ABSTRACT

Efficient use of energy and efficient use of raw materials are among the key factors for sustainability in the process industries. In the field of process synthesis and integration much progress has been made in developing design and optimization tools in order to improve the efficiency of chemical processes. Techniques such as hierarchical decomposition, pinch analysis and mathematical programming (MINLP) have made possible the development of improved processes in terms of energy and mass efficiency, environment and economics. However there is still room for improvement. The work in this thesis is part of the many efforts that are being made to develop systematic methods for synthesizing more efficient processes.

It has been shown that most of the features and cost of a process are usually fixed in the early stage of process design; therefore decisions made during this stage are crucial and thus there is a need for systematic methods that would guide decision making toward more efficient processes using as little information as possible. We have developed tools that combine fundamental thermodynamic concepts and a graphical approach in order to gain insight and provide a systematic way for not only determining process *targets* but understanding what is required in order to meet these *targets*. The approach used in this thesis is based on the idea that every process in which certain feed materials are converted into products has a certain amount of *heat* and *work* associated with it. Understanding the relationship between the *heat* and *work* can provide insight into the process and can give an indication of what the process structure would be.

Chemical processes are analyzed in terms of their *heat* and *work* requirement using the analogy of heat engine and a graphical approach. This approach looks at chemical processes holistically, where only the inlet and outlet streams are considered. Processes are represented and classified in different thermodynamic regions in a ΔH - ΔG space (gh-diagram) where their feasibility and reversibility are analyzed. This allows determining whether heat at an appropriate temperature is sufficient to meet the work requirement for a process, or if other means should be considered.

The gh-diagram is used to understand how process conditions such as pressure and temperature can be manipulated in order to meet heat and work requirements more reversibly. The relationship between process heat and work requirement and process complexity is revealed. The approach is applied to ammonia processes to understand the implications of process conditions and catalyst choice, on the heat and work requirement, process complexity and process efficiency.

The approach has been also used to analyze combustion processes and it has been shown that it is not possible to combust carbon based materials efficiently and a considerable amount of work potential is lost during the combustion process. However other substances have been explored and it has been showed that some of these have the potential for more reversible combustion. Opportunities to produce valuable chemicals such as fertilizers in addition to power production have been revealed.

This approach does not require much information or complex calculations and is suitable to be used in the early stage of process design for a quick insight into the process and analysis of alternatives.