Thermodynamical estimation of the bounds on performance of irreversible binary distillation

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ABSTRACT

The limits of the ability of a distillation system to seperate a binary mixture are considered for two different cases. In the first case the heat supply solely takes place at the column bottom and the heat removal at the condenser. In the second case the heat supply and removal is distributed over the column height. For both cases, the limiting column capacity and the minimum heat consumption are related to the external stream compositions and to the heat and mass transfer coefficients.

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1. Introduction

The investigation of the maximum performance of technical systems has been an important task for scientists for many years. Often bounds derived from a reversible consideration of the system are too high, so non-equilibrium approaches are used. Doing so, researchers got, during the last years, insight into the dissipation mechanism of systems like combustion waves [1], heat exchangers [2], anisotropic heat conductors [3], thermo acoustic engines [4], and geothermal power plants [5].

In this article a distillation column is considered. The investigation of distillation processes is an ongoing field of research: During the last years did studies on sweeping air membrane distillation [6], a solar distillation system [7], direct contact membrane distillation [8], multi-effect distillation [9], flat plate membrane-distillation [10], direct contact membrane distillation [11], or a randomly packed distillation column [12]. In contrast to other publications [13–22], here a continuous distillation column is considered, where the mass transfer can take place every in the column and is not organized in trays. The problem of optimal distillation design of such a column has been the subject of numerous studies [23–26]. The irreversibility of the process in a distillation column has been taken into account by correcting its reversible characteristics (by passing from the minimum reflux rate to the working reflux rate, from theoretical separation stages to real trays, and so on) through introduction of time-proved experimental coefficients. Some of the studies suggest design improvements to the process in order to reduce its cost and, accordingly, enhance its economic efficiency. However, the following questions arise here: What is the highest potential of such improvements? What advantages can they offer over the conventional organization of the process? What form should the optimal operating curve have, and how can this curve be realized without radically complicating the process? These problems are far from being solved completely. It should be mentioned that via analogous considerations processes like the growing of microorganisms can be understood better [27].

In our earlier works [28,29], based on results reported in [30], we determined the "ideal" form of the operating curve, for which the irreversibility of the process, characterized by entropy production, is the lowest at a given column capacity and integrated heat and mass transfer coefficients. In [31] the optimal separation sequence for a ternary mixture was investigated. Below, we make an attempt to take into account the irreversibility of the process in terms of heat and mass transfer kinetics in order to elucidate the effect of kinetic factors on the performance limits of the column (capacity and heat consumption). As we want to obtain an upper-bound estimate of the potential of the column, the assumptions simplifying the computational procedure and extending the applicability domain of the results will be made so that none of them adds to the irreversibility of the process. Only in this case can we claim that the performance parameters of a real column will not exceed the estimated upper bound. These assumptions lead to estimates biased upward, but these estimates are, nevertheless, much closer to the true values than the estimates based on consideration of solely reversible processes. Furthermore, the limiting capacity of the column can by no means be derived from reversible estimates.

Notation

g	flow rate, mol/s
$\bar{g}$	total mass transfer flux throughout the column height, mol/s
H	column height, m
h	molar enthalpy, J/mol
k	mass transfer coefficient per unit change in the lower boiling component concentration, mol/s
$\bar{k}$	effective mass transfer coefficient per unit height of the column, mol/(s m)
L	liquid flow rate, mol/s
l	coordinate characterizing position along the column height, m
P	pressure, Pa
p	power, W
q, q^0	total heat consumption and heat consumption in the reversible process, W
q_+, q_-	heat fluxes supplied to the column bottom and removed from the condenser, W
$q(x)$	heat flux density, W/m
R	universal gas constant, J/(mol K)
r	molar heat of evaporation, J/mol
s	coefficient of proportionality between the mass transfer flux and the driving force, mol/s
s_D, s_B, s_F	molar entropies in the condenser, bottom, and feed stream, J/(mol K)
T_+, T_-	temperatures of the vapor heating the bottom and of the water cooling the condenser, respectively, K

V	vapor flow rate, mol/s
W	water equivalent of the coolant flow rate, W/K
x	molar concentration of the lower boiling component in the liquid phase, mol/mol
y	molar concentration of the lower boiling component in the vapor phase, mol/mol
y^0	equilibrium concentration of the lower boiling component in the vapor phase, mol/mol
α	relative volatility
β	heat transfer coefficient, W/K
$\bar{\beta}$	total heat transfer coefficient, W/K
γ	parameter in the ideal operating curve equation
ε	draw-off ratio
μ	chemical potential, J/mol
σ	entropy production, W/K

Subscripts and superscripts

B	bottom
D	condenser
F	feed
i	flow number
q	heat transfer
g	mass transfer
j	component number
lim	limiting value

Here are the basic assumptions we make:

- Mass exchange is equimolar. This means that the transfer of a certain amount of the high boiling component from the vapor to the liquid phase corresponds to the transition of the same amount of the low-boiling component from liquid to vapor.
- In each cross section along the column height, the vapor and liquid flows have equal temperatures and pressures (which vary from one cross section to another).
- The effects of diffusion between adjacent cross sections are negligible, and the species flow in plug-flow regimes.
- The heat of the exiting streams is transferred to the entering streams, and the irreversibility of this heat transfer can be neglected.
- The liquid mixture to be separated is heated to its boiling point and, afterwards, fed into that cross section of the column in which it has the same composition as the reflux.

Thus, we will consider an "idealized" column, taking into account two sources of irreversibility, namely, heat transfer associated with heat supply to the stripping section of the column and heat removal from the rectifying section and mass transfer between the vapor and the reflux along the column height. Note that, if the mass transfer coefficient is derived from data for an operating column, it indirectly allows for the deviation from the plug flow pattern, mixing on trays, and diffusion between cross sections. In the next section, using thermodynamic balance equations for a binary distillation column, we will correlate the compositions and flow rates of the external streams with heat consumption in the case of heat supply to the column bottom and heat removal from the condenser. The limiting performance parameters of this column will be estimated. In the last section, we will investigate the limiting performance of the column that uses the ideal operating curve and report the laws of heat supply

and removal along the column height that make it possible to achieve this operating curve.

2. Performance of a traditional distillation column

2.1. Distillation model

In the traditional organization circuitry of rectification processes (see Fig. 1) the mixture's feed stream enters the column with flow velocity g_F and a certain concentration vector. Here, flow velocities are meant in terms of mol/s. In case of a binary mixture this vector can be characterized by two molar fractions. The heat flux q_+ is being supplied to the column's bottom (cube), whereby evaporation occurs, and a vapor stream with velocity V rises up the column and interacts with a liquid flow (reflux) with velocity
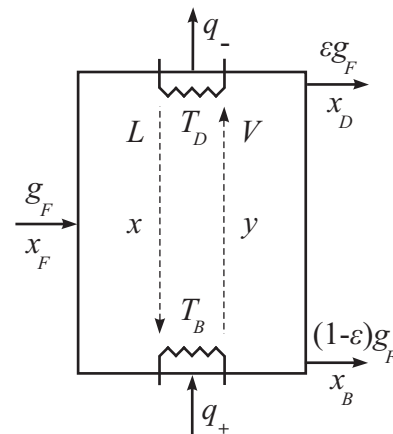
Fig. 1. The binary distillation column. Here L is the reflux flow and V is the vapour flow.