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Synthesis and design of reactive distillation columns with two reactive sections

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ABSTRACT

The synthesis and design of reactive distillation columns with two reactive sections (RDC–TRS) are attempted for the separations of reacting mixtures with somewhat unfavorable ranking of relative volatilities (RM–SURRV, i.e., two reactants are the light and heaviest components and two products the lightest and heavy ones). With the deliberate arrangement of the two reactive sections, the disadvantages by the unfavorable relative volatility can be substantially alleviated, facilitating consequently the reaction operation and separation operation involved. The separations of a hypothetical quaternary reaction, the esterification of acetic acid with methanol, and the transesterification of butyl acetate with ethanol are employed to evaluate the RDC–TRS. The process is found considerably superior to the reactive distillation column with a single reactive section and this demonstrates its feasibility and effectiveness in the separations of RM–SURRV. The RDC–TRS is found to present comparable or even improved performance in comparison with the reactive distillation column with an external recycle from bottom to reactive section and this corroborates it a potentially competitive alternative for the separations of the RM–SURRV. The RDC–TRS is also highlighted for the other kind of RM–SURRV (i.e., two reactants are the lightest and heavy components and two products the light and heaviest ones).

1. Introduction

The advantages of reactive distillation columns, e.g., the reduction of capital investment and operating cost, originate essentially from their capability of driving equilibrium-limited reactions to completion due to the in-situ separations of products from reactants in the reactive section (Doherty and Buzad, 1992; Malone and Doherty, 2000; Stankiewicz, 2003). In the case of the separations of reacting mixtures with the most favorable ranking of relative volatilities (RM–MFRRV, i.e., two reactants are the light and heavy components and two products the lightest and heaviest ones), such advantages can fully be exploited because of the light and heavy reactants unconverted are readily separated from the lightest and heaviest products (in the rectifying and stripping sections) and recycled back to the reactive section with the manipulations of reflux and reboil flow rates, respectively (Luyben, 2000; Kaymak and Luyben, 2004; Tung and Yu, 2007). This is indicated clearly in Fig. 1a in terms of the separation of a hypothetical quaternary reaction, $A+B\underset{k_B}{\overset{k_F}{\rightleftharpoons}}C+D$ ($\alpha_C>\alpha_A>\alpha_B>\alpha_D$). In the case of the separations of reacting mixtures with somewhat unfavorable ranking of relative volatilities (RM–SURRV, i.e., two reactants are the light and heaviest components and two products the lightest and heavy ones), such advantages can, however, only be partially exploited. Fig. 1b illustrates the detailed reason for the degradation of steady-state performance in terms of the separation of a hypothetical quaternary

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Notation

a	pre-exponential factor
A	hypothetical component
A_{vp}	vapor pressure constant (kPa)
B	hypothetical component
BPFR	bottom product flow rate (mol/s)
B_{vp}	vapor pressure constant (kPa K)
C	hypothetical component
D	hypothetical component
DFR	distillate flow rate (mol/s)
E	activation energy of the hypothetical ideal reaction (J/mol)
F	feed flow rate (mol/s)
IPFR	intermediate product flow rate (mol/s)
k	specific reaction rate (mol/(s mol))
k_{eq}	reaction equilibrium constant
L	liquid flow rate (mol/s)
M	kinetic holdup on a reactive stage (mol)
M_{REB}	kinetic holdup within reboiler (mol)
P	pressure (kPa)
Q_{reb}	heat duty of reboiler (MW)
R	ideal gas law constant (J/(mol K))
Rate	net reaction rate (mol/s)
RF	external recycle flow rate (mol/s)
RR	reflux flow rate (mol/s)
T	temperature (K)
V	vapor flow rate (mol/s)
x	liquid composition
y	vapor composition
ΔH_R	heat of a reaction (J/mol)

Abbreviations

BuAc	butyl acetate
BuOH	butanol
EtAc	ethyl acetate
EtOH	ethanol
HAc	acetic acid
H_2O	water
MeAc	methyl acetate
MeOH	methanol
RDC–ERBR	reactive distillation column with external recycle from bottom to reactive section
RDC–SRS	reactive distillation column with a single reactive section
RDC–TRS	reactive distillation column with two reactive sections
RM–MFRRV	reacting mixtures with the most favorable ranking of relative volatilities
RM–SURRV	reacting mixtures with somewhat unfavorable ranking of relative volatilities

Greek letters

α	relative volatility
β	feed splitting ratio
δ	Kronecker delta function
ε	error tolerance
ν	stoichiometric coefficient of a reaction

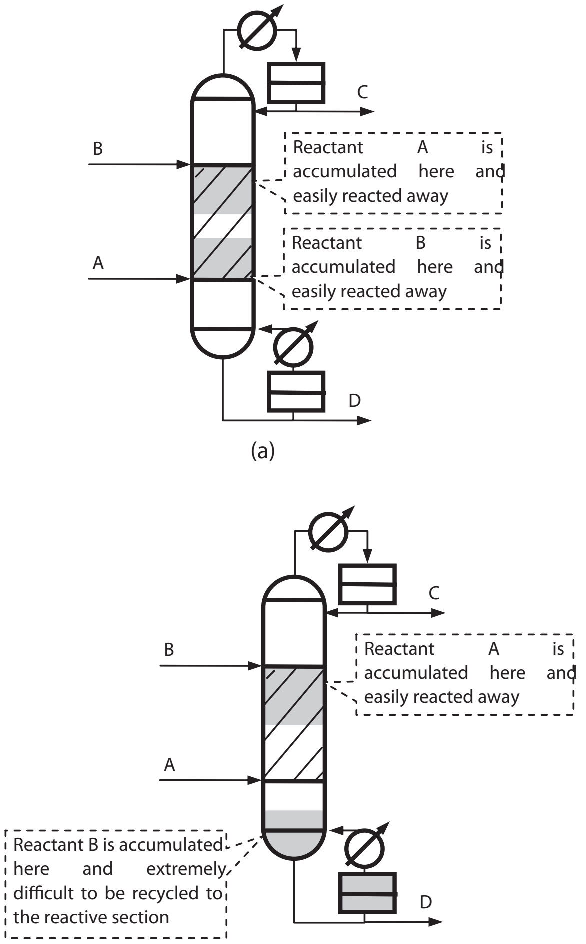
Subscripts

A	component index
B	component index
bot	bottom
C	component index
D	component index
d	distillate
i	component index
ip	intermediate product
j	stage index
m	feed stage index

Superscript

s	saturation
sp	product specification

reaction, $A+B \underset{k_B}{\overset{k_F}{\rightleftharpoons}} C+D$ ($\alpha_C>\alpha_A>\alpha_D>\alpha_B$). Although the light reactant *A* unconverted can readily be separated from the lightest product *C* in the rectifying section and recycled back to the reactive section through the manipulation of reflux flow rate, the heaviest reactant *B* unconverted is extremely difficult to be separated from the heavy product *D* in the stripping section and recycled back to the reactive section with the manipulation of reboil flow rate (it tends actually to accumulate at bottom). Thus, the unfavorable relative volatility between reactant *B* and product *D* accounts for the



(a)

(b)

Fig. 1 – Separations of the RM–MFRRV ($\alpha_C>\alpha_A>\alpha_B>\alpha_D$) and RM–SURRV ($\alpha_C>\alpha_A>\alpha_D>\alpha_B$) with the RDC–SRS: (a) RM–MFRRV, (b) RM–SURRV.