# ABSTRACT

Pinch Analysis, in the broadest sense, is concerned with the optimal use of resources (material or energy) in a multi-process system. Pinch Analysis based techniques have emerged for water systems over the past decade. A major assumption that has been made in applying these techniques is that a process system can be segregated into a set of process streams and a set of water streams. With this distinction in place, only the water streams are considered in the Pinch Analysis with the process streams represented implicitly. This approach has obvious limitations in situations where a clear distinction between process streams and water streams cannot be made.

The chlor-alkali process is an example of a system in which the clear distinction between process streams and water streams cannot be made. Water is intrinsically involved in the process, serving as a carrier medium for raw materials and eventually becoming part of the products produced by the complex. Hydrochloric acid and caustic soda are reagents which are both used within and produced by the complex. These reagents are required by the process at a range of concentrations and the concentrated reagent is diluted to the required concentrations using demineralised water. Within the chlor-alkali complex, a number of effluents containing the reagent species are available and are typically sent to drain. It is conceivable that these effluents might be recovered and used for dilution purposes instead of demineralised water. This would bring about a reduction in the amount of water and concentrated reagent used and the amount of effluent produced by the complex. Given the economic value of these reagents relative to water, their recovery, if feasible, is likely to dominate the optimal water-use and effluent generation strategy.

Current Water Pinch Analysis theory relies on the distinction being made between process streams and water streams and does not consider the recovery of reagents or the presence of desirable species within the system. In addition, the assumption is made that species are non-reactive; reactive species such as hydrogen chloride and sodium hydroxide, fall outside the scope of the current theory.

The objectives of this study have included the development of an approach which is able to address these limitations of the existing theory. This approach, termed Combined Water and Materials Pinch Analysis seeks to identify optimal use strategies for raw materials and reagents, in addition to water-use and effluent generation. The approach combines mathematical programming with conceptual insights from Water Pinch Analysis. The approach is based on the optimisation of a superstructure which represents the set of all possible flow configurations for water, reagents and raw materials between the various operations within the process system; this problem is solved as a nonlinear programming (NLP) problem using standard optimisation tools.

The application of the developed approach to the Sasol Polymers chlor-alkali complex at Umbogintwini, south of Durban, has been a further objective of this study. Given the variety of process operations present within the complex, which differ both in terms of their physical structure and function, individual process models for these operations were required. These models were described in terms of four basic functional elements, namely, mixing, flow separation, component separation and reaction, and incorporated into the superstructure. Given the complexity of the problem, the process system was divided into three subsystems which were optimised in isolation from each other. These results were subsequently integrated to reflect the performance of the subsystems in combination with each other. The results showed a potential reduction of 14% in water-use and 42% in effluent production by the complex, relative to the existing operating configuration. Amongst other savings in material use, the results indicated a 0.2% reduction in the use of salt, a 1.6% reduction caustic soda use and an 8.3% reduction in the use of hydrochloric acid. Economically, the potential saving identified was R 945 727 per annum, based on operating costs in the year 2000.

The final objective of this study was the interpretation of the pinch as it relates to the Combined Water and Materials Pinch Analysis problem. A general definition of the pinch was proposed; according to this definition, the pinch corresponds to that constraint or set of constraints which limits the performance of the system, that is, prevents it from further improvement. For the Combined Water and Materials Pinch Analysis problem, this performance is measured in terms of the operating cost. This definition is thus a departure from its usual thermodynamic interpretation of the pinch; in addition, the pinch is defined in terms of a constraint or a set of constraints instead of a point. These constraints are identified by an analysis of the marginal values provided by the optimisation algorithm. Marginal values are also used as a means of identifying process interventions which may be effected such that the performance of the system may be improved further.