Chemical Engineering Science 192 (2018) 380–390

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

On the dimensionality and complexity of multiple-feed attainable regions

Dean Kudakwashe Zimucha *, David Ming, Michelle Low

School of Chemical and Metallurgical Engineering, University of the Witwatersrand, Private Bag X3, P O Wits, Johannesburg 2050, South Africa

HIGHLIGHTS

- The relative position of each feed influences the dimensionality of the system.
- Independent feeds reveal achievable distinct pockets of state space.
- Multiple-feed AR consists of smaller single-feed ARs.

ARTICLE INFO

Article history:
Received 18 July 2017
Received in revised form 22 June 2018
Accepted 13 July 2018
Available online 18 July 2018

Keywords:
Optimal reactor design
Attainable region
Dimension
Multiple feeds

ABSTRACT

Much of the existing literature on attainable region (AR) theory has focused on finding it from a single feed. Yet, many industrial processes involve multiple feed streams and thus the total set of achievable states within a reactive process is affected by the number and type of feeds available. In this paper, we describe conditions for which multiple feeds change the dimension of the space belonging to the AR, allowing for an expansion of the region that would otherwise be infeasible from a single feed. Under specific conditions, we describe how multiple feeds may only alter the shape and size of the AR whilst preserving its dimension to that of a single feed AR. We determine the maximum number of the parallel reactors required to achieve these new states. This is obtained from the reaction stoichiometry and feeds alone, without consideration of reaction kinetics.

1. Introduction

Chemical reactors play a vital role in chemical engineering since they often dictate the quality of the product and cost of subsequent downstream purification processes. In chemical reactor design, the task of the designer is to develop a reactor (or a network of reactors) in a manner that is most appropriate for the design objective. Whether this is to maximise the production of the desired product, or to enhance the product quality at a minimum cost, the design process involves transforming raw material into higher-value products under economic and physical constraints.

Many chemical processes of industrial significance involve complex reactions in which many components interact over multiple reaction pathways. This behaviour makes it difficult to achieve the best performance of the system in a single reactor. Furthermore, we cannot design for the best performance when we have no knowledge of what it is, or how to achieve it. This is referred to as the reactor network synthesis (RNS) problem. RNS involves connecting multiple reactors in a network – often termed a *reactor structure* – such that the optimal output is produced (Feinberg, 1999). A reactor structure can achieve states that would not otherwise be achievable from a single reactor when multiple reactions are involved. The state of a process stream is the chemical and/or physical condition that characterises the process stream such as concentration or mass fraction.

Attainable Region (AR) theory provides a *geometric* interpretation for finding optimal reactor structures for a set of reactions with specified kinetics and a given feed (Ming, et al., 2016). The primary concern of AR theory is to understand the absolute performance limits of a reaction system. Horn (1964) conceptualised the AR as the set of all possible reactor effluent concentrations when reaction and mixing are allowed. The boundary of the AR forms the absolute performance limits of the system in state space (Glasser, et al., 1987). Therefore, we can determine the best possible performance of a process as well as evaluate the strength of existing designs by how far they are from the best. Furthermore, understanding the performance limits of a system ensures that we can set better performance targets. A performance target is

* Corresponding author.
E-mail addresses: dean.zimucha@students.wits.ac.za (D.K. Zimucha), david.ming@wits.ac.za (D. Ming), michelle.low@wits.ac.za (M. Low).

https://doi.org/10.1016/j.ces.2018.07.032
0009-2509/

Nomenclature

n	number of components in the system	ν_{ij}	stoichiometric coefficient of component j participating in reaction i
$\mathbf{C}$	concentration vector	d	number of independent reactions in the system
$\mathbf{C}^*$	final concentration of a mixture	ε	extent of reaction
$\mathbf{r}(\mathbf{C})$	rate vector	$\bar{\mathbf{P}}$	complement space of the AR
$\mathbf{C}^{\#}$	equilibrium concentration vector	z	number of independent feeds entering the system
$\mathbf{C}_f$	feed vector	m	maximum number of parallel reactor structures needed to achieve a point on the boundary of the multiple-feed AR
τ	residence time		
α	DSR side-stream flowrate		
$\mathbf{S}$	stoichiometric subspace		

an objective based on the design criteria such as minimising the reactor volume or maximising the production rate. Inherently, the strength of a reactor design is its ability to achieve the performance target. We can solve for multiple performance targets and find the physical reactor structures required to achieve them using the AR approach (Glasser, et al., 1987).

For a single-feed system, the maximum number of parallel and sequential reactors in the optimal reactor structure is determined from the reaction stoichiometry alone. The dimension of the AR also cannot exceed the total number of components. Using Carathéodory's theorem for convex hulls (Carathèodory, 1911), Feinberg & Hildebrandt (1997) describe how the maximum number of parallel reactor structures needed to achieve a point on the AR boundary is related to the *dimension* of the space belonging to the AR. One finds that for an AR existing in d-dimensional space, no more than $d-1$ parallel structures are needed to achieve a point on the AR boundary whereas no more than d parallel structures are needed to achieve a point in the interior of the AR. Fig. 1 illustrates how the dimension of the space belonging to the AR relates to the maximum number of parallel reactor structures needed to generate it.

The dimension of the space belonging to the AR is determined by the number of independent reactions in the system (Aris & Mah, 1963; Luenberger, 1969; Feinberg, 2000a,b; Gadewar, et al., 2001). Frumkin, et al. (2017) refined Feinberg's Equivalence Principle which allows one to decompose any arbitrary steady-state reactor-separator system into a new system comprising $R+1$ Continuous Flow Stirred Tank Reactors (CFSTRs), and a perfect separating system where R represents the number of independent chemical reactions. The number of CFSTRs in the new system is equal to the dimension of the AR. Zhou & Manousiouthakis (2008) proved, using the Infinite DimEnsionAl State-space (IDEAS) framework, that when component generation rates are linearly related, their corresponding concentrations in constant density reactor networks are also linearly constrained. Hence, the dimension of the AR can be systematically reduced, consequently minimising the computational workload for finding the AR. However, their work considered reactor networks with single network inlet/outlet streams.

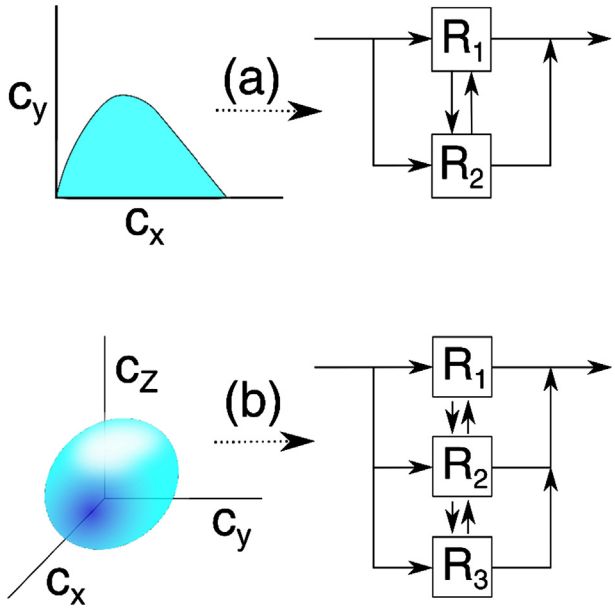

Fig. 1. The dimension of the space to which the AR belongs relates to the number of parallel reactor structures. (a) A two-dimensional AR indicates that two parallel reactor structures may be required, whereas (b) a three-dimensional AR indicates three parallel reactor structures.

We consider the influence of multiple feeds on the dimension of the AR, the achievability of states and the optimal physical reactor structure. Typically, AR construction methods operate from a single feed; assuming that all the available feed material enters the system via a single stream. This assumption accounts for the amount of feed material supplied to the system, but not the way in which it is fed. However, most chemical processes involve multiple feeds where raw material of different states is supplied at different points along the process. In higher-dimensional problems with many participating reactions and components, multiple feeds enhance the flexibility of the process as feed material can be simultaneously introduced in multiple reactor structures. Multiple feeds affect the dimension and complexity of the AR; as more feed streams are allowed into the system, the region of achievable states changes shape and dimension. Posada & Manousiouthakis (2008) developed an implementation of the IDEAS framework (Burri, et al., 2002; Manousiouthakis, et al., 2004) to identify the multi-feed AR in reduced dimension. Their work shows how the equilibrium curves of the reaction system define the boundary projections of the sub-dimensional single-feed AR. Conner & Manousiouthakis (2013) proposed a process network AR framework based on the IDEAS formulation for networks that feature multiple inlets, outlets with known flowrate ratio specifications. Our aim is to show how multiple feeds affect the dimension of the AR, the achievability of states and the optimal physical reactor structure.

2. Preliminaries and terminology

Our goal here is to provide preliminaries that will be frequently referred to in the paper. Readers familiar with these concepts can proceed to Section 3.

2.1. AR theory

In this section, we lay the foundation for concepts later employed in Section 3. Many of these concepts are adapted from (Ming, et al., 2016).