A REVISED METHOD OF ATTAINABLE REGION CONSTRUCTION UTILISING ROTATED BOUNDING HYPERPLANES

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Summary

An improved method of construction of the attainable region (AR), based on the method of bounding hyperplanes by Abraham and Feinberg[1,2], has been developed. The current implementation of the method utilises a rotation of a plane about existing extreme points of the AR to further eliminate unachievable regions from an initial bounding set. The algorithm has shown to be faster in two dimensional constructions and has been extended to include construction of candidate ARs involving non-isothermal kinetics in concentration and concentration-time space.

Keywords

Attainable Regions, polytopes, convex regions, bounding hyperplanes

Introduction

In 1964, F.J.M. Horn introduced the idea of the attainable region (AR)[3]. In general terms, the AR is the result of all possible outcomes for all possible conceivable designs (including those inconceivable designs which surpass current imagination) with respect to a specified input. The idea was meant to be a general one, with the notion that it would be suitable for a vast set of circumstances and disciplines [4].

Early work by Glasser et al.[5], Hildebrandt[6] and Hildebrandt and Glasser[7] laid much of the contemporary geometrical foundation of the attainable region as it is perceived today and sought to establish a definite interpretation of Horn's idea. Viewed as a geometric figure in space generated by the combination of reaction and mixing processes, the AR is a process synthesis tool used for the determination of optimal reactor network structures.

Work by Glasser et al.[5], Hildebrandt[6], Feinberg and Hildebrandt[4], and Feinberg[8,9] have shown that by use of three archetypal reactors alone - the continuously stirred tank reactor (CSTR), the plug-flow reactor (PFR) and the differential side-stream reactor (DSR), as well as allowing for the process of mixing among all network streams, the full set of all outcomes (the AR) may be constructed.

Description

Current methods of candidate AR construction fall into two broad categories. Methods which attempt to generate the AR from inside-out [5,10,11,12], and those from outside-in [2,13,14].

A method of candidate AR construction has been developed which is based on the method of bounding hyperplanes by Abraham and Feinberg[1,2]. The method utilises an outside-in approach to construct the AR with a large number of bounding hyperplanes approximating the true convex polytope representing the AR itself. .

The algorithm begins by first placing an upper bound in concentration space. This initial bounding space, referred to by Feinberg[2] as the stoichiometric subspace, is the starting polytope which is regarded as the bounding set of all concentrations in n-dimensional concentration space achievable through chemical reaction and determined by the set of reaction equations specific to the process under consideration. With each successive iteration, unattainable regions, that is, regions which form part of the stoichiometric subspace but which are physically unachievable through any conceivable reaction network, are 'cut away' resulting in a successively smaller and tighter bounding set. The elimination process is achieved by successive introduction of bounding hyperplanes, which divide the current polytope into two regions. The hyperplanes are orientated in a way which division of the two regions results in one of the two halves containing only unachievable concentrations. This region is then discarded and the newly introduced hyperplane is added to the current set of constraints forming the bounding set. After repeated stages of refinement, a convex polytope is

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produced containing only those output compositions achievable i.e. the AR.

The original method developed by Abraham and Feinberg introduces a bounding hyperplane at a corner of the polytope, with a fixed orientation calculated on an average of the hyperplane orientations which shape the corner. The plane is then moved into the current bounding set until stopping criteria are met.

In the same manner as the original, the revised method's main feature incorporates the use of a number of hyperplanes which successively eliminate regions from an initial bounding set. What differs in the revised approach however, is in the choice of hyperplane orientation and positioning in space.

The authors propose a method of hyperplane rotation, utilising the extreme points of the convex polytope generated from previous iterations as edges from which the hyperplane can be rotated about. New extreme points to the AR are found through a rotation of a plane, where existing extreme points are combined with new ones to build the polytope face by face. By choice of a rotation about an edge, the area swept out during elimination iterations is shown to reject larger portions of the unattainable set. What results is a modified method which demonstrates improved calculation times for a specified set of reaction kinetics and feed specifications when compared to the original method of bounding hyperplanes of Abraham and Feinberg.

The method is currently under early stages of development and as a result, capable of candidate AR construction in two dimensions only. In spite of these limitations however, the method has been successfully adapted to handle construction of candidate regions for non-isothermal kinetics. Elimination via a rotation implies no dependence or knowledge of an existing corner to the current polytope, and hence reliance on a closed polytope is not a requirement. As a consequence of this, construction of unbounded ARs, such as those which are formed in concentration-residence time space are also possible with the revised method.

Candidate ARs for isothermal rate kinetics including the classical van de Vusse and Trambouze examples, as well as more complicated cases involving multiple steady states have been considered and have been successfully validated with the regions generated by the standard approaches of Hidebrandt[6], Seodigeng et al.[12], Goddor et al.[15], Kauchali et al.[10], Manousiouthakis and Justanieah[13], Zhou and Manousiouthakis[14], and Abraham and Feinberg[1,2]. Temperature dependent van de Vusse kinetics have been considered with this new method and the associated candidate ARs and the optimal operating temperature profile have been constructed, and shown to agree with the operating profiles of Godorr et al.[15].

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