Electrification of Thermal Chemistry and Catalysis for Intensified Chemical Manufacturing

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Electrification of thermal chemistry enables spatial and temporal control of heat generation in chemical reactors. Grid electricity can diversify industrial energy supply and potentially reduce carbon emissions. Microwave and Joule heating can produce localized high-temperature zones and rapid thermal pulses that are difficult to achieve with conventional furnace heating. These heating modes can alter catalyst stability, reaction pathways, and product selectivity. This dissertation examines these effects across four reactions.

First, indirect microwave heating is investigated for nonoxidative propane dehydrogenation over $PtSn/SiO_2$, with a SiC monolith absorbing microwaves and transferring heat to the catalyst. Without co-fed hydrogen, the microwave-heated bed exhibits higher propylene selectivity and slower deactivation than the furnace-heated bed. At equal coke loading, coke deposits are located farther from the metal nanoparticles under microwave heating, consistent with more active sites remaining accessible. Localized conventional heating also suppresses gas-phase cracking, but the greater performance improvement under microwave heating suggests more effective heat localization.

Next, direct microwave heating is examined using reduced rutile TiO_2 as both a microwave absorber and a CO_2 hydrogenation catalyst. Oxygen removal generates Ti^{3+} polarons that dissipate electromagnetic energy through charge transport and oxygen vacancies that participate in surface redox reactions. Although both originate from reduction, microwave absorption and catalytic activity peak at different reduction states, revealing distinct roles of electronic defects and surface vacancies. Direct microwave exposure also accelerates oxygen

removal and enables CO_2 hydrogenation at substantially lower measured temperatures than conventional heating, achieving complete CO selectivity and reaction rates comparable to those of noble-metal catalysts. These findings establish a physical basis for designing reducible oxides that couple electromagnetic energy directly to catalysts while controlling their redox activity.

Turning to Joule heating, continuous and pulsed operation are examined for noncatalytic ethane cracking using carbon fiber paper as an internal heater. Direct heat generation within the reaction zone enables millisecond-scale cracking at high temperatures, limiting the time available for secondary reactions that consume ethylene. At temperatures above 1000 °C and residence times below 10 ms, the measured ethylene yield reaches 56%, compared with 53% for conventional steam cracking at 850 °C and 100 ms. Kinetic and CFD modeling identify rapid downstream quenching as essential and predict ethylene yields above 64% with an improved reactor design. Pulsed operation consumes half the average power of continuous operation at comparable conversion, whereas continuous heating achieves higher ethylene selectivity.

Finally, tandem methane coupling and CO_2 reduction are investigated using pulsed Joule heating. Rapid thermal pulses enable the simultaneous production of C_2 hydrocarbons and CO through nonoxidative methane coupling and the reverse water-gas shift reaction. Compared with continuous heating, pulsed operation reduces power consumption by 60% while suppressing aromatic formation and heating element degradation. Microkinetic modeling shows that short pulses favor C-C coupling over reforming and aromatization because these reactions proceed on different timescales. This noncatalytic route extends methane dry reforming beyond syngas production, potentially providing C_2H_2, CO, and H_2O as feedstocks for downstream C_3 oxygenate synthesis.

Together, these studies demonstrate how spatial and temporal control of heat generation can improve catalyst stability, steer reaction selectivity, and reduce energy consumption, revealing the complementary benefits of electrification for thermal chemical processes.