Generation of Hydrogen Production Cycles Through Water Splitting*

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The decreasing supply of fossil fuels and their negative environmental impact has resulted in a significant amount of research for alternative energy sources. One of the most promising and studied researched alternatives is hydrogen fuel. Current methods to produce hydrogen either are inefficient or use fossil fuels in the process. One of the most promising methods for hydrogen generation is from the use of water-splitting cycles.

Water splitting cycles involve the formation of hydrogen and oxygen from the decomposition of water. The cycles utilize a combination of thermally driven chemical reactions. For the thermal decomposition of water alone, a temperature of more than 2500°C is required. If a two or more reaction cycle is utilized, the temperature of each reaction can be greatly reduced from 2500°C. The only net reactant of the cycle is water and net products are molecular hydrogen and oxygen. The most important aspect of the cycle is all other reactants are regenerated as products in other reactions of the cycle. Research funded by the Department of Energy has identified and ranked currently known potential water-splitting cycles. The negative aspect of all these cycles is the presence of one or more high temperature reactions. These high temperature steps will require large heat utilities accompanied by high operational costs. The proposed solution is to couple the cycles with the new generation of nuclear reactors. These reactors will likely not be built until at least 2030 and alternative production methods are warranted.

A computer algorithm using VBA was developed in this project to generate low temperature water splitting cycles. The program was successful in generating cycles for five different configurations. The program initiated combinations from 100 molecules, and also generated molecules from functional groups. The molecules were enumerated into a given reaction configuration the program checked the cycle feasibility by evaluation of both atomic balance considerations and thermodynamic constraints.

A total of about 1000 unique cycles were found from all of the configurations tested. For instance, cycles generated from the 2 reactant-2 product configuration reached a maximum efficiency of 72 % and other configurations yielded high efficiencies, but most had a high number of reactant molecules. These cycles likely will not be practical on a large scale because the kinetics are assumed to be very low. The best reaction found with the most practical potential was generated in a 3 reaction scheme with one reaction proceeding via electrolysis. The efficiency was near 90% with a small number of reactant molecules, possibly indicating favorable kinetics. The inclusion of separation work into the higher efficiency cycles reduced the efficiency by about 10% for each case. When excess reactants were used in situations with low reaction conversion, the conversion increased as much as 60%.

This study has demonstrated the ability to produce feasible water splitting cycles to generate hydrogen; however, potential cycles will require further analysis to realize the practical application. Foremost is the determination of reaction kinetics, selectivity, and more accurate predictions of separation work. The results from this work are promising and the expanse of the work could lead to important developments for the production of hydrogen to replace fossil fuel energy supply.

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