Abstract

As the global population approaches 10 billion by the mid-century, supplying all the needs of the human race from the Earth's limited land area and resources with minimized greenhouse gas emission will be the essential challenge of sustainability. In a sustainable economy, all renewable energy, in combination with carbon sources and other elements from the nature, such as water, air and land, will be used synergistically to produce building blocks for human beings. These building blocks, including electricity, heat, fuels, hydrogen, etc., will enable the production of all the end uses for human beings. The challenge for chemical engineers is to come up with processes and synergistic strategies to enable such a sustainable future.

Shale gas can serve as both energy resource and chemical feedstock for the transition period towards a sustainable economy and has the potential to be a carbon source for the long term. Natural gas liquids contained in shale gas provide abundant feedstock for chemical and fuel production and could bring extra value for remote shale gas basins. Unlike current shale gas processing where large scales are preferred, simple and intensified processes with least processing steps and least pieces of equipment are favored for remote shale plays. While conventional shale gas processing usually follows a four-section hierarchy of "gas treatment - NGL recovery - NGL fractionation - NGL activation", four innovative configurations are proposed for simpler and intensified process design, including NGL co-processing, integrated NGL recovery and activation, switched NGL recovery and activation, and eliminated NGL recovery. A two-step conversion of NGLs to liquid hydrocarbons via dehydrogenation followed by oligomerization is used as an example to show how these innovative process designs evolve. Simulation results show that the loss of ethane, the NGL component with the highest concentration, could be largely reduced by the innovative process configurations. At the same time, higher yield of liquid products, fewer processing steps, reduced pieces of equipment and elimination of energy and capital-intensive units can be achieved. The intensification of process here would benefit the modularization of shale gas plants and make it possible for distributed production of liquid hydrocarbons onsite for remote shale locations.

While shale gas being the carbon source for a sustainable future, renewable energy, especially solar and wind energy, will become the dominant energy resources for a sustainable economy. However, both solar and wind energy are dilute resources and harvesting them requires vast

tracts of land, which could potentially compete with agricultural production for food. As a bookend case study, we investigate the land requirement for a 100% solar economy. The contiguous United States is used as an example and our analysis takes into account several issues that are usually ignored, such as the intermittent solar availability, estimation of future energy demand, actual power production from solar farms and available land types. Results show that it will be difficult for currently available land to meet the energy needs using current solar park designs for the entire contiguous United States and for nearly half of the individual states, which include well over half of the total US population. Barring radical improvements in agricultural output that could greatly reduce the land devoted to agriculture, the competition for land between energy and food seems inevitable, posing a major challenge to a future solar economy. If we extend the study to Germany, the United Kingdom and China, we could see that the challenge exists for both developed and developing countries.

To resolve the issue, a concept of "Aglectric" farming is proposed, where agricultural land produces electricity without diminishing existing agricultural output. Both wind turbines and photovoltaic (PV) panels can be used to generate electricity on agricultural land. While the use of the current PV panels is known to have a negative impact on crop growth, we propose several innovative PV systems using existing and new materials, innovative installation paradigms and module designs. Through extensive modelling of PV shadows throughout a day, we show that some of our designed PV systems could mitigate the loss of solar radiation while still maintaining substantial power output. Thus, it should be possible to design and install these PV systems on agricultural land to have significant power output without potentially diminishing agricultural production. We also show that PV aglectric farms alone will have the potential of realizing a 100% solar economy without land constraint. Together with regular PV parks and wind aglectric farms, PV aglectric farms will serve as an important option for a renewable future.

With its high energy density and zero greenhouse gas emission, hydrogen is the key energy carrier in a sustainable future. We introduce a process design strategy for the production of hydrogen by high temperature water electrolysis using concentrated solar thermal energy. At the same time, co-production of hydrogen and electricity is investigated where hydrogen can be produced by both thermochemical cycles and high temperature electrolysis. The process design features the process integration between hydrogen production and power generation. Process simulation is performed in an integrated Matlab and Aspen Plus platform. Efficiencies are analyzed for various processes.

Synergy is the key feature of all the studies in the dissertation. Process intensification for shale gas conversion and process integration for solar hydrogen production are examples of synergy at the process level. Coproduction of hydrogen and electricity and coproduction of electricity and food are examples of synergy at the building block level. Potential synergistic use of solar, wind and shale resources is an example of synergy at the resource level. Synergy is the keyword of the sustainable future we are pursuing.