증류탑 간이 설계법

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Short-cut Method for Distillation Columm Design

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요 약

새로운 증류탑 간이 설계법이 개발되었다.

$$N = \frac{\ln S\left[\dfrac{R - 1/(\alpha - 1)}{R - R_m}\right]^{1.075}}{\ln \alpha\left[\dfrac{R}{R + R_m(\alpha - 1)}\right]^{0.5}}$$

어 교뱅은 2성분계 뿐만 아니라 다성분계에서도 유용하다.

Abstract

A new short-cut method for distillation column design has been developed to calculate the

number of theoretical plates. The proposed model is as follows:

$$N = \frac{\ln S\left[\dfrac{R - 1/(\alpha - 1)}{R - R_m}\right]^{1.075}}{\ln\alpha\left[\dfrac{R}{R + R_m(\alpha - 1)}\right]^{0.5}}$$

This model is useful for multicomponent systems as well as binary systems.

I. Introduction

Method to obtain the number of theoretical plates(NPT) can be divided into four types; empirical method using charts, empirical method using equations, analytical method using equations and rigorous stage-to-stage method. However, in the latter two types the procedures are too tedious, while the former two types may lead to uncertainty about their reliability because of the lack of the theoretical background and the limited column specifications. Thus, it is not surprising that the great efforts have been directed toward developing theoretically sound short-cut method to calculate NTP.

Short-cut method to calculate NTP is studied by a number of investigators.[1-9]

Gilliland's graphical correlation[1] is most widely used. Eduljee[2] proposed a single equation representing Gilland's plot as follows:

$$\frac{N - N_m}{N + 1} = 0.75\left[1 - \left(\frac{R - R_m}{R + 1}\right)^{0.5608}\right]$$

(1)

Smoker,[10] Stoppel,[11] Underwood,[12,13] Strangio and Treybal[14] derived exact analytical equations for binary systems, but their equations are all the same practically. Strangio and Treybal applied their equations to multicomponent systems. The accuracy was within that of Gilliland's plot.

Recently, Jafarey et al.[3] reported a short-cut method based on Smoker's equations and Underwood's minimum reflux ratio for high purity separations[15] as follows:

$$N = \frac{\ln S}{\ln\alpha\left(\dfrac{R X_F}{1 + R X_F}\right)^{0.5}}$$

(2)

The equation of Jafarey et al. is excellent in a sense of the sound theoretical backup for preliminary designs, but their equation is unreasonable in respect that it does not become infinity at minimum reflux and for this reason it leads to unreliability in the neighborhood of minimum reflux.

In this paper, a new short-cut method is presented based on Smoker's equations and Underwood's minimum reflux ratio for high purity separations. The accuracy of this method is not so good as Eduljee's version of Gilliland's plot, but this method is for preliminary design calculations for both binary and multicomponent systems.

II. General Design Equation

Although in practice multicomponent systems are important ones, binary systems have attracted much attention, and give a number of informations capable of application to multicomponent systems.

For binary systems with saturated liquid feed and high purity separations, Underwood's minimum reflux ratio[15] is as follows:

$$R_m = \frac{1}{(\alpha - 1)}\left\{\frac{X_D}{X_F} - \frac{\alpha(1 - X_D)}{1 - X_F}\right\}$$

$$\cong \frac{1}{(\alpha - 1)X_F} \tag{3}$$

Jafarey et al. approximated Smoker's equations with assumption of high purity separations as follows(eqs 16 and 17 in their paper):

$$N_R \cong \frac{\ln\left(\frac{X_D}{1 - X_D}\right)\left(\frac{1 - X_F}{X_F}\right)\left(\frac{R/R_m - X_F}{R/R_m - 1}\right)}{\ln\alpha\left(\frac{R}{R + 1}\right)} \tag{4}$$

$$N_S \cong \frac{\ln\left(\frac{1 - X_W}{X_W}\right)\left(\frac{X_F}{1 - X_F}\right)\left[\frac{R/R_m - (1 - \alpha X_F)}{R/R_m - 1}\right]}{\ln\alpha\left[\frac{(R + 1)X_F}{1 + RX_F}\right]} \tag{5}$$

The following equation is obtained from eqs 4, 5 and 6 with assumption of $N_R \cong N_S \cong N/2$.

$$N \cong \frac{\ln S\left(\frac{R/R_m - X_F}{R/R_m - 1}\right)\left(\frac{R/R_m - X_F}{R/R_m - 1} + \phi\right)}{\ln\alpha\left(\frac{RX_F}{1 + RX_F}\right)^{0.5}} \tag{6}$$

where

$$\phi = \frac{(\alpha + 1)X_F - 1}{R/R_m - 1} \tag{7}$$

Jafarey et al. obtained their design equation by dropping the reflux-dependent terms in numerator of eq 6.

Distillation column by its inherent nature has two limits of operation based on the reflux ratio, one limit is fixed by minimum reflux, and the other limit by total reflux. The equation of Jafarey et al. is unreasonable in respect that it does not become infinity at minimum reflux. In other words, the term $1/(R/R_m - 1)$ in the numerator of eq 6 is critical, which is very significant in the neighborhood of minimum reflux. At total reflux, the effects of two reflux-dependent terms in the numerator of eq 6 on NTP are usually small as compared with the effect of S. And ϕ in the second reflux-dependent term seems to make eq 6 complicated to some extent. If we assume that ϕ in the numerator ef eq 6

does not affect NTP significantly as compared with S and $(R/R_m - X_F)/(R/R_m - 1)$, we may drop ϕ to simplify eq 6. Hence, eq 6 becomes

$$N \cong \frac{\ln S\left(\frac{R/R_m - X_F}{R/R_m - 1}\right)^2}{\ln\alpha\left(\frac{RX_F}{1 + RX_F}\right)^{0.5}} \tag{8}$$

But ϕ factor may affect NTP significantly in the neighborhood of minimum reflux. On the other hand, we would expect in practical problems that eq 6 results in a conservative design as a result of the assumption of high purity separations. Thus, we should correct one or both of reflux-dependent terms in eq 8 for compensation of the overpurification and the effect of ϕ. By the way, it is the reflux-dependent term in the numerator that should be corrected under the consideration of the fact that it dominates NTP in the neighborhood of minimum reflux. Thus, design equation becomes

$$N = \frac{\ln S\left(\frac{R/R_m - X_F}{R/R_m - 1}\right)^{n'}}{\ln\alpha\left(\frac{RX_F}{1 + RX_F}\right)^{0.5}} \tag{9}$$

where n' is a function of system parameters.

In addition, we would expect that X_F in eq 9 which appears in both of the numerator and denominator might cause significant error in application of pseudobinary technique to multicomponent systems. With eqs 3 and 6, we can obtain the following equation by similar procedures as the case of eq 9.

$$N = \frac{\ln S\left[\frac{R - 1/(\alpha - 1)}{R - R_m}\right]^n}{\ln\alpha\left[\frac{R}{R + R_m(\alpha - 1)}\right]^{0.5}} = \frac{\ln S'}{\ln\alpha'} \tag{10}$$

where

n = correction factor, a function of system parameters

$$S' = S\left[\frac{R - 1/(\alpha - 1)}{R - R_m}\right]^n \tag{11}$$

$$\alpha' = \alpha\left[\frac{R}{R + R_m(\alpha - 1)}\right]^{0.5} \tag{12}$$

If ϕ is negligible in eq 6, n and n' fall on the interval, $n, n' \leq 2$.

At total reflux eq 12 reduces to Fenske's expression for minimum NTP,[16] and at minimum reflux, moreover, it results in an infinite NTP. Any separation with operating reflux can be exactly converted into an equivalent separation with total reflux by using a modified relative volatility and a modified separation factor.[12]

III. Analysis of Data

There are two limiting cases in distillation column design: $R/R_m = 1$; and $\alpha = 1$. In both cases, NTP becomes infinity. Thus, parameters R/R_m and α should be chosen carefully in application of approximate equations.

To determine the value of the exponent n in eq 10 by the method of least-squares fitting, system parameters are selected: $\alpha = 1.1$, 1.5 and 2.5; $X_F = 0.25$ and 0.50; $X_D = 0.98$ and 0.95; $X_W = 0.02$ and 0.05; and $R/R_m = 1.75, 1.30, 1.20, 1.10, 1.05$ and 1.30. There are 108 possible systems with the given parameters(see Table 1). For R/R_m, since the optimum reflux ratio usually falls on the interval $1.03 \leq R/R_m \leq 1.37$,[17] the relatively narrow intervals of R/R_m in the neighborhood of 1.1 are considered to obtain more accurate results in that region. For α, NTP becomes too large on the interval $1 \leq \alpha < 1.1$ and too small on the interval $\alpha > 2.5$, generally.

We can obtain $n = 1.075$ from the data analysis of the 108 systems using the least-squares criterion which requires that

$$Q = \sum_{i=1}^{108}\left[\frac{N_i,\ eq\ 10 - N_i,\ Smoker}{N_i,\ Smoker}\right]^2 \tag{13}$$

be a minimum. Thus we obtain

$$N = \frac{\ln S\left[\dfrac{R - 1/(\alpha - 1)}{R - R_m}\right]^{1.675}}{\ln\alpha\left[\dfrac{R}{R + R_m(\alpha - 1)}\right]^{0.5}} \tag{14}$$

By similar procedures, an alternate equation can be obtained from eq 9 as follows:

$$N = \frac{\ln S\left(\dfrac{R/R_m - X_F}{R/R_m - 1}\right)^{0.853}}{\ln\alpha\left(\dfrac{R X_F}{1 + R X_F}\right)^{0.5}} \tag{15}$$

Table 1 shows the comparison of predictions for NTP of several models. Mean values of the relative errors of eqs 14 and 15 are 6.48% and 6.41%, respectively, while those of Eduljee's version of Gilliland's plot and Jafarey et al. are 3.07% and 16.98%, respectively.

Table 2 shows confidence limits[18] of n and n'. As it can be seen in Table 2, we can conclude that the difference between eq 14 and the equation of Jafarey et al. is statistically significant.

Table 3 shows the effect of ϕ, which appears in eq 6, on the relative errors of eqs 14 and 15. The relative errors tend to decrease as $(\alpha + 1)X_F$ increases and R/R_m decreases. Particularly, the relative errors depend largely on X_F, that is because of the assumption of $N_R \cong N_S$. Thus, a particular attention must be given on the intervals, $X_F < 0.25$ and $X_F > 0.5$, when these design equations are applied. In addition to the results of Table 3, we would expect that these design equations give better results generally as S increases, under the consideration of their derivation steps.

Table 4 shows the results of calculations of 22 multicomponent systems culled from references,[1,19,20] which are obtained by pseudobinary technique.[7,9,14,21] At least in these examples eq 14 seems to give comparable results with Gilliland's plot. But eq 15 gives worse results than the equation of Jafarey et al. because of the numerator correction term.

Table 1. Comparison of Predictions for NTP, Binary$(q=1)$

No.	Specifications* $(\alpha, X_F, X_D, X_W, R/R_m)$	Smoker	Gilliland (Eduljee)	Jafarey	eq 14	eq 15
1	aaaaa	115.865	115.407	116.581	126.231	125.437
2	aaaba	99.030	101.410	102.392	112.201	111.247
3	aabba	87.109	87.434	89.843	98.050	98.863
4	abaaa	120.165	116.041	117.328	123.122	123.896
5	ababa	105.905	101.968	103.047	109.092	109.615
6	abbba	91.570	87.961	91.493	94.578	98.263
7	baaaa	28.334	28.033	28.163	30.461	30.302
8	baaba	24.216	24.674	24.735	27.075	26.874
9	babba	21.353	21.342	21.740	23.657	23.923
10	bbaaa	29.281	28.764	28.408	29.699	29.998
11	bbaba	25.889	25.321	24.950	26.313	26.541
12	bbbba	22.411	21.969	22.291	22.783	23.940
13	caaaa	13.399	13.298	13.015	14.045	14.003
14	caaba	11.475	11.741	11.431	12.483	12.419
15	cabba	10.157	10.228	10.084	10.903	11.293
16	cbaaa	13.727	14.209	13.199	13.679	13.938
17	cbaba	12.215	12.553	11.593	12.117	12.332
18	cbbba	10.601	11.056	10.515	10.453	11.293
19	aaaab	143.202	143.254	135.952	156.605	154.616
20	aaabb	120.259	125.908	119.404	140.342	138.069
21	aabbb	107.366	108.593	105.833	123.879	125.037
22	abaab	149.497	144.166	137.295	151.198	152.053
23	ababb	132.490	126.711	120.584	134.936	135.342
24	abbbb	115.194	109.351	108.885	117.781	124.355
25	baaab	35.268	35.090	32.639	37.579	37.120
26	baabb	29.729	30.914	28.666	33.676	33.147
27	babbb	26.061	26.777	25.425	29.720	30.039
28	bbaab	36.475	36.109	33.052	36.259	36.605
29	bbabb	32.525	31.816	29.029	32.357	32.582
30	bbbbb	28.250	27.648	26.373	28.188	30.119
31	caaab	16.734	16.861	14.895	17.123	16.940
32	caabb	14.242	14.916	13.082	15.344	15.127
33	cabbb	12.775	13.029	11.630	13.535	13.741
34	cbaab	17.045	18.047	15.176	16.495	16.807
35	cbabb	15.356	15.973	13.329	14.716	14.960
36	cbbbb	13.299	14.099	12.298	12.748	14.045
37	aaaac	158.129	158.464	143.586	170.933	168.104
38	aaabc	131.753	139.290	126.110	153.798	150.628
39	aabbc	118.474	120.148	112.221	136.428	137.549
40	abaac	164.842	159.465	145.203	164.521	165.138

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41	ababc	146.595	140.170	127.530	147.386	147.464
42	abbbc	127.916	120.980	115.931	129.168	136.968
43	baaac	38.946	38.884	34.322	40.853	40.182
44	baabc	42.654	34.270	30.144	36.758	36.005
45	babbc	29.423	29.697	26.825	32.600	32.879
46	bbaac	40.160	39.986	34.806	39.294	39.584
47	bbabc	35.976	35.245	30.569	35.198	35.348
48	bbbbc	31.322	30.637	27.945	30.781	33.016
49	caaac	18.423	18.713	15.556	18.495	18.212
50	caabc	15.661	16.566	13.663	16.641	16.319
51	cabbc	14.133	14.481	12.178	14.751	14.927
52	cbaac	18.706	19.960	15.874	17.757	18.053
53	cbabc	16.950	17.678	13.942	15.903	16.121
54	cbbbc	14.675	15.603	12.939	13.819	15.287
55	aaaad	186.560	186.812	153.720	194.489	189.772
56	aaabd	153.611	164.229	135.010	176.201	171.062
57	aabbd	139.808	141.681	120.779	157.633	158.218
58	abaad	192.891	187.880	155.734	186.661	186.313
59	ababd	172.698	165.169	136.779	168.373	167.358
60	abbbd	151.803	142.568	125.457	148.722	158.017
61	baaad	45.797	45.867	36.490	46.188	45.048
62	baabd	38.133	40.445	32.049	41.844	40.606
63	babbd	34.753	35.067	28.641	37.427	37.520
64	bbaad	46.824	47.018	37.072	44.295	44.351
65	bbabd	42.292	41.463	32.560	39.952	39.839
66	bbbbd	37.014	36.047	30.002	35.205	37.510
67	caaad	21.470	22.031	16.375	20.716	20.216
68	caabd	18.252	19.523	14.382	18.768	18.223
69	cabbd	16.637	17.078	12.861	16.637	16.847
70	cbaad	21.689	23.279	16.741	19.828	20.029
71	cbabd	19.838	20.635	14.704	17.879	17.991
72	cbbbd	17.192	18.194	13.744	15.644	17.311
73	aaaae	217.370	215.560	160.144	215.852	208.802
74	aaabe	177.447	189.520	140.652	196.838	189.310
75	aabbe	163.246	163.515	126.248	177.513	176.950
76	abaae	221.875	216.588	162.424	207.081	205.106
77	ababe	200.047	190.425	142.655	188.066	185.337
78	abbbe	177.248	164.368	131.596	167.496	177.304
79	baaae	53.045	52.849	37.827	51.030	49.321
80	baabe	43.999	46.619	33.223	46.535	44.716
81	babbe	40.509	40.431	29.768	41.957	41.724
82	bbaae	53.663	53.936	38.473	48.918	48.583
83	bbabe	48.850	47.580	33.790	44.423	43.900
84	bbbbe	43.023	41.355	31.289	39.467	42.157

85	caaae	24.603	25.251	16.863	22.747	21.987
86	caabe	20.959	22.393	14.811	20.743	19.935
87	cabbe	19.274	19.592	13.269	18.693	18.598
88	cbaae	24.748	26.387	17.259	21.761	21.795
89	cbabe	22.823	23.405	15.159	19.757	19.694
90	cbbbe	19.834	20.604	14.230	17.426	19.172
91	aaaaf	240.858	235.415	163.046	230.223	221.261
92	aaabf	195.787	206.988	143.201	210.880	201.416
93	aabbf	181.370	178.592	128.731	191.215	189.482
94	abaaf	243.296	236.359	165.454	221.013	217.523
95	ababf	220.457	207.819	145.316	201.671	197.385
96	abbbf	196.456	179.375	134.400	180.682	190.304
97	baaaf	58.497	57.620	38.422	54.310	52.141
98	baabf	48.463	50.838	33.745	49.747	47.464
99	babbf	44.910	44.095	30.272	45.099	44.558
100	bbaaf	58.710	58.606	39.097	52.097	51.401
101	bbabf	53.724	51.710	34.339	47.534	46.643
102	bbbbf	47.544	44.932	31.867	42.485	45.122
103	caaaf	26.923	27.404	17.077	24.141	23.174
104	caabf	22.987	24.311	14.998	22.112	21.096
105	cabbf	21.262	21.270	13.448	20.036	19.794
106	cbaaf	27.011	28.411	17.486	23.110	22.989
107	cbabf	25.041	25.209	15.358	21.081	20.861
108	cbbbf	21.821	22.165	14.443	18.708	20.451
mean of relative errors(%)		0.00	3.07	16.98	6.48	6.41
maximum of relative errors(%)		0.00	8.70	38.67	16.73	16.69

* Key: For a, $\alpha=1.10$; $X_F=0.25$; $X_D=0.98$; $X_W=0.02$; $R/R_m=1.75$. For b, $\alpha=1.50$; $X_F=0.50$; $X_D=0.95$; $X_W=0.05$; $R/R_m=1.30$. For c, $\alpha=2.50$; $R/R_m=1.20$. For d, $R/R_m=1.10$. For e, $R/R_m=1.05$. For f, $R/R_m=1.03$.

Table 2. Confidence Limits of n and n' *

	$\bar{x}$	s^2	95% confidence limits
n	1.005	0.202	$0.920 \le \mu \le 1.090$
n'	0.732	0.184	$0.651 \le \mu \le 0.813$

* $\bar{x}$, s^2, μ denote sample mean, sample estimate of the population variance and population mean, respectively.

Table 3. Effect of ϕ on Relative Errors(%) of eq 14

$(\alpha+1)X_F-1$	R/R_m-1*					
	0.75	0.30	0.20	0.10	0.05	0.03
-0.475^a	11.6(11.4)	13.8(13.1)	13.3(12.2)	10.6(8.7)	6.3(3.7)	2.9(−0.3)
-0.375^a	10.0(10.0)	11.2(9.9)	9.4(8.4)	6.1(4.3)	1.8(−0.8)	−1.4(−4.6)
-0.125^a	7.0(7.3)	5.3(5.0)	3.7(2.9)	0.1(−1.6)	−3.9(6.3)	−6.6(−9.7)
0.050^b	2.9(4.6)	1.7(3.9)	0.4(2.6)	−2.6(−0.8)	−6.1(5.0)	−8.6(−8.1)
0.250^b	1.6(3.9)	−0.4(2.4)	−2.0(0.7)	−5.3(−3.0)	−8.7(−7.2)	−11.1(−10.2)
0.750^b	−0.8(3.0)	−3.8(0.5)	−5.7(−1.4)	−9.2(−5.4)	−12.5(−9.7)	−14.8(−12.6)

　* Each value is mean of three equivalent relative errors. Each value in parentheses is equivalent value of eq 15.

　a; $X_F=0.25$.　b; $X_F=0.50$.

Table 4. Comparison of Predictions for NTP, Multicomponent ($q=1$)*

Source	No. of Component**	R	R_m	Stage-to-stage		Gilliland (Eduljee)	Jafarey	eq 14	eq 15
				N_m	N				
Ex II^a	5(0.35)	7	5.2	19	35	34.0	30.5	35.4	33.8
		10			27	26.8	26.3	28.5	27.7
Ex III^a	3(0.60)	2	0.98	11.2	17	17.6	16.7	16.5	17.2
Ex VII^a	3(0.45)	1.6	1.25	9	18	19.4	17.6	17.6	19.6
		2.1			15	13.5	15.1	14.7	16.1
		5.14			11	11.0	11.2	11.0	11.5
Ex VIII^a	5(0.35)	12.0	6.0	43.1	58	59.1	80.4	60.5	83.8
		19.0			52	51.7	61.9	52.8	63.3
Ex XI^a	5(0.23)	20	7.0	29	35	35.5	39.8	37.2	41.0
		35			32	33.0	34.6	33.3	35.1
Ex X^a	4(0.60)	5	2.3	20.2	29	28.2	29.0	27.9	29.7
		15			22	22.3	22.7	22.4	22.9
Ex XI^a	5(0.25)	2.57	2.26	10.8	25.8	26.0	29.4	24.3	35.2
Ex XII^a	3(0.15)	5.67	1.5	7.7	9.5	9.8	12.2	9.8	12.4
		9.0			8.8	8.8	10.4	9.0	10.6
Ex XIII^a	3(0.30)	9	1.85	8.6	10.5	10.0	10.9	10.2	11.1
Ex XIV^a	5(0.58)	3	0.9	13.0	17	17.2	18.0	16.3	18.3
Ex XVI^a	6(0.46)	4.0	3.3	18.7	39	38.7	45.7	37.2	52.8
		6.0			30	27.7	32.3	28.0	34.3
		10.0			25	23.1	25.5	23.5	26.3
Ex 9-2^b	5(0.20)	2.52	0.98	7.0	10.0	10.1	16.3	9.7	17.1
Ex 7-1^c	4(0.23)	3.70	2.80	8.6	18.0	16.6	18.9	17.3	22.3
mean of relative errors(%) ·················· 0.00						3.07	12.11	3.57	17.19
maximum of relative errors(%) ··············0.00						10.00	63.00	6.67	71.00

　* All vacant entries in the table are identical to values above.
　a; Gilliland(1940).　b; Smith(1963).　c; Van Winkle(1967).
　** Values in the prentheses are X_F values.

Ⅳ. Conclusion

A short-cut method for distillation has been developed to calculate the number of theoretical plates. The proposed model is as follows:

On the intervals, $1.1 \leq \alpha \leq 2.5$, $1.03 \leq R/R_m \leq 1.75$, $0.25 \leq X_F \leq 0.50$, $0.95 \leq X_D \leq 0.98$ and

$$N = \frac{\ln S \left[\dfrac{R - 1/(\alpha - 1)}{R - R_m} \right]^{1.075}}{\ln \alpha \left[\dfrac{R}{R + R_m(\alpha - 1)} \right]^{0.5}}$$

$0.02 \leq X_W \leq 0.05$, the relative error of the proposed model decreases as $(\alpha + 1)X_F$ increases and R/R_m decreases. On the given intervals, mean of the relative errors of the proposed model is 6.48%, while those of Eduljee's version of Gilliland's plot and Jafarey et al. are 3.07% and 16.98%, respectively. Since the error of proposed model depends largely on X_F, it may be dangerous to use this model on the intervals, $X_F \langle 0.25$ and $X_F \rangle 0.50$.

For multicomponent systems, the proposed model gives comparable results with Gilliland's plot.

Nomenclature

N: number of theoretical plates(NTP)

N_m: minimum number of theoretical plates

N_R: number of theoretical plates in rectifying section

N_S: number of theoretical plates in stripping section

n, n': functions of system parameters, which appear in eqs 10 and 9, respectively

Q: defined by eq 13

q: liquid fraction of feed

R: reflux ratio

R_m: minimum reflux ratio

S: separation factor, $X_D(1 - X_W)/[X_W(1 - X_D)]$

S': defined by eq 11

X_D: top composition

X_F: feed composition

X_W: bottom composition

α: relative volatility

α': defined by eq 12

ϕ: defined by eq 7

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