ABSTRACT

Chemical processes impose a heavy burden on the world's natural resources, because they use raw materials to manufacture various products and require energy to drive them. Because these processes are also inefficient, much benefit to both industry and energy conservation can be derived from improvements in their design.

This dissertation presents a technique that can be used to analyze the reactions that take place (often more than one, and in competition) in a reactor. This is done via the graphical representation of what occurs during a chemical process in terms of mass balance calculations used together with basic thermodynamic principles. This technique allows the researcher to identify which of the many possible reactions taking place in a reactor is/are likely to dominate in that particular chemical process, and the degree of transformation that is achievable.

The graphical technique postulates that the chemical species involved create lines that define the reaction's attainable boundaries in a G–H space. This makes it possible to evaluate the operating process; identify sources of inefficiency within it; establish systematic performance targets; and improve process performance. A collateral benefit is the contribution these improvements can make not only to the sustainability of the chemical processing industry but to conserving raw material sources and reducing negative environmental impacts.

The most crucial element of the graphical technique is its use to locate the attainable region (AR) for chemical processes in a reactor. In this case it is a thermodynamically achievable region in the state space within which the reactor can function without violating thermodynamic boundaries, using only the process of reactions and mixing.

After finding the AR, we can interpret its boundary in terms of the likely limiting extents of reaction through mass balance calculations. By these means we can deduce the process reaction pathways. The technique is two-dimensional, allowing for easy and rapid interpretation of the results, such as the effects of changing the process feed and operating conditions. It also provides insight into the likely reactions achievable in the reactor under different process conditions.

This approach was applied to the simultaneous methanol synthesis from syngas and water gas shift (WGS) reactions. The graphical plots show that the introduction of either water or CO_2 or both to the feed opens up the mass balance region, resulting in WGS activity, which generates more reaction path alternatives, as does the reverse (RWGS) reaction. They also demonstrate that the change in Gibbs free energy across the reactor and the reaction pathways leading to the product are interlinked. The quantities involved y can be useful to the engineer in setting performance targets for chemical processes.

The examples of graphical analysis supplied in this dissertation show that reaction path analysis could become an important tool in the preliminary stages of process design, because it can identify the most desirable reaction routes.