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# $CO_2$-assisted propane dehydrogenation: Unravelling the reaction mechanism via transient kinetic techniques

## Keywords
$CO_2$-assisted PDH, Temporal Analysis of Products, Reaction mechanism.

## Aim
This thesis investigates propane dehydrogenation with $CO_2$ co-feed ($CO_2$-assisted PDH) over Pt-Sn catalysts. The aim is to unravel the propane-to-propylene conversion mechanism on the catalyst surface in the presence of $CO_2$, and the general interplay with the catalyst structure. This will be accomplished by transient techniques - such as Temporal Analysis of Products (TAP) - combined with several other catalyst characterization techniques.

## Justification
Propylene is the second most important olefin in industry. Currently, it is mainly produced as by-product in refinery conversion processes. However, to meet the rising demand, its on-purpose production becomes increasingly important. A commercial example hereof is propane dehydrogenation (PDH), in which propane is catalytically converted to hydrogen and propylene. Catalysts based on platinum (Pt) are established as highly active for this process, but suffer from low selectivity. This leads to rapid coke formation and deactivation. Moreover, PDH is an equilibrium limited process.
A first possible improvement is the addition of a promotor element to the catalyst, with tin (Sn) as commercial example. When alloyed with Pt, improvements in propylene yield are obtained through electronic and geometric effects.

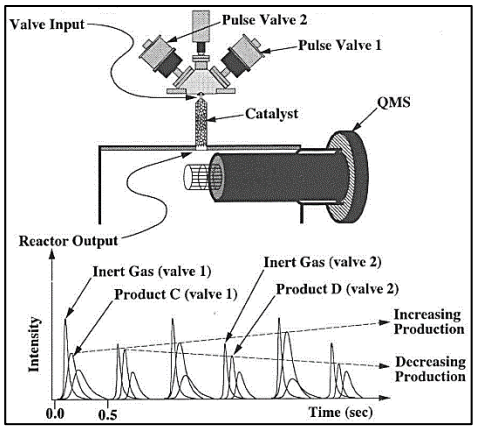

*Figure 1: Temporal Analysis of Products perturbs the catalyst surface via very small gas pulses. [1]*

A second and more recently explored improvement is the use of a $CO_2$ co-feed ($CO_2$-assisted PDH). As soft oxidant, $CO_2$ breaches the thermodynamic limitations through $H_2$ consumption, and it oxidizes coke depositions.
So far, the mechanistic understanding of $CO_2$-assisted PDH is still limited and very catalyst-specific. The current scientific debate is therefore not only related to the nature of the chemical conversion, occurring at the catalyst surface, but also relates to the catalyst structure itself. Understanding the reaction mechanism, the catalyst structure and their interplay in presence of $CO_2$ can provide useful insight to further develop and improve this process. Such insights can be provided by Temporal Analysis of Products, a unique in-house setup (TAP, Figure 1).

## Program
- Literature study on $CO_2$-assisted PDH and its catalysts.
- Synthesis of Pt-Sn catalysts.
- Catalyst characterization by means of Transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD) and $H_2$ temperature programmed reduction ($H_2$ TPR).
- Steady-state and transient kinetic techniques (Temporal Analysis of Products) are combined with the above characterization techniques to determine the mechanism of propane-to-propylene conversion, the catalyst structure and their interplay, with special attention to the role of $CO_2$.

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*[1] J. T. Gleaves, G. S. Yablonskii, P. Phanawadee, and Y. Schuurman, "TAP-2: An interrogative kinetics approach," Appl. Catal. A Gen., vol. 160, no. 1, pp. 55–88, 1997*