

Abstract

Traditional work in batch processes has focused mainly on the optimisation of batch reactors and the scheduling of batch processes. Recent development in the application of attainable region (AR) theory has allowed for its entry into this landscape. As time is a crucial consideration in the study of these systems, furthering the application of AR theory to batch reactors required the incorporation of time into the ARs. This was previously done in terms of residence time for continuous systems. With its use in batch systems this work sought to investigate how the time component differs within ARs between batch and continuous systems. It demonstrated that while residence time could be undergo linear mixing, the time in batch systems could not due to its nature. Therefore the ARs generated in concentration-residence time and concentration-time space would differ slightly. A way to circumnavigate this was proposed in that the AR be plotted in terms of concentration and residence time following which the continuous reactor structure is obtained. From this the batch structure can be determined by substituting the equivalent reactor types.

Production rates were also introduced as a method of interpreting an AR plotted in concentration-residence time space. By minimising the time taken to reach a particular point in the AR, one may effectively increase the rate at which the desired product can be produced. The developed concepts were applied to two example systems with the aim of obtaining the batch reactor structure for the most productive point that satisfied a given objective. Success was achieved for 2D single reaction system as well as a more complex 3D two biological reaction system. The more complex system led to the development of non-conventional attainable regions in terms of another process variable; in this case pH was used to demonstrate the concept although other variables such as temperature and pressure may be used in a similar fashion. Such plots may be used to further optimise the reaction system or identify a particular region in which to operate. Further development of AR theory to batch reactors has indeed allowed its use in conjunction with optimisation and scheduling of batch processes. Most notably, scheduling may utilise the obtained batch structure as part of the process to be scheduled or use the indicated reaction time.