

Attainable regions of reactive distillation—Part I. Single reactant non-azeotropic systems

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Abstract

Reactive distillation (RD), a promising multifunctional reactor, can be used to improve the selectivity of the desired product by manipulating the concentration profiles in the reactive zone of the column. In this work, a new approach has been proposed to obtain the feasible regions of RD for the reactive systems involving single reactants, e.g. dimerization, aldol condensation, etc. Two new models namely the reactive condenser and the reactive re-boiler have been proposed. These models indicate the best location of the reactive zone in a column. Multistage versions of these models namely, reactive rectification and reactive stripping further expand the feasible region and are capable of representing the performance offered by a conventional RD unit. Several hypothetical non-azeotropic ideal systems have been extensively studied using these models and it has been shown that selectivity close to 100% is attainable over the entire range of conversion for a series as well as a combination of series and parallel reactions with positive reaction orders. Two industrially important cases of aldol condensation of acetone and dimerization of isobutylene have also been addressed using this approach. For porous catalysts, the presence of intra-particle diffusion resistance may limit the feasible region and even in the case of ideal non-azeotropic systems it may not be possible to obtain 100% selectivity. A methodology to incorporate pore diffusion effects is also illustrated.

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1. Introduction

Reactive distillation (RD) as the name suggests is the integration of reaction and separation in a single piece of equipment. Such integration can be effectively used to improve the selectivity of a series or combination of series and parallel reactions especially when the intermediate product is the desired one. RD, when designed judiciously, can offer significantly high yields compared to the conventional reactor systems in such case. One can conveniently manipulate the concentration profiles of various species in the reactor, which involves in situ separation, to obtain better selectivity for the desired product. The multiple reactions involved in the system may be irreversible or a combination of reversible and irreversible reactions.

Attainable region (AR) approach, first introduced by Horn (1964), is used to assess the reactor network feasibility. It has been extensively studied and investigated by Hildebrandt, Glasser and their co-workers. Glasser et al. (1987) defined AR, essentially a plot of yield vs conversion, as the region in concentration space which can be obtained by any combination of conventional reactors and mixing. This AR is sometimes called the “kinetically attainable region” to distinguish it from the “thermodynamically attainable region,” which is determined by equilibrium constraints (Shinnar and Feng, 1985). To identify a region as AR, Glasser et al. (1987) defined a reaction vector. Simple steady state models for the isothermal CSTR (Eq. (1)) and PFR (Eq. (2)) with constant volume were applied to construct the AR in concentration space:

$$c - c_0 = \tau r(c), \quad (1)$$

$$\frac{dc}{d\tau} = r(c), \quad c(t=0) = c_0, \quad (2)$$

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where r is the reaction vector. The direction of reaction vector indicates the direction of change of concentration in the concentration space.

For ideal reactors certain geometric properties were identified:

- The reaction vector is tangent to every point on the PFR performance locus.
- The reaction vector is collinear with the vector obtained from the difference of feed concentration and exit concentration at each point on the CSTR performance locus.
- The feed to the PFR section in recycle reactor lies on the line joining the feed and exit streams of the system representing mixing of two concentration vectors.

The necessary conditions derived by Glasser et al. (1987) to identify region as attainable, are:

- The region is convex.
- No reaction vector on the region points outwards.
- In the complement of the AR no reaction vector when extrapolated intersects the AR.

AR approach is not an optimization technique. It can, however, provide insights for devising a superstructure in an optimization problem. Lakshamanan and Biegler (1996) used the AR properties to formulate a reaction network and Pahor et al. (2000) suggested an iterative procedure using AR analysis to update the superstructure in MINLP formulation. AR approach only identifies the feasible region for the production of a desired product. It serves an important purpose of generating process alternatives at the conceptual design stage. The approach has been successfully applied to assess reactor network synthesis.

Nisoli et al. (1997) combined the concept of AR for reaction-mixing system with the geometric methods used for the feasibility of separations. A systematic approach was developed to identify compositions that can be achieved by combining reaction, mixing and separation in co-current devices. The reaction-separation devices considered were: CSTR with vapor removal and PFR with vapor removal. They modified the reaction vector for systems with simultaneous reaction and separation to give a reaction-separation vector. This reaction-separation vector was also shown to follow the same geometric properties as that defined by Glasser et al. (1987). The steady state equations of CSTR with vapor removal and PFR with vapor removal are given by

$$x - x_0 = DaR(x, y), \quad (3)$$

$$\frac{dx}{d\eta} = R(x, y), \quad x(t=0) = x_0, \quad (4)$$

where R is the reaction-separation vector which is a combination of reaction and separation effects. It was further modified by Gadewar et al. (2002) for the cascade of two phase CSTRs. The countercurrent cascade model of two phase CSTRs was considered as the surrogate for stripping and rectifying sections by Gadewar et al. (2002). For the consecutive series reaction

they showed that the suggested model offers enhanced selectivity when the reactant is heavier than the desired product. We extend this work further to encompass other reacting systems and propose a new approach to construct AR of RD on a conversion vs selectivity plot.

The work emphasizes on a single reactant system involving multiple reactions with intermediate product as the desired one. Such systems are relatively simple to analyze and hence considered as case studies to begin with. However, we believe, the approach can be extended to other cases as well. Several simplified model reactor-separator units have been proposed that are capable of surpassing the performance of the conventional flow reactors depending on the kinetics and vapor-liquid equilibrium of a given reacting system. With this method it is expected that one can avoid use of rigorous optimization techniques, at least at a conceptual level, as RD with its complex behavior and large number of design and operating parameters is still a challenging problem for current optimization routines (Gangadwala et al., 2006). These simplified models not only help in knowing the AR but also indicate the location of reactive zone in the RD column before going for a rigorous design and simulation exercise. The model systems are also simple enough so that direct laboratory experiments can be conveniently performed in such units, in the absence of kinetic and thermodynamic data, to obtain the desired representative results.

2. Model development

Each segment or a stage of RD column can be viewed as a combination of a reactor and separator units, which repeats along the length of the column as shown in Figs. 1 and 2. This reactor-separator combination traveling along the length of the column (Figs. 1a and 2a) is in a sense analogous to the batch reactor separator units shown in Figs. 1b and 2b progressing along the time co-ordinate. The units shown are a combination of two stages, namely re-boiler and condenser, of which one

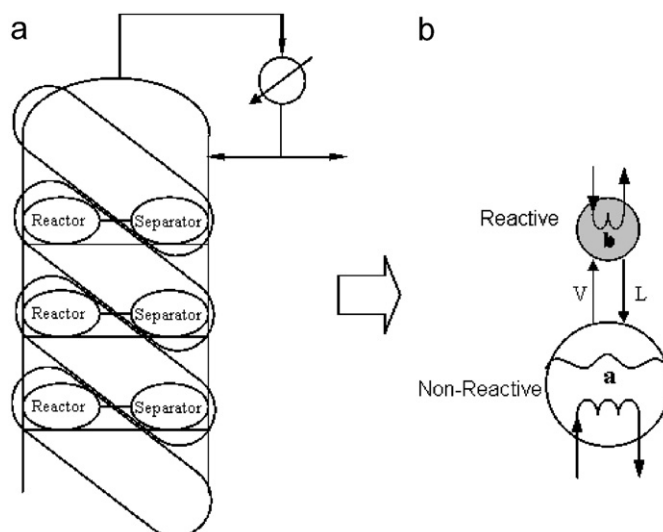


Fig. 1. (a) Rectifying section of RD column and (b) reactive condenser unit.

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