Solutions for R&D to Design

Distillation Column Composition and Temperature Calculations by Sequential Step Calculation

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Introduction

- The required number of theoretical stages and the reflux ratio of a distillation column can be determined using the Fenske equation (Tips to Scale-up & Design #1009), the Underwood equation (Tips to Scale-up & Design #1011), the Gilliland correlation or the Brown-Martin correlation.
- In order to calculate the diameter of a continuous distillation column and to study energy savings, the vapor-liquid composition and temperature distributions in the column are required, but they cannot be obtained by calculation using the above equations.
- In this study, we will introduce a sequential step calculation method using the Thiele-Geddes method, which is one of the shortcut distillation calculation methods.

Thiele-Geddes Method

- Sequential Calculation Method:

① Set the number of rectifying section stages and the number of stripping section stages in advance, and assume a temperature for each stage (input an initial value) to determine the vapor-liquid equilibrium ratios (K_i).

② Calculate the compositions in the column sequentially from the top of the column and the bottom of the column, and determine the distillate composition ($x_{i,D}$) and the bottom liquid composition ($x_{i,W}$), and the composition of all stages from the vapor-liquid equilibrium relationship when the feed stage is reached.

③ Correct the temperatures of each stage so that the sum of the compositions is 1.

Nowadays, it is possible to easily obtain a convergent solution by using the Excel solver, or equation solver software and the like, but the above mentioned calculation appeared to be too complicated when first announced in 1933, and it seems it was not widely applied before a long time (*1).

*1: “Taseibun-Kei no Jouryu” *in Japanese*: “Multi-Component Distillation”, Reprinted new version, Separation Technology Series 7, Mitsuho Hirata, Hiroshi Sagara

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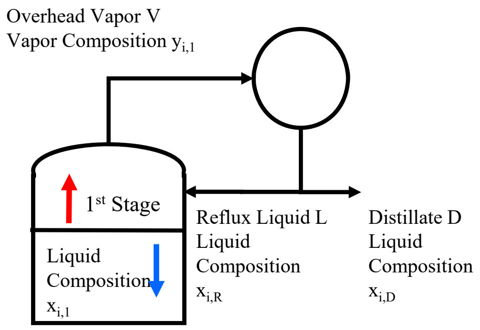
Thiele-Geddes Method Equation Derivation 1

Mass balance and vapor-liquid relationship for distillation column rectifying section:



$$V = L + D \qquad \cdots ①$$

$$V \cdot y_{i,n} = L \cdot x_{i,n-1} + D \cdot x_{i,D} \qquad \cdots ②$$

Balance equations

$$K_{i,n} = \frac{y_{i,n}}{x_{i,n}} \qquad \cdots ③$$

Equilibrium relationship

$y_{i,n}$: Composition of Component i Rising from Rectifying Section Stage n
$x_{i,n-1}$: Liquid Composition of Component i Descending from Rectifying Section Stage n-1
$x_{i,D}$: Overhead Composition of Component i
$K_{i,n}$: Vapor-Liquid Equilibrium Ratio of Component i at Stage n
V : Overhead Vapor Flow Rate [kmol/h]
L : Reflux Flow Rate [kmol/h]
D : Distillate Flow Rate [kmol/h]

Eq. 4 is obtained by rearranging Eq. 2 and substituting Eq. 1

$$\frac{y_{i,n}}{x_{i,D}} = \frac{L}{V} \cdot \frac{x_{i,n-1}}{x_{i,D}} + \frac{V-L}{V}$$

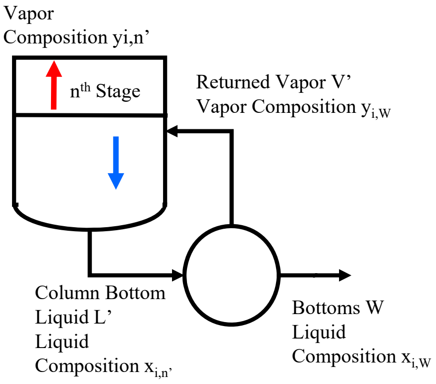
$$= \frac{L}{V} \cdot \left(\frac{x_{i,n-1}}{x_{i,D}} - 1 \right) + 1 \qquad \cdots ④$$

Dividing both sides of Eq. 3 by xi,D gives Eq. 5

$$\frac{x_{i,n}}{x_{i,D}} = \frac{1}{K_{i,n}} \cdot \frac{y_{i,n}}{x_{i,D}} \qquad \cdots ⑤$$

Thiele-Geddes Method Equation Derivation 2

Mass balance and vapor-liquid relationship for distillation column stripping section:



$$V' = L' - W \quad \cdots ⑥$$

$$V' \cdot y_{i,n+1'} = L' \cdot x_{i,n'} - W \cdot x_{i,W} \quad \cdots ⑦$$

Balance equations

$y_{i,n+1'}$: Vapor Composition of Component i Rising from Stripping Section Stage
$x_{i,n'}$: Liquid Composition of Component i Descending from Stripping Section Stage n
V' : Returned Vapor Flow Rate [kmol/h]
L' : Column Bottom Liquid Flow Rate [kmol/h]
W : Bottoms Flow Rate [kmol/h]

Eqs. 8 and 9 can be obtained by modifying the equations in the same way as the rectifying section

$$\frac{x_{i,n'}}{x_{i,W}} = \frac{V'}{L'} \cdot \left(\frac{y_{i,n+1'}}{x_{i,W}} - 1 \right) + 1 \quad \cdots ⑧$$

$$\frac{y_{i,n'}}{x_{i,W}} = K_{i,n'} \cdot \frac{x_{i,n'}}{x_{i,W}} \quad \cdots ⑨$$

In other words, if $x_{i,D}$ and $x_{i,W}$ are determined, the composition of each stage can be calculated.

Thiele-Geddes Method Equation Derivation 3

Ratio of distillate composition ($x_{i,D}$) to bottoms composition ($x_{i,W}$):
If the feed is a boiling point liquid (V/F = 0), the composition ($y_{i,n+1}$) below the lowermost stage of the rectifying section (the feed stage) and the composition ($y_{i,n-1'}$) of the stage above the uppermost stage of the stripping section (the feed stage) are the same.

$$y_{i,n-1'} = y_{i,n+1} \quad \cdots ⑩$$

$y_{i,n+1}$: Vapor Composition of Component i Below the Bottom Stage of the Rectifying Section
$y_{i,n-1'}$: Vapor Composition of Component i Above the Top Stage of the Stripping Section

Eq 11 is obtained by multiplying both sides of Eq. 10 by the ratio of the compositions at the top and the bottom of the column ($x_{i,D}$ / $x_{i,W}$)
With this, the ratio of the compositions x_i, D and x_i, W can be calculated.

$$\frac{x_{i,D}}{x_{i,W}} = \left(\frac{y_{i,n-1}}{x_{i,W}} \right) \Big/ \left(\frac{y_{i,n+1}}{x_{i,D}} \right) \quad \cdots ⑪$$

Thiele-Geddes Method Equation Derivation 4

Distillate composition ($x_{i,D}$) and bottoms composition ($x_{i,W}$):
Consider the mass balance equations around the entire column

$$F = D + W \qquad \cdots ⑫$$

$$F \cdot x_{i,F} = D \cdot x_{i,D} + W \cdot x_{i,W} \qquad \cdots ⑬$$

Total balance equations

Substituting Eq. 12 into Eq. 13 and rearranging gives Eq. 14

$$1 = \frac{F \cdot x_{i,F}}{D \cdot x_{i,D} + (F - D) \cdot x_{i,W}}$$

$$x_{i,D} = \frac{F \cdot x_{i,F} \cdot x_{i,D}}{D \cdot x_{i,D} + (F - D) \cdot x_{i,W}} = \frac{F \cdot x_{i,F}}{D + (F - D) \cdot x_{i,W} / x_{i,D}}$$

$$= \frac{F/D \cdot x_{i,F}}{1 + (F/D - 1) \cdot x_{i,W} / x_{i,D}} = \frac{x_{i,F}}{D/F + (1 - D/F) \cdot x_{i,W} / x_{i,D}}$$

$$\boxed{\therefore x_{i,D} = \frac{x_{i,F}}{D/F + (1 - D/F) \cdot \left(x_{i,W} / x_{i,D}\right)}} \qquad \cdots ⑭$$

Eq. 15 is obtained by making the same rearrangement for the bottoms composition ($x_{i,W}$)

$$\boxed{x_{i,W} = \frac{x_{i,F}}{W/F + (1 - W/F) \cdot \left(x_{i,D} / x_{i,W}\right)}} \qquad \cdots ⑮$$

Thiele-Geddes Method: Organization of Calculation Procedure

The equations obtained with the calculation procedure are organized as follows:

① Give the number of theoretical stages of the rectifying and stripping sections, and the top and bottom temperatures.

② From the investigated conditions, calculate the flow rate ratios by calculating the vapor and liquid flow rates in the rectifying and stripping sections.

$$\frac{L}{V}, \frac{V'}{L'}, \frac{D}{F}, \frac{W}{F}$$

③ Assume the temperatures in the distillation column and obtain the vapor-liquid equilibrium ratios at these temperatures. For an ideal solution, according to Raoult’s law, the vapor-liquid equilibrium ratios can be obtained by the following equation.

$$K_i = \frac{y_i}{x_i} = \frac{P_i^0}{P}$$

P_i^0 : Saturated Vapor Pressure of Component i [kPaA]
P : Distillation Column Operating Pressure [kPaA]

④ Calculate the ratios of the vapor phase compositions and the liquid phase compositions to the distillate composition (xi,D) in the rectifying section.

$$\frac{y_{i,n}}{x_{i,D}} = \frac{L}{V} \cdot \left(\frac{x_{i,n-1}}{x_{i,D}} - 1 \right) + 1 \qquad \frac{x_{i,n}}{x_{i,D}} = \frac{1}{K_{i,n}} \cdot \frac{y_{i,n}}{x_{i,D}}$$

Thiele-Geddes Method: Organization of Calculation Procedure

⑤ Calculate the ratios of the vapor phase compositions and the liquid phase compositions to the bottoms composition ($x_{i,W}$) in the stripping section.

$$\frac{x_{i,n'}}{x_{i,W}} = \frac{V'}{L'}\cdot\left(\frac{y_{i,n+1'}}{x_{i,W}} - 1\right) + 1 \qquad \frac{y_{i,n'}}{x_{i,W}} = K_{i,n'}\cdot\frac{x_{i,n'}}{x_{i,W}}$$

⑥ Calculate the ratio of the distillate composition ($x_{i,D}$) and the bottoms composition ($x_{i,W}$).

$$\frac{x_{i,D}}{x_{i,W}} = \left(\frac{y_{i,n-1}}{x_{i,W}}\right)\Big/\left(\frac{y_{i,n+1}}{x_{i,D}}\right)$$

⑦ Calculate the distillation composition ($x_{i,D}$) and the bottoms composition ($x_{i,W}$).

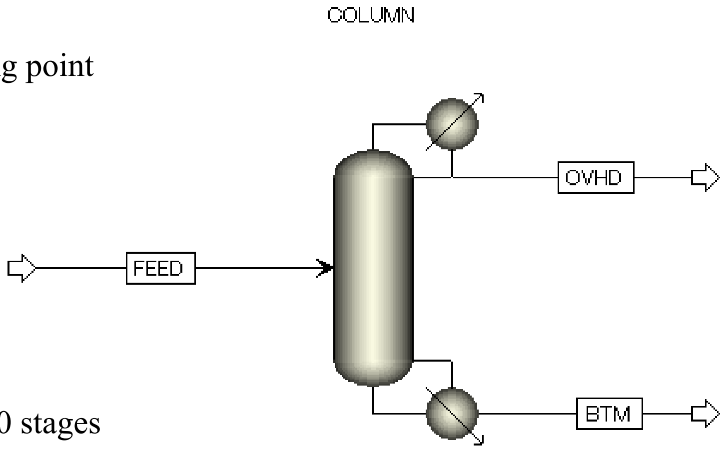
$$x_{i,D} = \frac{x_{i,F}}{D/F + (1 - D/F)\cdot\left(x_{i,W}/x_{i,D}\right)} \qquad x_{i,W} = \frac{x_{i,F}}{W/F + (1 - W/F)\cdot\left(x_{i,D}/x_{i,W}\right)}$$

⑧ Calculate the composition of each stage and find the sum of the compositions.

⑨ Find the temperature at which the sum of compositions becomes 1 in all stages by convergence calculation.

Verification Calculation: Subject of Examination

Calculations are carried out using an Excel solver on a four component hydrocarbon mixture. In this study, in order to simplify the calculations, the vapor-liquid equilibrium ratios (K_i) were determined by Raoult's law (the saturation vapor pressure uses the extended Antoine equation).
Also, the column is assumed to have an equimolar flow.



Feed condition: Liquid at boiling point

C3	5 kmol/h
n-C4	40 kmol/h
n-C5	30 kmol/h
n-C6	25 kmol/h

Distillation column:
Distillate flow rate: 45 kmol/h
Reflux ratio: 4
Number of theoretical stages: 10 stages
Pressure: 700 kPaA

Step.1 (Number of Theoretical Stages and Flow Ratio Calculation Specifications)

Ihhg#Vwuhdp#Frqglwlrqv

	Ihhg#Iorz Udwh ^np ro2k`	Suhvvxuh ^nSdD`	Ydsru#iudfwlrq
q0F6	8	:33	3
q0F7	73		
q0F8	63		
q0F9	58		
Wrwdo	433		

+4,#Ghwhuplqdwlrq#ri#Glvwloodwlrq#Froxpq#Frqglwlrqv

	Whpshudwxuh ^°C`	Suhvvxuh ^nSdD`	Glvwloodwh#Udwh ^np ro2k`	Uhiox{#Udwlr	Wrwdo#Qxpehu ri#Wkhruhwlfdo Vwdjhv	Qxpehu#ri Wkhruhwlfdo Uhfwli|lqj Vwdjhv	Qxpehu#ri Wkhruhwlfdo Vwulsslqj Vwdjhv
Wrs	8717	:33	78	7	43	7	8
Erwwrp	45414	:33					

+5,#Iorz#Udwlr#Fdofxodwlrq

Uhfwli|lqj#Vhfwlrq		Vwulsslqj#Vhfwlrq		Iorz#Udwh#Udwlrv			
Oltxlg#Iorz Udwh#O ^np ro2k`	Ydsru#Iorz Udwh#Y ^np ro2k`	Oltxlg#Iorz Udwh#O* ^np ro2k`	Ydsru#Iorz Udwh#Y* ^np ro2k`	O2Y	Y*2O*	G2I	Z2I
4;3	558	5;3	558	31;	31;37	3178	3188

- The calculation is carried out with a total of 10 stages in which the feed stage is added to the 4 stages of the rectifying section and 5 stages of the stripping section.
- Feed conditions: Vapor fraction = 0 indicates a liquid in which the components are preheated to the boiling point. In these conditions, the following calculation holds: Liquid flow rate in the stripping section (L’) = Liquid flow rate in the rectifying section (L) + Feed flow rate (F).
- Since the equimolar conditions are assumed in the column, the flow rate of the rectifying section can be obtained by the following equations:
  Rectifying section liquid flow rate (L) = Distillate flow rate (D)×Reflux ratio (R)
  Rectifying section vapor flow rate (V) = D×(1 + R)

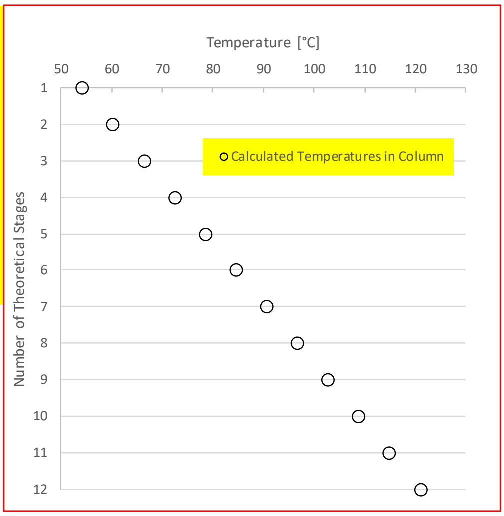
Step.2 (Temperature Assumption in Column, K Value Calculation)

+6,#Ydsru0Oltxlg#Htxloleulxp#Frqvwdqw#Fdofxodwlrq#+Nl@\|l2{l,

	Frqghqvhu	Uhfwli|lqj#vhfwlrq				Ihhg#Vwdjh	Vwulsslqj#Vhfwlrq					Uherlohu
Wkhruhwlfdo Vwdjh#q		4	5	6	7	8	9	:	;	<	43	
Whpshudwxuh	8717	931797	99185:	:518<4	:;1988	;71:4;	<31:;5	<91;78	4351<3<	43;1<:6	4481369	45414
q0F6	519<6	61388	61785	61;;9	7168<	71;:6	81764	91369	919<4	:16<<	;1496	;1<;9
q0F7	31:<7	31<56	4139;	4155;	41738	41934	41;49	51385	51643	518<4	51;<:	6155<
q0F8	31593	31644	3169;	31767	3183;	318<4	319;7	31:;:	31<35	4135<	4149<	41656
q0F9	313<3	31444	31468	31496	314<8	31565	315:7	31655	316:8	31769	31836	318:;

- The initial values of temperatures inside the column are assigned to have a linear distribution between the temperatures at the top and the bottom of the column.
- The K values are obtained from Raoult’s law using the vapor pressure of each component.

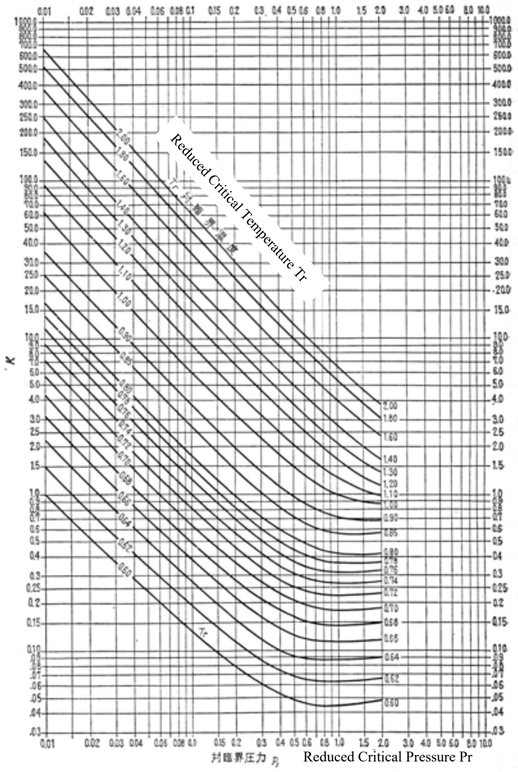
Note: Since this system is a pressurized system, it is necessary to consider the non-ideality of the vapor phase in order to make calculations more accurate.



$$K_i = \frac{y_i}{x_i} = \frac{P_i^0}{P}$$

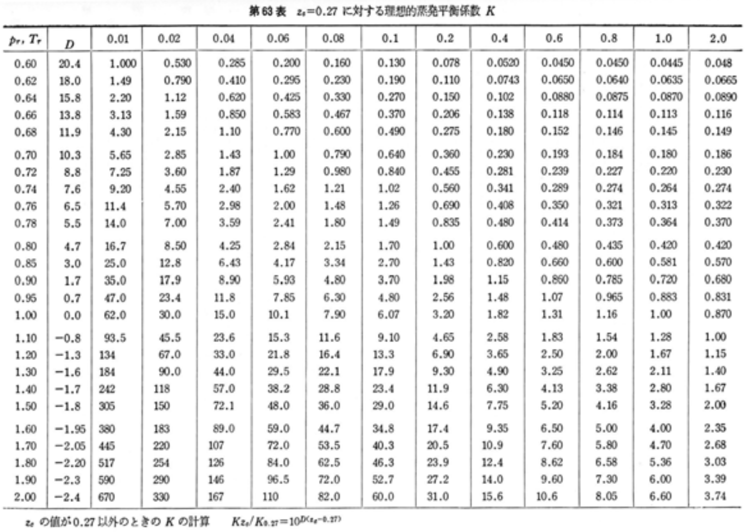
$$\ln(P_i^0) = A + \frac{B}{T + C} + D \cdot T + E \cdot \ln(T) + F \cdot T^G$$

Reference: Vapor-Liquid Equilibrium Ratio (K_i)



第 252 図 蒸発平衡係数 K (z_e=0.27)
Fig. 252 Vapor-Liquid Equilibrium Ratios K (z_e=0.27)

Table 63 Theoretical Vapor-Liquid Equilibrium Ratios K for z_e=0.27


第 63 表 z_e=0.27 に対する理想的蒸発平衡係数 K

p_r, T_r	D	0.01	0.02	0.04	0.06	0.08	0.1	0.2	0.4	0.6	0.8	1.0	2.0
0.60	20.4	1.000	0.530	0.285	0.200	0.160	0.130	0.078	0.0520	0.0450	0.0450	0.0445	0.048
0.62	18.0	1.49	0.790	0.410	0.295	0.230	0.190	0.110	0.0743	0.0650	0.0640	0.0635	0.0665
0.64	15.8	2.20	1.12	0.620	0.425	0.330	0.270	0.150	0.102	0.0880	0.0875	0.0870	0.0890
0.66	13.8	3.13	1.59	0.850	0.583	0.467	0.370	0.206	0.138	0.118	0.114	0.113	0.116
0.68	11.9	4.30	2.15	1.10	0.770	0.600	0.490	0.275	0.180	0.152	0.146	0.145	0.149
0.70	10.3	5.65	2.85	1.43	1.00	0.790	0.640	0.360	0.230	0.193	0.184	0.180	0.186
0.72	8.8	7.25	3.60	1.87	1.29	0.980	0.840	0.455	0.281	0.239	0.227	0.220	0.230
0.74	7.6	9.20	4.55	2.40	1.62	1.21	1.02	0.560	0.341	0.289	0.274	0.264	0.274
0.76	6.5	11.4	5.70	2.98	2.00	1.48	1.26	0.690	0.408	0.350	0.321	0.313	0.322
0.78	5.5	14.0	7.00	3.59	2.41	1.80	1.49	0.835	0.480	0.414	0.373	0.364	0.370
0.80	4.7	16.7	8.50	4.25	2.84	2.15	1.70	1.00	0.600	0.480	0.435	0.420	0.420
0.85	3.0	25.0	12.8	6.43	4.17	3.34	2.70	1.43	0.820	0.660	0.600	0.581	0.570
0.90	1.7	35.0	17.9	8.90	5.93	4.80	3.70	1.98	1.15	0.860	0.785	0.720	0.680
0.95	0.7	47.0	23.4	11.8	7.85	6.30	4.80	2.56	1.48	1.07	0.965	0.883	0.831
1.00	0.0	62.0	30.0	15.0	10.1	7.90	6.07	3.20	1.82	1.31	1.16	1.00	0.870
1.10	−0.8	93.5	45.5	23.6	15.3	11.6	9.10	4.65	2.58	1.83	1.54	1.28	1.00
1.20	−1.3	134	67.0	33.0	21.8	16.4	13.3	6.90	3.65	2.50	2.00	1.67	1.15
1.30	−1.6	184	90.0	44.0	29.5	22.1	17.9	9.30	4.90	3.25	2.62	2.11	1.40
1.40	−1.7	242	118	57.0	38.2	28.8	23.4	11.9	6.30	4.13	3.38	2.80	1.67
1.50	−1.8	305	150	72.1	48.0	36.0	29.0	14.6	7.75	5.20	4.16	3.28	2.00
1.60	−1.95	380	183	89.0	59.0	44.7	34.8	17.4	9.35	6.50	5.00	4.00	2.35
1.70	−2.05	445	220	107	72.0	53.5	40.3	20.5	10.9	7.60	5.80	4.70	2.68
1.80	−2.20	517	254	126	84.0	62.5	46.3	23.9	12.4	8.62	6.58	5.36	3.03
1.90	−2.3	590	290	146	96.5	72.0	52.7	27.2	14.0	9.60	7.30	6.00	3.39
2.00	−2.4	670	330	167	110	82.0	60.0	31.0	15.6	10.6	8.05	6.60	3.74

z_e の値が 0.27 以外のときの K の計算　$K_{z_e}/K_{0.27}=10^{D(z_e-0.27)}$

Calculation of K when the value of z_e is different than 0.27

A table of K-value estimations based on reduced critical states (derived from Tr and Pr) is shown. About 60% of the hydrocarbons are said to be concentrated around Zc = 0.27, which seems to be particularly effective for hydrocarbon-based mixtures.

“Kagaku Hannou, Kougaku II Neturikigaku” *in Japanese*: “Chemical Reaction Engineering II Thermodynamics” P. 404-409, Maruzen (1964)

Step.3 (Composition Ratio, $x_{i,D}$, $x_{i,W}$ Calculation)

+7,#Uhfwli|lqj#Vhfwlrq#Frp srvlwlrq#Udwlr#+{q#ru#|q#2{G ,#Fdofxodwlrq

Frp srvlwlrq Udwlr	{U2{G	|42{G	{42{G	|52{G	{52{G	|62{G	{62{G	|72{G	{72{G	|I2{G	{I2{G
q0F6	41333	41333	3165:	31795	31467	3163:	313:<	31596	31393	3157;	31384
q0F7	41333	41333	413;6	41399	31k<<	31k<<	31;47	31;84	31938	319;7	3175:
q0F8	41333	41333	61554	51::9	:1874	91566	4716:7	4419<<	56137<	4;196<	641888
q0F9	41333	41333	<133;	:173:	871;73	7713:5	5:31757	549186<	443<17<:	;;:1:<;	6;581:53

+8,#Vwulsslqj#Vhfwlrq#Frp srvlwlrq#Udwlr#+{q#ru#|q#2{Z ,#Fdofxodwlrq

Frp srvlwlrq Udwlr	|Z 2{Z	{432{Z	|432{Z	{<2{Z	|<2{Z	{;2{Z	|;2{Z	{:2{Z	|:2{Z	{92{Z	|92{Z	{I2{Z	|I2{Z
q0F6	;1k;9	:174;	93187;	7;1;84	6941773	5<31973	4<771:47	48951k46	<767168:	:8;416:9	744::13<:	663;;1k68	4945781337
q0F7	6155<	51:<4	;13;:	919<8	4:167;	471469	65198:	59176;	87158;	761:<9	:<187<	97144<	4351995
q0F8	41656	41593	417:6	416;3	41753	4166;	4153:	41499	31k4;	31k67	3196<	31:43	3174<
q0F9	318:;	31994	31666	31797	31535	3168<	31468	31638	313<;	315:8	313:8	3158:	31393

+9,#{l/G2{l/Z ,#Fdofxodwlrq

	{G2{Z
q0F6	97<6:81k7
q0F7	483133:747
q0F8	313557;995
q0F9	91:4;:H038

+:,#{l/G/#{l/Z #Fdofxodwlrq

	{G	{Z
q0F6	31444	31333
q0F7	31;;5	31339
q0F8	31345	31869
q0F9	31333	31788

- The rectifying section is calculated from the top of the column and the stripping section is calculated from the bottom using the equations derived from the Thiele-Geddes method.
- By this, each composition of the distillate and bottoms can be determined at the assumed temperature.

Step.4 (Stage per Stage Composition Calculation, Minimization of Objective Function)

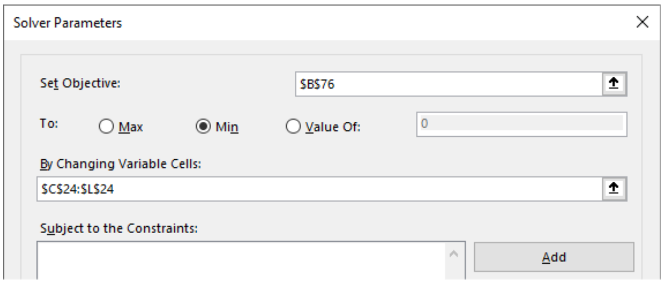
+;04,#Oltxlg#Skdvh#Frpsrvlwlrq#Fdofxodwlrq												
Frpsrvlwlrq	{G	{4	{5	{6	{7	{8	{9	{:	{;	{<	{43	{Z
q0F6	31444	31369	31348	3133<	3133:	31339	31334	31333	31333	31333	31333	31333
q0F7	31;;5	31k88	31;;4	31:4:	31867	316::	3158:	31488	313;6	3136<	31349	31339
q0F8	31345	3136<	313<4	314:6	315:;	316;3	31833	31958	31:49	31:6<	319:8	31869
q0F9	31333	31333	31335	3133;	31367	3144:	31458	3146;	31496	31544	31633	31788
Wrwdo	41338	41363	31k;;	31k3;	31;85	31;:<	31;;7	31k4<	31k96	31k;<	31k<4	31k<9
Huuru	031338	031363	31345	313<5	3147;	31454	31449	313;4	3136:	31344	3133<	31337

+;05,#Ydsru#Skdvh#Frpsrvlwlrq#Fdofxodwlrq											
Frpsrvlwlrq		|4	|5	|6	|7	|8	|9	|:	|;	|<	|43
q0F6		31444	31384	31367	3135<	3135;	3133:	31335	31333	31333	31333
q0F7		31;;5	31k73	31;;4	31:83	31936	3179;	3164<	314<5	31435	3137;
q0F8		31345	31366	313:8	31474	31557	31675	317<5	31979	31:94	31:;<
q0F9		31333	31333	31334	3133:	3135:	31367	31378	31394	313<5	31484
Wrwdo		41338	41358	31k<4	31k5:	31;;6	31;84	31;8:	31k33	31k87	31k;:
Huuru		031338	031358	3133<	313:6	3144:	3147<	31476	31433	31379	31346

Vxp#ri
Vtxduhv#ri
Huuruv
314758:;

- Calculate the vapor and liquid compositions of each stage.
- An objective function is set so that sum of the compositions of each stage is 1, and a least squares calculation using the temperature in the column as the operation variable is performed by using the Excel solver.
- Objective function =Σ $(1-x_{i,n})^2 + \Sigma(1-y_{i,n})^2$

Note that $x_{i,n}$ includes $x_{i,D}$ and $x_{i,W}$.



Solver Parameters

Set Objective: $B$76

To: ○ Max ● Min ○ Value Of: 0

By Changing Variable Cells: $C$24:$L$24

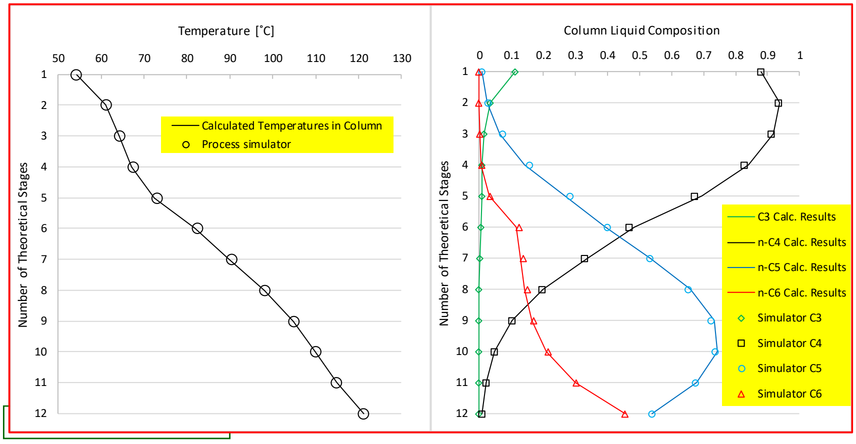
Subject to the Constraints:

Calculation Results

+;04,#Oltxlg#Skdvh#Frpsrvlwlrq#Fdofxodwlrq												
Frpsrvlwlrq	{G	{4	{5	{6	{7	{8	{9	{:	{;	{<	{43	{Z
q0F6	31444	31369	31348	31343	3133;	31339	31334	31333	31333	31333	31333	31333
q0F7	31;;3	31k6;	31k4<	31;74	319<6	317;8	3166;	314<<	31436	3137;	31353	3133:
q0F8	3133;	31359	31398	31476	3159;	316<6	31867	3198<	31:65	31:75	319:<	3186<
q0F9	31333	31333	31334	31339	31364	3144:	3145:	31474	31498	31543	31633	31788
Wrwdo	31k<<	41333	41333	41333	41333	41333	41333	41333	41333	41333	31k<<	41333
Huuru	31334	31333	31333	31333	31333	31333	31333	31333	31333	31333	31334	31333

+;05,#Ydsru#Skdvh#Frpsrvlwlrq#Fdofxodwlrq											
Frpsrvlwlrq		|4	|5	|6	|7	|8	|9	|:	|;	|<	|43
q0F6		31444	31384	31368	31363	3135;	3133;	31335	31333	31333	31333
q0F7		31;;3	31k5:	31k44	31;7<	31:64	31935	3174<	31579	31459	3138;
q0F8		3133;	31355	31386	31449	31549	3168:	31866	319;;	31:;3	31:<4
q0F9		31333	31333	31334	31338	31358	31367	3137:	31398	313<7	31484
Wrwdo		31k<<	41333	41333	41333	41333	41333	41333	41333	41333	41333
Huuru		31334	31333	31333	31333	31333	31333	31333	31333	31333	31333

Vxp#ri
Vtxduhv#ri
Huuruv
31333335



- A comparison with the results of the general-purpose simulator was carried out (the simulator calculation also applied Raoult’s law).
- It was confirmed that the compositions and the temperatures match well.
- It can be seen that the assumption of equimolar flow is valid, since the biggest difference between the results of Excel and the simulator is whether equimolar flow can be assumed.

Reference: Impact of K Values

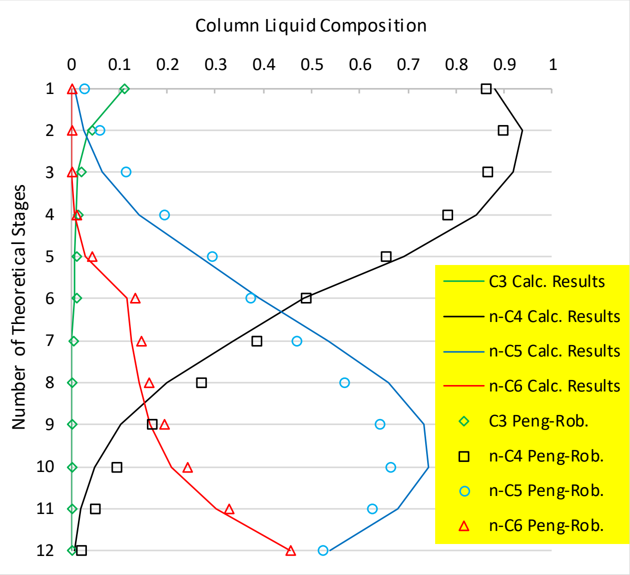
- Thiele-Geddes method K value calculation: Raoult's law

$$K_i = \frac{y_i}{x_i} = \frac{P_i^0}{P}$$

- K value calculation of general purpose simulator: Peng-Robinson equation of state

$$K_i = \frac{y_i}{x_i} = \frac{\phi_i^L}{\phi_i^V}$$

φ_i^V : Fugacity Coefficient of Component i in the Vapor Phase
φ_i^L : Fugacity Coefficient of Component i in the Liquid Phase



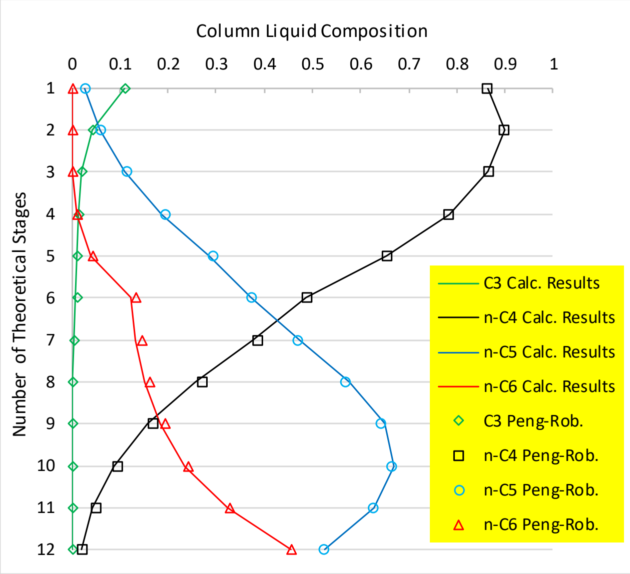
A comparison was done with the results when using the Peng-Robinson equation of state for calculation of the general purpose simulator. When the K values in the simulator are determined by the Peng-Robinson method, there is a difference with the results calculated by the Thiele-Geddes method since the non-ideality on the vapor phase side is taken into account.

参考：K値の影響2

- Thiele-Geddes method K value calculation: Peng-Robinson equation of state (Using the calculated values of the simulator)

- K value calculation of general purpose simulator: Peng-Robinson equation of state

$$K_i = \frac{y_i}{x_i} = \frac{\phi_i^L}{\phi_i^V}$$



The comparison with the results calculated by replacing the K values used for the calculation of the Thiele-Geddes method with the values obtained by the simulator is shown. The results of the general-purpose simulator and Thiele-Geddes method extensively agree.
It can be seen that the K values are important to determine the correct compositions and temperatures in the column.

Conclusion

- In this document, we derived the equations of the Thiele-Geddes method, which is a sequential calculation method.
- The Thiele-Geddes method uses the number of theoretical stages and the reflux ratio, and allows finding, without giving distillate and bottoms compositions, the internal column temperatures and compositions that are required for further calculating the diameter and energy saving measures of a continuous distillation column.
- The calculation requires the vapor-liquid equilibrium ratios (K_i), and the K values have a considerable effect on the calculation accuracy. Therefore, measures must be taken when this method is applied to systems other than ideal solutions or systems in which the K values are generalized as a function of reduced critical points or temperature.
- In addition, since the column calculation is done assuming equimolar flow, it is necessary to verify the impact of this assumption when applying this method to systems with highly non-ideal liquids.