

ABSTRACT

Gençer, Emre PhD, Purdue University, August 2016. Enabling a Sustainable Economy through Energy Systems Modeling: Solar-centric Efficient, Integrated and Continuous Process Synthesis and Optimization. Major Professor: Rakesh Agrawal.

The expected increase in food, energy and water demand due to increase in population and change in consumption habits in conjunction with diminishing fossil fuel reserves and increasing greenhouse gas emissions urge the development and implementation of alternative energy conversion techniques using renewable energy for a sustainable economy. Among renewable energy sources, solar energy is prominent due to its abundance. A sustainable economy can be created by producing building blocks foundational to meeting all basic human needs of daily existence. However, intermitencies and limitations on land area dedicated to harness solar energy are the major obstacles on widespread implementation of solar energy conversion technologies. To address these challenges this dissertation has identified energy efficient, synergistically integrated, continuously operable process designs and process synthesis methods for harnessing renewable energy sources for various end uses.

Hydricity, a paradigm that proposes synergistic coproduction of solar thermal power and hydrogen is introduced. Hydricity concept is realized by judiciously integrating solar water power (SWP) cycle, solar thermal hydrogen production techniques, and turbine-based hydrogen power cycle and by suitably improving each one for compatibility and beneficial interaction. When the proposed integrated process is operated in a standalone, solely power production mode, the resulting solar water power cycle can generate electricity with unprecedented efficiencies of 40 - 46%. Similarly, in standalone hydrogen mode, pressurized hydrogen is produced at efficiencies approaching $\sim 50\%$. In the coproduction mode, the coproduced hydrogen is

stored for uninterrupted solar power production. When sunlight is unavailable, we envision that the stored hydrogen is used in a turbine-based hydrogen water power (H_2WP) cycle with the calculated hydrogen-to-electricity efficiency of 65 - 70%, which is comparable to the fuel cell efficiencies. The H_2WP cycle uses much of the same equipment as the solar water power cycle, reducing capital outlays. The overall sun-to-electricity efficiency of the hydricity process, averaged over a 24 hour cycle, is shown to approach $\sim 35\%$, which is nearly the efficiency attained by using the best multi-junction photovoltaic cells along with batteries. In comparison, our proposed process has the following advantages: (i) It stores energy thermochemically with a two- to threefold higher density, (ii) coproduced hydrogen has alternate uses in transportation/chemical/petrochemical industries, and (iii) unlike batteries, the stored energy does not discharge over time and the storage medium does not degrade with repeated uses.

For uninterrupted renewable power supply, carbon storage cycles (CSC), which involves cyclic transformation of carbon atoms between carbon dioxide and carbon fuel is studied. CSC has the potential to achieve high storage efficiency ($\sim 54 - 59\%$) for GWh-level energy storage with much reduced storage volumes compared to other options. Detailed process simulations of DME storage cycle is performed which results in $\sim 57\%$ storage efficiency.

Fresh water need is an increasing need, integration strategies of multi stage flash (MSF) desalination process with solar thermal power and hydrogen production processes are established. In addition to integration with SWP cycle and modified SWP cycle, high pressure desalination alternatives are also designed and analyzed. To continuously produce fresh water, MSF desalination process is integrated with hydrogen and electricity coproduction process whereby stored hydrogen is converted to electricity by modified H_2WP cycle while coproducing fresh water when solar energy is not available.

To supply FEW demand for a full earth, the potential of a novel approach for the utilization of the entire solar spectrum by directing solar photons to maximize FEW

production from a land area is studied. The proposed solar spectrum unbundling FEW systems (SUFEWS) can enhance quality of life while reducing the overall environmental impact of meeting these needs. SUFEWS implementation on a relatively small portion of agricultural land area can supply the entire electricity and fresh water demand without reducing the food production capacity.

Towards reducing the CO₂ emissions associated with the transportation sector, synergistic carbon and energy efficient process designs for integrated biomass and natural gas (NG) to liquid fuel conversion is synthesized by formulating and solving a process superstructure optimization problem. The solution of the Mixed Integer Nonlinear Programming (MINLP) model identifies optimal process configurations that are capable of producing ~ 15% more liquid fuel output than the combined fuel output of individual standalone processes converting the same amount of biomass and NG. This synergy originates from synthesizing additional liquid fuel by combining the residual biomass carbon with the excess hydrogen per carbon available from the NG feed.