

Process Intensification and Renewable Energy for Low-Carbon Propane Dehydrogenation

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Propylene is a building block for polypropylene and many commodity chemicals. As steam crackers shift from naphtha to ethane feedstocks, their propylene output diminishes, motivating on-purpose propane dehydrogenation (PDH). PDH is strongly endothermic and equilibrium-limited, so it requires high reaction temperatures. In conventional plants, this heat comes from burning fossil fuels. Solar heat or renewable electricity can replace fired heat and lower carbon emissions. Integrating a hydrogen-selective membrane offers an additional route to intensification. Removing hydrogen in situ relaxes equilibrium limitations and raises the achievable conversion at lower temperatures, reducing the energy intensity of propylene production. This dissertation uses reactor and process models, from the catalyst layer to the plant, to develop design guidelines for these routes to low-carbon PDH.

First, a transient model of a Joule-heated, washcoated reactor identifies design principles for electrified PDH. Narrow channels with thin washcoats limit transport losses, while feed preheating, insulation, and heat recovery govern temperature uniformity and energy efficiency. The catalyst reaches operating temperature within minutes, and this fast response makes the reactor compatible with intermittent renewable electricity for power-to-chemicals applications.

Next, an experimentally validated membrane-reactor model guides the design of modules in which carbon molecular sieve hollow fibers remove hydrogen during ethane dehydrogenation over Co@DeAl-BEA and propane dehydrogenation over Pt-Zn/S1. Comparing the reaction, residence, and permeation time scales optimizes the fiber count and catalyst configuration. The model also points to practical modifications, such as sealing the excess fiber length that leaks hydrocarbons and fixing the bundle with a wire mesh.

The optimized membrane reactor is then integrated into a commercial-scale plant heated by concentrated solar power with molten-salt storage. Process simulation, hourly solar dispatch, and techno-economic analysis show that the membrane plant uses less heat and electricity than conventional PDH and emits 65% less CO₂. Its economics, however, are dominated by the cost of the membrane modules. Hydrogen permeance is the main lever, which points to more permeable Pd-Ag membranes despite their deactivation in propylene.

Finally, a coupled finite-volume model tests whether temperature stratification can suppress coking of the Pd–Ag membrane in an electrified reactor. The membrane can operate more than 250 K cooler than the catalyst. The catalyst–membrane gas gap, external heat exchange, and membrane emissivity govern the degree of stratification. A strongly stratified reactor keeps the membrane almost fully active over 24 h and produces more propylene, but at a higher energy cost. Hydrogen removal, however, accelerates catalyst coking and lowers propylene output over 24 h.

Together, the models show that renewable energy and process intensification make PDH a promising route to low-carbon propylene. For economic feasibility, membrane performance and stability are crucial, while the design of electrified reactors must account for energy efficiency and transport limitations. These developments would enable cost-competitive propylene production with little or no fossil-fired heat, advancing the decarbonization of the chemical industry.