

https://dspace.org/

Improving batch reactors using attainable regions: Towards automated construction of the attainable region and its application to batch reactors

Ming, David

2015-05-12
http://hdl.handle.net/10539/17709

Downloaded from a DSpace repository. https://dspace.org/

Abstract

The Attainable Region is the set of all achievable states, for all possible reactor configurations, obtained by reaction and mixing alone. It is a geometric method that is effective in addressing problems found in reactor network synthesis. For this reason, Attainable Region theory assists towards a better understanding of systems of complex reaction networks and the issues encountered by these systems.

This thesis aims to address two areas in Attainable Region theory:

1. To help improve the design and operation of batch reactors using Attainable Regions.

2. To further advance knowledge and understanding of efficient Attainable Region construction methods.

Using fundamental concepts of mixing and attainability established by Attainable Region theory, a graphical method of identifying opportunities for improving the production rate from batch reactors is first presented. It is found that by modifying the initial concentration of the batch, overall production performance may be improved. This may be achieved in practice by retaining a fraction of the final product volume and mixing with fresh feed material for subsequent cycles. This result is counter-intuitive to the normal method of batch operation. Bypassing of feed may also be used to improve production rate for exit concentrations not associated with the optimal concentration. The graphical approach also allows optimisation of batches where only experimental data are given.

An improved method of candidate Attainable Region construction, based on an existing bounding hyperplanes approach is then presented. The method uses a plane rotation about existing extreme points to eliminate unachievable regions from an initial bounding set. The algorithm is shown to be faster and has been extended to include construction of candidate Attainable Regions involving non-isothermal kinetics in concentration and concentration-time space.

With the ideas obtained above, the application of Attainable Regions to batch reactor configurations is finally presented. It is shown that with the appropriate transformation, results developed from a continuous Attainable Region may be used to form a related batch structure. Thus, improvement of batch reactor structures is also possible using Attainable Regions. Validation of candidate Attainable Regions is carried out with the construction algorithm developed in this work.