DODGE and HUFFMANN [3] introducing a further restriction.

3) The equilibrium curve of nearly ideal mixtures — e.g. that of hydrocarbons — can be approximated by the function $f(x) = \frac{x}{1 + (\alpha - 1)x}$ where $\alpha = \text{const}$. The *Dodge—Huffmann* integral — in the book of ROBINSON and GILLILAND [4] called the "Lewis Method" — results as follows:

$$(N_L)_{\text{rect}} = \frac{1 + \frac{b_1}{2}}{\sqrt{b_1^2 - 4 a_1 c_1}} \ln \left[\frac{x_D + A_1}{x_T + A_1} \cdot \frac{x_T + B_1}{x_D + B_1} \right] - \frac{1}{2} \ln \frac{a_1 x_D^2 + b_1 x_D + c_1}{a_1 x_T^2 + b_1 x_T + c_1} \quad (2a)$$

where

$$A_1 = \frac{b_1 - \sqrt{b_1^2 - 4 a_1 c_1}}{2 a_1},$$

and

$$B_1 = \frac{b_1 + \sqrt{b_1^2 - 4 a_1 c_1}}{2 a_1}$$

$$a_1 = -(\alpha - 1)$$

$$b_1 = (\alpha - 1) \cdot \left(1 - \frac{x_D}{R}\right) + \frac{\alpha}{R}$$

$$c_1 = -\frac{x_D}{R};$$

and

$$(N_L)_{\text{exh}} = \frac{1 + \frac{b_2}{2}}{\sqrt{b_2^2 - 4 a_2 c_2}} \ln \left[\frac{x_T + A_2}{x_M + A_2} \cdot \frac{x_M + B_2}{x_T + B_2} \right] - \frac{1}{2} \ln \frac{a_2 x_T^2 + b_2 x_T + c_2}{a_2 x_M^2 + b_2 x_M + c_2} \quad (2b)$$

where

$$A_2 = \frac{b_2 - \sqrt{b_2^2 - 4 a_2 c_2}}{2 a_2},$$

and

$$B_2 = \frac{b_2 + \sqrt{b_2^2 - 4 a_2 c_2}}{2 a_2}$$

$$a_2 = 1 - \alpha$$

$$b_2 = (\alpha - 1) \left[1 + \frac{\beta}{R + 1 + \beta} x_M \right] - \alpha \frac{\beta}{R + 1 + \beta}$$

$$c_2 = \frac{\beta}{R + 1 + \beta} x_M, \quad \text{and} \quad \beta = \frac{x_D - x_T}{x_T - x_M}.$$

According to graphical solutions and computations, the value N_L obtained by the Lewis'-integral, or by the explicit form derived by *Dodge* and *Huffmann*, approximates the "real" value N only if α is sufficiently small. (The condition 2 for the concentration change per plate is satisfied for small values of α only.)

2. A new analytical determination of the number of theoretical plates

Condition 2 — being to severe in actual circumstances — restricts the utility of the final integral.

Assuming equal molal flow only a new integral has been obtained for the calculation of the number of theoretical plates in a former paper [1] on

the analytical determination of the problem. The well-known mathematical method, the substitution of optional sections of the $y = f(x)$ equilibrium curve using a polygon of chords is applied (by drawing lines through the smoothed points of measurements) and the partial results obtained for the single chords are summed up further. In the system of equations, constructed from the equations of the chords referring to experimental data and from those of the material balance concerning the single plates; the *number of the equations* — being equal to the number of plates to be found — is considered unknown and assuming linear operating line — it can be expressed by a recursive formula. Using the mean value theorem of the differential calculus, and increasing the number of chords of the substituting polygon, the sums in the expression for the number of equations converge to the following integrals:

$$N \simeq N_I = (N_I)_{\text{rect}} + (N_I)_{\text{exh}} = \int_{x_r}^{x_D} \frac{f'(x) - g'(x)}{\ln \frac{f'(x)}{g'(x)}} \frac{dx}{f(x) - g(x)} + \int_{x_M}^{x_r} \frac{f'(x) - g'(x)}{\ln \frac{f'(x)}{g'(x)}} \frac{dx}{f(x) - g(x)} \quad (3)$$

where $y = f(x)$ is the equation of the smoothed equilibrium line and $y = g(x)$ is that of the operating line.

The above restriction for the integral N_I , i.e. replacing the curve $f(x)$ by a chord within a single stage — is admissible for every not extremely curved equilibrium line or for relative high numbers of theoretical plates and as a difference to Lewis' integral it ought to be valid for higher values of α as well, in consequence of the above mentioned mean-value theorem. For high numbers of the theoretical plates the integral N_I is a closer approaching to the "real" number N , determinable principally by graphical method only, but showing great technical difficulties for this reason.

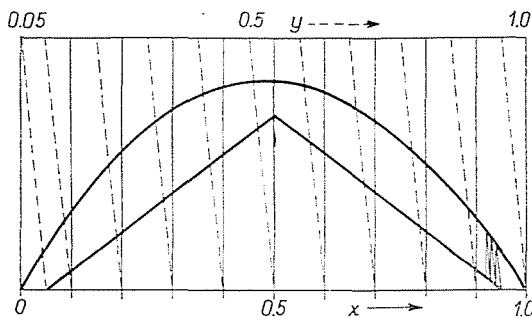


Fig. 1. Graphical determination of the number of theoretical plates on a bevel-angle co-ordinate system

Values calculated according to the integral (the method of calculation will be shown later) agree with those of the number of theoretical plates N determined by graphical method assuming equal molal flow. The accuracy of the graphical plotting was enhanced by using a large-scale bevel-angle $x - y$ co-ordinate system (cf. Fig. 1). The validity of Lewis' integral for $f'(x) = g'(x)$ — i.e. only if the equilibrium line runs parallel with the linear operating line — was proved. As a difference from Lewis' integral the expression for N_I (3) can be integrated numerically only, due to the logarithmic function figuring in it. This integral is, however, a generalization of the Lewis one and in the special case $f'(x) \rightarrow g'(x)$ it tends to the Lewis' integral N_L (1).

3. Approximative integration of N_I for $\alpha = \text{const.}$ and $R = \text{const.}$

The integral N_I regarded as the best approximation for the "real" number of theoretical plates N , can be calculated to any required accuracy, if the integration is carried out by a computer. The integral should be expressed, however, also in an explicit form following the example of LEWIS, or that of DODGE and HUFFMANN. Using an interpolation formula fitting smoothly the measured equilibrium points, the function $y = f(x)$ can be approximated. The adaptation of constant relative volatility $\alpha = \text{const.}$ is the simplest expedient, it is a restriction, however. On the contrary to LEWIS, the concentration change is not supposed to be the same from plate to plate, the only assumption is the linearity of the function $y = f(x)$ within a stage.

Thus

$$f(x) = \frac{\alpha \cdot x}{1 + (\alpha - 1)x},$$

and

$$g(x) = \frac{x_D}{R+1} + \frac{R}{R+1} \cdot x.$$

Applying the approximative relation [5]

$$\ln \left[\frac{f'(x)}{g'(x)} \right] \cong \frac{f'(x) - g'(x)}{[f'(x) \cdot g'(x)]^{0.5}} = S_2$$

the integrand in (3) becomes a rational function which may be integrated by elementary functions.

As it was shown in [5], the geometric mean is a good approximation for the so-called logarithmic mean in a suitable interval:

$$\frac{f'(x) - g'(x)}{\ln \left[\frac{f'(x)}{g'(x)} \right]} \cong [f'(x) \cdot g'(x)]^{1/2}.$$

Substituting into the integral (3), and introducing the denotation

$$N_a = \int [f'(x) \cdot g'(x)]^{1/2} \frac{dx}{f(x) - g(x)},$$

we get

$$N_I \cong N_a$$

or

$$N_I = N_a - N_R$$

where N_R is the "residuum", the error of the calculation, due to the substitution, which can be estimated.

After integration

$$N_a = (N_a)_{\text{rect}} + (N_a)_{\text{exh}} \quad (4i)$$

is obtained, where

$$(N_a)_{\text{rect}} = \sqrt{\frac{R+1}{R(b_r^2 - 4a_r c_r)}} \ln \left[\frac{x_D + A_1}{x_D + B_1} \cdot \frac{x_T + B_1}{x_T + A_1} \right] \quad (4a)$$

$$(N_a)_{\text{exh}} = \sqrt{\frac{\alpha \cdot (R+1)}{(R+1+\beta) \cdot (b_e^2 - 4a_e c_e)}} \ln \left[\frac{x_T + A_2}{x_T + B_2} \cdot \frac{x_M + B_2}{x_M + A_2} \right]. \quad (4b)$$

The expressions for A and B are the same as the corresponding formulae used by LEWIS, or by DODGE and HUFFMANN; the symbols a_r , b_r , c_r and a_e , b_e , c_e respectively slightly differ from those of Lewis.

$$a_r = (1 - \alpha)R; \quad a_e = (1 - \alpha) \cdot \left(1 + \frac{\beta}{R+1} \right);$$

$$b_r = (\alpha - 1) \cdot (R - x_D), \quad b_e = (\alpha - 1) - \frac{\beta}{R+1} [1 - x_M(\alpha - 1)]$$

$$c_r = -x_D; \quad c_e = \frac{\beta}{R+1} \cdot x_M$$

The derived approximative integral formula (N_a) is similar to that of LEWIS (N_L) but being simpler, the integration is less laborious.

Numerical calculations showed, that from 20 plates upwards Eq. (2) and Eq. (4) approximating the more exact expression N_I , give a slightly different result from that of the graphical construction made stepwise for N and the difference between N_a and N_I can be estimated. The quoted paper [5] contains the estimation of the error in N_a referring to N_I ; ($N_R = N_a - N_I$).

N_I — being a more general term than N_L — gives more exact results than that of Lewis in spite of its approximative character. It should be noted, however, that Lewis' criteria for the concentration change, being constant from plate to plate for small values of $f - g$, i.e. at high number of theoretical

plates, judged too severe at first, do not seem to be important in the light of numerical results. The reality of Lewis' restrictions is demonstrated by it.

For $\alpha \geq 2$, the error of the Lewis' integral becomes significant; the error of the approximative term N_a becomes negligible as long as the error N_R caused by the above mentioned substitution

$$\ln(1+z) \cong S_2(z) \quad \text{where} \quad z = \frac{f'(x) - g'(x)}{g'(x)}$$

remains sufficiently small.

4. Determination of the value N_{\min}

FENSKE's equation [7] is known for the analytical determination of N_{\min} ($R = \infty$, or $g = x$, $g' = 1$):

$$N_{\min} = \frac{\ln \frac{x_D(1-x_M)}{x_M(1-x_D)}}{\ln \alpha_m} \quad (5)$$

$$\alpha_m = \sqrt[N]{\alpha_1 \cdot \alpha_2 \cdot \alpha_3 \cdot \dots \cdot \alpha_N}$$

The equation of FENSKE is of general validity, even the theorem of equal molal flow is disregarded in it, thus the value of the calculated N_{\min} renders the value of N_{\min} obtained graphically.

In practical application, however, the change of the values of α_n from plate to plate causes difficulties, therefore the equation is applied for $\alpha = \text{const.}$ only:

$$N_{\min} = \frac{\ln \frac{x_D(1-x_M)}{x_M(1-x_D)}}{\ln \alpha} \quad (5a)$$

A similar equation to that of FENSKE can be derived from the integral N_L of LEWIS (cf. Eq. 2) as well [4].

$$\lim_{R \rightarrow \infty} N_L = (N_L)_{\min} = \frac{\alpha}{\alpha - 1} \ln \frac{x_D(1-x_M)}{x_M(1-x_D)} \quad (6)$$

α must be equal or nearly equal to unity to get the equation proposed by FENSKE.

The integral N_I will be integrable taking into account the restriction $(\alpha - 1)x \ll 1$; further $g = x$ and $g' = 1$ respectively; thus the equation of Fenske is obtained in the following form:

$$\lim_{R \rightarrow \infty} N_I = (N_I)_{\min} = N_{\min} = \frac{\ln \frac{x_D(1-x_M)}{x_M(1-x_D)}}{\ln \alpha} \quad (7)$$

Considering the approximative integral N_a , the adequate form of the equation of FENSKE is as follows:

$$\lim_{R \rightarrow \infty} N_a = (N_a)_{\min} = \frac{\sqrt{\alpha} \cdot \ln \frac{x_D(1-x_M)}{x_M(1-x_D)}}{\alpha-1} \quad (8)$$

Comparing Eqs (7) and (8), it is easy to observe: the expression $\frac{\alpha-1}{\sqrt{\alpha}}$ is in $(N_a)_{\min}$ instead of the adequate expression $\ln \alpha$ in N_{\min} ; according to the approximative relation [5]:

$$\frac{\alpha-1}{\ln \alpha} \cong \sqrt{\alpha}.$$

Thus, $(N_a)_{\min}$ can be used instead of the expression N_{\min} as long as the logarithmic mean can be approximated by the geometric mean with satisfying accuracy.

5. Gilliland's universal graph for the determination of the number of theoretical plates

The well-known form of GILLILAND's generalized diagram is as follows:

$$\frac{N - N_{\min}}{N + 1} = \varphi \left(\frac{R - R_{\min}}{R + 1} \right) \quad (9)$$

where R denotes the reflux.

According to the opinion of the author: ". . .there should be no unique correlation of this form . . ." [6] the approximative integral N_a and the formula of Lewis N_L as well shows that the universal character of Gilliland's diagram cannot be supported theoretically; i.e. neither the function $N_L(R)$, nor the function $N_a(R)$ can be expressed in the form (9).

Our attempts didn't even succeed in finding the reason, why GILLILAND's data are clustered in a relative narrow band. GILLILAND's diagram is to be applied carefully for the extreme values of α and β .

The verification of the universality of Gilliland's diagram was tried using numerical examples calculated with the approximative integrals N_a .

The results can be summed up as follows:

- a) for $\alpha = \text{const. (1.18 — 2.5)}$ and
 $R = \text{const. (1.03 — 23)}$

	α	R	x_T	x_D	x_M	β	No.
+	1.18	23.03	0.25	0.85	0.07	3.33	11
					0.15	6.0	12
×	2.5	5	0.5	0.85	0.001	0.7	21
				0.95		0.902	22
				0.05		1.0	23
				0.25		1.8	24
○	2	3.5	0.5	0.95	0.05	1	31
					0.4	4.5	32
●	2	1.03	0.5	0.66	0.05	0.37	41
				0.75		0.55	42
				0.66	0.25	0.66	43
					0.35	1.11	44

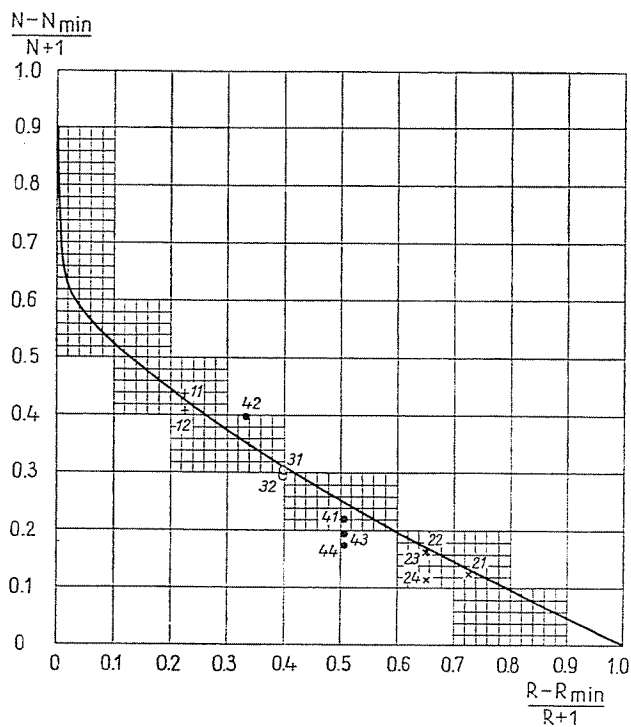


Fig. 2. Gilliland's curve

No.		β	α	x_T	x_D	x_M	$\frac{R}{R_{min}}$
11	-----	3.7	1.05	0.25	0.99	0.05	variable
12	=====		3.0				
21	+	1.0	2.5	0.5	0.95	0.05	1.2
22			1.18				1.21
23			1.5				1.43
24			2				2.06
25			2.5				4.55
31	○	0.66	1.18	0.46	0.72	0.07	1.3
32			2.0	0.50	0.66	0.25	∞ only for stripping

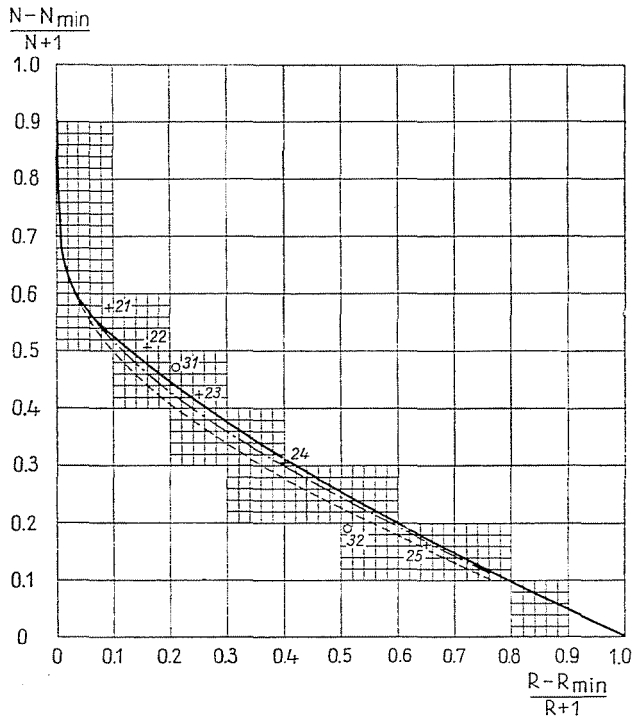


Fig. 3. Gilliland's diagram

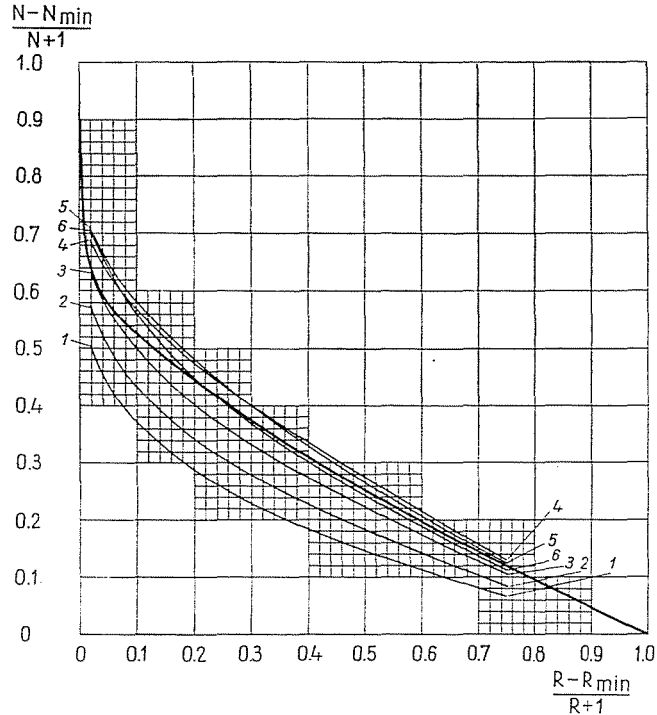


Fig. 4. Gilliland's diagram

$$\left. \begin{array}{l} 1. \beta = 17,8 \\ 2. \beta = 8,4 \\ 3. \beta = 3,7 \\ 4. \beta = 0,88 \\ 5. \beta = 0,3428 \\ 6. \beta = 0,175 \end{array} \right\} \alpha = 1,05$$

the values of the function in (9) are varying in a large interval depending on the parameter β (0.37 — 6.0) (cf. Fig. 2)

b) for $\beta = \text{const.}$ and
 $1.05 < \alpha < 3$

the values of the function in (9) are varying in a relative narrow band being close or less close to the GILLILAND's diagram depending on β (cf. Fig. 3)

c) for $\alpha = 1.05$
 $x_D = 0.99$
 $x_M = 0.05$

large deviations (50—100 per cent) can be found depending on extremely scattered values of x_T and β respectively ($\beta = 0.175 — 17.8$) (cf. Fig. 4).

It is to be emphasized, that these significant deviations from Gilliland's curve are due to the extreme values supposed here to act, and which were chosen with intent so as to eschew "inner compensation" and so as to give a bias to the curve.

Though Gilliland himself did mention that in the construction of his diagram "extreme" conditions were considered as much as possible, it seems likely that, in most of the cases, the narrow band was due to inner compensations.

Since, deservedly, Gilliland's diagram is widely popular in instructional circles, we thought it not amiss to suggest these critical notes on it.

Summary

The formulae proposed by LEWIS, and DODGE and HUFFMANN, respectively impose rather strict restrictions on the determination of the number of theoretical plates of columns for the rectification of binary mixtures. These relations are referring to relative low volatility (α) or high number of theoretical plates (N) only.

The results, obtained by our method, are summed up as follows:

1. A generalization of the integral of LEWIS is proposed.
2. Constant molecular flow is the only condition imposed, obtaining the integral valid for each equilibrium curve $y = f(x)$, and for each N respectively.
3. Analytical approximation N_a to integral N_I is proposed for $\alpha = \text{const}$. The error of the approximative formula can be estimated.

The universal diagram of GILLILAND was controlled by calculations using the expression N_a .

Symbols

N	'real' number of theoretical plates
N_L	Lewis' approximative integral for the number of theoretical plates (Eq. (1)), integrated by Dodge and Huffmann (Eq. (2))
N_I	Authors' approximative integral (Eq. (3))
N_a	approximative expression of the approximative integral N_I (Eq. (4))
N_R	$N_a - N_I$: The error in N_a referred to N_I
R	Reflux ratio

Subscripts:

$-D$	Refers to distillate
$-M$	Refers to bottom
$-T$	Refers to feed
$-R$	Index of N_R
$-m$	Refers to mean value of α
$-r$	Refers to rectifying column
$-c$	Refers to exhausting (stripping) column

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