OPTIMIZATION-BASED SYNTHESIS AND ANALYSIS OF HYDROGEN PRODUCING ALTERNATIVE THERMOCHEMICAL CYCLES

By

Ryan Joseph Andress

An Abstract of a Thesis Submitted to the Graduate

Faculty of Rensselaer Polytechnic Institute

in Partial Fulfillment of the

Requirements for the Degree of

DOCTOR OF PHILOSOPHY

Major Subject: CHEMICAL AND BIOLOGICAL ENGINEERING

The original of the complete thesis is on file
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Examining Committee:

Lealon L. Martin, Thesis Adviser

B. Wayne Bequette, Member

Patrick T. Underhill, Member

Maximilian B. Gorensek, Member

Rensselaer Polytechnic Institute
Troy, New York

May 2011
(For Graduation August 2011)

ABSTRACT

Hydrogen has been identified as a future carrier of sustainable energy sources. However, economically feasible, carbon-free hydrogen production has yet to be realized on a large-scale. With thermodynamic limitations inhibiting the thermal efficiency of direct production from water, fossil fuel based processes remain prominent. In an effort to use high-quality renewables (i.e. nuclear and solar energy) for the production of hydrogen from water, thermochemical cycles have been identified as a promising technology to overcome those thermodynamic barriers. Thermochemical cycles use a sequence of thermodynamically feasible reactions, within a realizable temperature range, to accomplish the overall reaction of water-splitting. Water-splitting is a favorable production method because only oxygen is produced as a by-product.

This research specifically deals with the analysis of alternative thermochemical cycles (i.e. alternatives to the baseline hybrid sulfur and sulfur-iodine cycles). Here, a systems engineering approach is taken to screen candidate systems for thermochemical cycles that are competitive with a combined bottoming cycle - water electrolysis hydrogen production process. The methodology developed encompasses two tasks: (i) the systematic identification of thermodynamically feasible alternative thermochemical cycles and (ii) a standardized multi-level evaluation procedure. Task (i) is accomplished via the formulation of a mathematical program to identify feasible reaction clusters using a thermodynamic database. Two key contributions of this work are the ability to identify all feasible cycles for a given system and the formulation of a hybrid cycle generation algorithm. Task (ii) employs simulation software and heat pinch analysis to evaluate cycles based on thermal efficiency. Case studies on the Fe-Cl, Ca-Br, and Cu-Cl are presented to illustrate and develop the methodology. A comprehensive screening and analysis of three reaction cycles from the V-Cl system results in the identification of three promising cycles with higher-level efficiencies that exceed 30%. Recommendations are made for the future analysis of these cycles and for identifying additional viable V-Cl cycles.