Distillation Theory and Its Application to Optimal Design of Separation Units

Distillation Theory and Its Application to Optimal Design of Separation Units presents a clear, multidimensional, geometric representation of distillation theory that is valid for all types of distillation columns for all splits, column types, and mixtures. This representation answers such fundamental questions as:

- What are the feasible separation products for a given mixture?
- What minimum power is required to separate a given mixture?
- What minimum number of trays is necessary to separate a given mixture at a fixed-power input?

Methods of the general geometric theory of distillation, encoded in software, provide quick and reliable solutions to problems of flowsheet synthesis and to optimal design calculations. DistillDesigner software allows refinement and confirmation of the algorithms of optimal design.

This book is intended for students and specialists in the design and operation of separation units in the chemical, pharmaceutical, food, wood, petrochemical, oil-refining, and natural gas industries, and for software designers.

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Preface

This book is devoted to distillation theory and its application. Distillation is the most universal separation technique. Industrial distillation consumes a considerable part of the world power output. The distillation theory enables one to minimize power and capital costs and thus opens up new ways of designing economical separation units. The most important constituent of the distillation theory is the geometric approach, which reveals general rules governing the variation of component concentrations along the distillation column. In other words, it provides general rules for the arrangement of distillation trajectories in the so-called concentration space, in which every point represents some mixture composition. A considerable part of the book is concerned with these general rules, which are used as the basis in developing new methods and algorithms for the optimal design of separation units.

The geometric approach to distillation was put forward by the German scientists Ostwald and Schreinemakers in the early twentieth century. During the years that followed, it has been developed by scientists from various countries. However, until recently, the geometric approach found little use in the design of distillation units. The progress in this field was made by developing the pure computational approach, more specifically, ways of describing the liquid–vapor equilibrium and algorithms for solving sets of distillation equations. This approach has been fruitful: it has resulted in universal computer programs that enable one to design a distillation column (system) of any type for separation of any kind of mixture. However, the pure computational approach gives no answer to a number of fundamental questions that arise in the optimal design of distillation processes, particularly in the case of azeotropic distillation. These questions are the following: (1) What are the feasible separation products for a given mixture? In other words, what components can be present in or absent from the separation products? (2) What minimum power is required to separate a given mixture into the desired components? (3) What minimum number of trays is necessary to separate a given mixture into the desired components at a fixed-power input? Answers to these questions have been provided only by a general geometric theory of distillation.

Until recently, this theory had not advanced to a sufficient extent. Solutions were only obtained for particular cases. For many years, the author and his colleagues, relying on the results obtained by other researchers, have been putting a great deal of effort into elaborating general methods of the geometric theory to answer the fundamental questions listed above. An analysis of thermodynamically reversible distillation, the conception of "sharp" separation, the formulation of conditions under which distillation trajectories can tear-off from the boundaries of the concentration simplex, and the conditions of joining of column section trajectories have been particularly important steps in constructing the geometric theory of distillation. We have proposed a clear multidimensional geometric representation of distillation, which is valid for all types of distillation columns and complexes, for mixtures of any number of components and azeotropes, and for all splits. This representation provided answers to all the fundamental questions, which were previously enumerated. This success encouraged the author to write the present book.

The optimal design of a distillation plant includes the optimization of the sequence of the most economic columns and complexes for separation for a given mixture (flowsheet synthesis) and optimization of the operating and design parameters of these columns and complexes (optimal design calculations). Methods of the general geometric theory of distillation, encoded in software, provide quick and reliable solutions to both problems. The creation of this book necessitated the development of DistillDesigner software that allowed us to refine, check, and confirm the algorithms of optimal designing and also to provide for a significant portion of illustrations and exercises. The problems are solved neither by conventional "blind" methods nor by trial-and-error methods based on the designer's intuition. They are solved in a systematic way, and the solution has a geometric image so the designer can see that it is really optimal. The creation of the software product led, in its turn, to a revision of the general statements of the geometric distillation theory.

Furthermore, the book considers problems that are beyond the framework of the geometric theory of distillation but are still of importance from both the theoretical and practical standpoints.

Among these problems is the problem of maximizing energy savings by optimizing the type of separation unit and by maximizing heat recovery and the problem of the maximum yield of the most valuable products in the separation of thermolabile mixtures (e.g., the maximum yield of the light product in oil refining). Application of optimal design methods based on the general geometric theory of distillation and use of new, most economic distillation units and separation sequences bring the practice of separation to a much higher level.

This book is intended for a wide variety of specialists in the design and operation of separation units in the chemical, pharmaceutical, food, wood, petrochemical, oil-refining, and natural gas industries, and for those engaged in creating software for separation unit design. The circle of these specialists comprises software engineers, process designers, and industrial engineers. The software engineer will find new computational algorithms, the process designer will be provided with a useful guide in his or her search for economic engineering solutions, and the industrial engineer will find ways of reducing the process cost. This book can serve as a manual for students and postgraduates who want to refine their understanding of distillation.

The book has many illustrations, without which understanding of the geometric theory would be impossible. The visualization of trajectory location in the concentration space has great practical significance, as it allows the process designer to understand the main peculiarities of separation of each particular mixture. Developing the geometric theory of distillation necessitated the introduction of some new terms. Furthermore, for some concepts, there are no unique, commonly accepted terms. For these reasons, the book is supplemented with a short glossary, which is believed to be useful for the reader. For better understanding of the subject, each chapter has an introduction that presents the problems to be considered, their brief history, and a conclusion, which summarizes the basic results. Besides that, each chapter contains questions for review and exercises with DistillDesigner software. The most important chapter for understanding the geometric theory of distillation is Chapter 5. The chapters preceding it are basically introductory, and those that follow speak mostly of the application of the theory.

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More information

Nomenclature

A	separation work
A	stationary point of bond chain
A	vertex of product simplex
B	bottom stream (flow rate), kmol/sec
$C^{(k)}$	k-component boundary element of concentration simplex
C_n	concentration simplex for n-component mixture
d	dimension of trajectory bundle
D	overhead stream (flow rate), kmol/sec
E	entrainer stream (flow rate), kmol/sec
F	feed stream (flow rate), kmol/sec
h	enthalpy of liquid, kJ/kg or kcal/kg
H	enthalpy of vapor, kJ/kg or kcal/kg
h	heave key component
$i_D : i_B$	split in column (i_D and i_B – components of overhead and bottom products respectively)
$i : j$	split in section (i and j present and absent component of section product or pseudoproduct respectively)
K	equilibrium ratio
k	number of product components at sharp distillation
k	key component
k	key stationary point (pseudocomponent)
K_j^{∞}	equilibrium ratio of component j at infinite dilution
K^t	equilibrium ratio in tear-off point
l	light key component
L	liquid stream (flow rate), kmol/sec
m	number of product components at sharp distillation

m	number of stationary points of bond chain
n	number of components in a mixture
N	number of equilibrium stages
N^+ or N^-	stable or unstable node respectively
N_D^+ or N_D^-	stable or unstable node of overhead boundary element of concentration simplex or of distillation region respectively
N_B^+ or N_B^-	stable or unstable node of bottom boundary element of concentration simplex or of distillation region respectively
N_r^+ or N_r^-	stable or unstable node of rectifying trajectory bundle respectively
N_s^+ or N_s^-	stable or unstable node of stripping trajectory bundle respectively
N_e^+ or N_e^-	stable or unstable node of extractive trajectory bundle respectively
P	pressure, Pa
q	fraction of liquid in feed
Q	heat flow rate, kJ/sec or kcal/sec
qS	quasisaddle
R	reflux ratio
$R_{\min}$	minimum reflux ratio
$R_{\lim}^1$ or $R_{\lim}^2$	first or second boundary minimum reflux ratio respectively
$R_{\min}^t$ or $R_{\max}^t$	minimum or maximum reflux ratio for trajectory tear-off respectively
$\underset{ijk}{\mathrm{Reg}}$	region
Reg_{ord}	component order region
$\mathrm{Reg}_D^{(k)}$ or $\mathrm{Reg}_B^{(k)}$ or $\mathrm{Reg}_{D,E}^{(k)}$	k-component possible overhead or bottom or overhead-entrainer product region respectively
$\overset{j}{\underset{i}{\mathrm{Reg}}}_D$ or $\overset{j}{\underset{i}{\mathrm{Reg}}}_B$ or $\overset{j}{\underset{i}{\mathrm{Reg}}}_{D,E}$	i-present components and j-absent components possible overhead or bottom or overhead-entrainer product region respectively
$\overset{j}{\underset{i}{\mathrm{Reg}}}_{bound,D}$ or $\overset{j}{\underset{i}{\mathrm{Reg}}}_{bound,B}$ or $\overset{j}{\underset{i}{\mathrm{Reg}}}_{bound,D,E}$	boundary of possible overhead or bottom or overhead-entrainer product region respectively, i-present components, and j-absent components
$\mathrm{Reg}_r^{t(k)}$ or $\mathrm{Reg}_s^{t(k)}$ or $\mathrm{Reg}_e^{t(k)}$	k-component tear-off region of rectifying or stripping or extractive section respectively
Reg^∞	distillation region at infinite reflux
$\mathrm{Reg}_{bound,D}^\infty$, $\mathrm{Reg}_{bound,B}^\infty$	top or bottom boundary element of distillation region at infinite reflux respectively
$\mathrm{Reg}_{sep,r}^{\min,R}$, $\mathrm{Reg}_{sep,s}^{\min,R}$	separatrix min-reflux region for rectifying or stripping section for given reflux R respectively

$\text{Reg}^{sh,R}_{sep,r}$, $\text{Reg}^{sh,R}_{sep,s}$	separatrix sharp split region for rectifying or stripping section for given reflux R respectively
$\text{Reg}^{R}_{w,r}$, $\text{Reg}^{R}_{w,s}$ $\text{Reg}^{R}_{w,e}$	rectifying or stripping or extractive section working region at given reflux R respectively
$\text{Reg}^{i:j}_{sh,r}$, $\text{Reg}^{i:j}_{sh,s}$, $\text{Reg}^{i:j(E)}_{sh,e}$	sharp split region for rectifying or stripping or extractive section for split $i:j$ respectively
$\text{Reg}^{h}_{rev,r}$, $\text{Reg}^{l}_{rev,s}$, $\text{Reg}^{m}_{rev,e}$	reversible distillation region for rectifying section with h heavy component or stripping section with l light component or extractive section with m middle component respectively
Reg_{att}	attraction region
Reg_{L-L}	two liquid phases region
Reg_{pitch}	region of pitchfork
Reg_{simp}	product simplex at infinite reflux
Reg_{sub}	subregion of distillation at infinite reflux
Reg_{tang}	tangential pinch region
S	reboil ratio
S	entropy
S	saddle
S^1	tear-off point of section trajectory at sharp split
S^2	tear-off point of section trajectory at minimum reflux
$S^1 - S^2 - N^+$	boundary element of trajectory bundle at sharp split
$S^2 - N^+$	boundary element of trajectory bundle at minimum reflux
SN	saddle-node
S_r or S_s or S_m	saddle point of rectifying or stripping or intermediate trajectory bundle respectively
T	temperature, K
V	vapor stream (flow rate), kmol/sec
x	mole fraction of liquid phase
x^t_{rev}	tear-off point of reversible distillation trajectory
x'_D	pseudoproduct point
x^{∞}_{f} or $x^{\min}_{f}$	composition on first plate under feed cross section at which number of stripping section plate is infinite or minimal respectively
x^{∞}_{f-1} or $x^{\min}_{f-1}$	composition on first plate above feed cross section at which number of rectifying section plate is infinite or minimal respectively
x^{branch}_{rev}	branch point of reversible distillation trajectory
(x^{sh}_{f}) or (x^{sh}_{f-1})	composition on first plate under or above feed cross section at sharp split respectively

$[x_f^{sh}]$ or $[x_{f-1}^{sh}]$	composition segment on first plate under or above feed cross section at sharp split respectively
y	mole fraction of vapor phase
z	mole fraction of liquid–vapor mixture
1, 2, 3 . . .	components 1, 2, 3 . . . respectively
1, 2; 1,3 . . .	mixtures of components 1 and 2; 1 and 3 . . . respectively
1-2, 1-2-3 . . .	boundary elements of concentration simplex
12, 13 . . .	binary azeotropes of components 1 and 2; 1 and 3 . . . respectively
123, 124 . . .	ternary azeotropes of components 1, 2, and 3; 1, 2, and 4 . . . respectively
123, 132 . . .	regions of component order

Greek and Other Symbols

ε	component recovery
Δ	difference
λ	eigenvalue of distillation matrix
σ	excess reflux factor
∞	infinity
α	relative volatility
Σ	sum
θ	the root of an Underwood equation for both sections
φ or ψ	the root of an Underwood equation for rectifying or stripping section
η	product purity
η	thermodynamic efficiency
Δx_f^{sh} or Δx_{f-1}^{sh}	composition interval on plate under or above feed cross section
$\alpha_{12}, \alpha_{13} \ldots$	volatility of component 1 relative of component 2, of component 3 . . .
$N^- \overset{S}{\Rightarrow} N^+$	distillation bundle included stationary points N^-, S, N^+
$x_{f-1} \Downarrow\Rightarrow x_f$	mixing in feed cross section
$\rightarrow$	bond, trajectory of distillation, one-dimensional trajectory bundle
$\Rightarrow$	set of all bonds (or of all distillation trajectories) of distillation bundle
$\Leftrightarrow$	flows between sections of distillation complex
$\Updownarrow$	decanter

Subscripts and Superscripts

az	azeotrop
ad	adiabatic

B	bottom product
con	condenser
D	overhead product
e	component of entrainer
E	entrainer
e	first plate under entrainer cross section
e-1	first plate above entrainer cross section
F	feed
f	first plate under feed cross section
f-1	first plate above feed cross section
h	heave key component *h*
Haz	heteroazeotrop
i	component of mixture
i, *D*	component *i*, which is present in product *D*
imp	impurity
int	intermediate condenser or reboiler
irr	irreversible
j	component *j*, which is absent on the boundary element of concentration simplex
j, *DE*	component *j*, which is absent in product *D* and entrainer *E*
j	plate of column
j	stationary point
k	component of mixture
k	plate of column
key	key component
l	light key component of mixture
L1, *L2*	first, second liquid phases
M	intermediate product
m	intermediate section
m	middle volatility component of mixture
new	new value at iterations
old	old value at iterations
pinch	pinch
pr	preferable
r	rectifying
reb	reboiler
rev	reversible
s	stripping
st	stationary point
t	tear-off point
*t*1, *t*2	first and second tear-off points of reversible distillation trajectories respectively
(*k*)	*k*-component boundary element of concentration simplex, *k*-component point, product point with *k* product components

w	working region, working trajectory
1,2,3 . . .	component 1,2,3 . . . ; section 1,2,3 . . . ; feed 1,2; variant 1,2,3; column 1,2,3 . . . respectively

Nomenclature to Figures

A	endpoint of tear-off segment of distillation trajectories
$A_1, A_2, A_3 \ldots$	vertexes of possible product composition regions
Az	azeotropes
boxed digits	component order regions
C-1, C-2 . . .	columns
dash-dotted line	line of material balance
dashes	tray compositions on composition profiles
dotted line	trajectory of reversible distillation
dotty line	separatrix
double segment	possible composition of overhead product or trajectory tear-off segment of top section
thick black segment	possible composition of bottom product or trajectory tear-off segment of bottom section
gray segment	tear-off segment of extractive distillation trajectories
$F + E$	composition point of feed and entrainer mixture
F_0	composition point of initial feed
$F_1 + F_2$	composition point of mixture of feeds F_1 and F_2
H	height of column
HD	heave diesel oil
HN	heave naphta
LD	light diesel fuel
LN	light naphta
little black or white circle	stable or unstable node of concentration simplex respectively
little cross circle	saddle of concentration simplex
little cross square	bottom composition point
little square	overhead composition point
little triangle	feed composition point
short segment with arrow	tie-line liquid–vapor
st	steam
thick line	trajectory of distillation
thin line	equivolatility line
(1), (2) . . .	column (1) or (2) respectively
(1), (2) . . .	split (1) or (2) respectively
$\alpha_{12}, \alpha_{13} \ldots$	equivolatility line of components 1 and 2, 1 and 3 . . . respectively