

Energy Systems Analysis for a Solar Economy
Dharik S. Mallapragada
(Advisors: Rakesh Agrawal, Fabio H. Ribeiro and W. Nicholas Delgass)

The use of solar energy for human needs faces challenges owing to its relatively low energy intensity and intermittent availability, coupled with the constrained availability of renewable carbon and land resources. This study uses systems analysis tools to identify carbon and energy efficient transformations of solar energy for different purposes, including transportation fuels and grid-scale energy storage. These efforts have been complemented with a feasibility analysis of existing fossil-energy and other hybrid pathways.

In an era of limited fossil resources, liquid fuels from sustainably available (SA) biomass could meet the energy needs of the transportation sector. We present a method for synthesizing augmented biofuel processes, which improve biomass carbon conversion to liquid fuel (η_{carbon}) compared to standalone biofuel processes by using supplemental solar energy in the form of H_2 , heat, and electricity. For any target η_{carbon} , our method identifies a process, which is guaranteed to consume the least amount of solar energy among all competing designs, thereby minimizing the land area requirement for biofuel production. A non-convex mixed integer nonlinear programming (MINLP) model allowing for simultaneous mass, heat, and power integration, is built over a process superstructure and solved using global optimization tools. As a case study, we consider biomass thermochemical routes of gasification/Fischer-Tropsch (FT) synthesis and fast-hydrolysis/hydrodeoxygenation. For $\eta_{carbon} = 70-95\%$, the synergistic gain of the optimal integrated process is evidenced from the $\sim 28-156\%$ lower solar energy consumption compared to augmented gasification/FT processes. To accommodate for the intermittent supply of solar heat and H_2 , we suggest two alternative processing options: 1) flexible operation between low and high carbon recovery modes, or 2) adapting a novel energy storage concept based on the cyclic transformation between liquid carbon dioxide and a liquid carbon molecule for round the clock augmented biofuel production.

If 100% SA biomass carbon conversion via augmented processes cannot meet the demand for renewable liquid fuel, additional carbon (i.e. atmospheric CO_2) and land resources must be allocated for this end use. Here, the metric of Sun-to-Fuel (STF) efficiency is shown to be useful in identifying energy and land use efficient routes for converting atmospheric CO_2 to liquid fuel.

The availability of H_2 is essential for the supply of fuels and chemicals in a solar economy. Using thermodynamic modeling, we estimate the achievable Sun-to- H_2 (STH_2) efficiency for water-splitting processes harnessing solar energy predominantly as heat. The estimated STH_2 efficiencies of 35-54% for direct and two-stage (using Fe_3O_4/FeO) thermal water-splitting are greater than the achievable values for electrolytic or single bandgap photoelectrochemical water-splitting.

Reconciling today's energy system with the future solar economy vision demands an energy transition roadmap. For the transportation sector, we propose an energy efficient transition using compressed natural gas that eventually can be substituted with compressed methane derived from biomass. Alternatively, if liquid fuel use remains dominant, we identify synergistic processes for integrated biomass and natural gas conversion to liquid fuel during the interim period.