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Selectivity engineering with single feed multi-side draw hybrid reactive distillation columns

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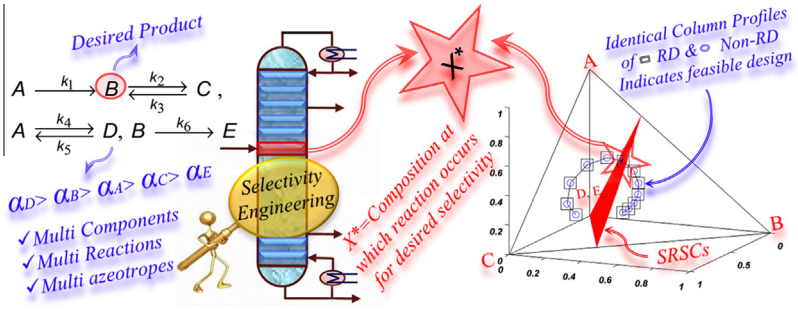
HIGHLIGHTS

- Conceptual design of multi-side draw hybrid reactive distillation columns.
- The design procedure is a combination of graphical method and simulations.
- The algorithm typically generates multiple designs of desired selectivity.
- The developed algorithm can be applied directly to multi azeotropic systems.
- Methodology is illustrated for transesterification of dimethyl carbonate with ethanol.

GRAPHICAL ABSTRACT



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ABSTRACT

In multireaction systems reactive distillation (RD) not only increases the reactant conversion and purity but also proves very helpful to achieve the selectivity of the desired product. Designing a reactive distillation column for a multicomponent multireaction system is a challenging task, especially when the reactant is intermediate boiling or saddle in the residue curve map of the mixture. In the previous work (Hasan et al., 2014), we introduced simple hybrid RD column and hybrid RD column with single side draw to obtain a desired selectivity in single reactant multireaction schemes. In this work, we extend the approach further to include multi-side draw hybrid RD configuration and present, a new synthesis and design methodology. The developed algorithm is a combination of geometric method and simulation based design. We determine a surface of reactive stage compositions (SRSCs) such that if the reaction takes place at any of the compositions that belongs to SRSCs then the desired selectivity is ensured. Further, we also show that a single feed multi-side draw hybrid RD configuration is capable to give a desired selectivity in multi-reactant multireaction schemes wherein, both the reactants are saddle in the corresponding residue curve map. This is illustrated using an industrially relevant example of transesterification of dimethyl carbonate with ethanol to achieve the desired selectivity toward ethyl methyl carbonate. The results provide a good starting point for rigorous simulation. The algorithm presented here is applicable to any number of components and can be directly applied to even multi azeotropic systems as well. Though at this stage its applicability is restricted to the single feed configurations, we believe that the developed approach can be conveniently extended to multi-feed configurations with appropriate modifications.

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Notations

F	feed flow rate (mol/s)
k	rate constant
k_{ref}	rate constant for the reference reaction
N	total number of stages
NC	number of components
Nfl	feed stage location
Nr	total number of reactive stages
Nrl	reactive stage location
r_k	actual reaction rate for kth reaction, mole/(time × mass of catalyst)
$r'_k (= r_k/k_{ref})$	normalized reaction rate
W_{cat}	mass of catalyst
x_i^*	reactive stage composition of ith component
Xf	feed composition
X^*	reactive stage composition
D:F	distillate to feed ratio
V:F	vapor boil-up to feed ratio
Sd1	side-draw location at location 1
Sd2	side-draw location at location 2
SD1	side-draw to feed ratio at location 1
SD2	side-draw to feed ratio at location 2
Greek letters	
α	relative volatility
$\upsilon_{i,k}$	stoichiometric coefficient of *ith* component in *kth* reaction
$\upsilon_{T,k}$	sum of the stoichiometric coefficient in *kth* reaction
Subscripts	
A, B, C, D	components involved in reaction
az	azeotrope
i	ith component
ref	reference component
Abbreviations	
CSTR	continuous stirred tank reactor
Da	Damkohler number
DMC	dimethyl carbonate
DEC	diethyl carbonate
EtOH	ethanol
EMC	ethyl methyl carbonate
FOC	family of curves
LFSCs	locus of liquid feed stage compositions
MeOH	methanol
Non-RD	non-reactive distillation column
RD	reactive distillation column
SRSCs	surface of reactive stage compositions

1. Introduction

Reactive distillation (RD) which integrates reaction and distillation is a promising multi-functional reactor which has a potential of giving desired selectivities when designed astutely. The development of a systematic design procedure for reactive distillation columns to obtain higher or desired selectivity in case of simple and complex reaction schemes has been the theme of our work published in the past [2–9]. If the reactant is unstable or stable node in the corresponding residue curve map then the simple configurations such as reactive rectification or reactive stripping can be used. However, for the cases wherein reactant is saddle, complex RD configurations are to be employed to achieve the desired performance. For such mixtures, Hasan et al. [1] recently proposed a design algorithm for simple hybrid RD columns as well as hybrid RD column with single side draw to achieve a desired selectivity in case of single reactant multicomponent multi-reaction schemes. This algorithm is limited to the cases wherein maximum of two products undergo further side reaction (s). In the present work, we remove this restriction and extend the method further to include cases wherein, more than two products undergo further side reaction(s) and this requires the inclusion of multi-side draw hybrid reactive distillation columns. As a result, a new synthesis and design methodology is developed for multi-side draw hybrid reactive distillation columns, to achieve a desired selectivity in case of single reactant multireaction schemes wherein, the reactant is a saddle in the corresponding residue curve map. The developed algorithm is a combination of geometric method and simulation based design. It is based on the visualization of the locus of liquid feed stage compositions (LFSCs), obtained by simulation. We search for the intersection of LFSCs with a surface in composition space such that, if the reaction takes place at any of the compositions on this surface then the desired selectivity is achieved.

The developed algorithm is also applicable to even multi-azeotropic systems as well. In case of multi-azeotropic systems, nonideal vapor–liquid equilibrium and distillation boundaries are responsible for the contraction of the feasible reactive stage composition region required for the design of RD column. It is shown with the help of a hypothetical example of complex van de Vusse type reaction scheme that the developed methodology is capable of finding the design configurations of multi-side draw hybrid RD column to obtain desired selectivities. The algorithm developed here can be successfully applied to multireactant multi-reaction schemes too wherein, both the reactants are of intermediate volatility. This is illustrated with the help of a commercially important process of transesterification of dimethyl carbonate with ethanol. We would like to note here that in our previous [1–9] work we introduced different RD models in order to obtain higher or desired selectivity in case of different types of complex reaction schemes. The overall objective is to develop a complete algorithm that is applicable for a wider range of reaction networks and suggest general norms that can serve as a ready reference for process designers. The selection of type of reactive distillation column for selectivity engineering (i.e. simple or complex RD column, hybrid or fully reactive column) strongly depends on the volatility of reactants and on the number of products that undergo further side reactions in a given complex reaction scheme, which is evident from our previous work [1–9]. It is for this reason that a unified generalized theoretical that will encompass any given scheme, though useful, may be difficult to develop at this stage. We have therefore considered specific feature(s) of the reactive system at a time and developed suitable methods in our work so far. Fig. C shows the broader picture and current state of this work. In this work, we restrict ourselves to single feed hybrid RD configurations with multi-side draws and consider both zeotropic as well as multi azeotropic mixtures. Our next step is to include multifeed hybrid RD configuration to extend the approach for a wider range of reaction networks as most of the real industrial problems consist of multireactant complex reaction schemes in which reactants need not be of intermediate volatility.

The article is organized as follows: we start with a geometric interpretation of CSTR and multi-side draw hybrid RD column and introduce the reader to the concept of surface of reactive stage compositions (SRSCs) which forms a basis for the proposed design algorithm. A step-wise design algorithm is illustrated for the two examples of complex van de Vusse type reaction scheme involving zeotropic and multi-azeotropic mixtures. Further, with the help of