High-temperature TAP reactor studies of ammonia oxidation

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Preferred background of candidates: experimentalist - chemistry, materials science, catalysis; modeling – physical chemistry, chemical kinetics, mathematical modeling.

Number of available projects: 1-2 projects are available for experimental and/or modeling work. Greater synergy is expected within a combined project, if two candidates with suitable expertise apply, but individual projects are self-contained and also highly encouraged.

Preferred project period: July-August

Project(s) outline:

Ammonia (NH_3) is a key energy vector in the emerging hydrogen-based economy and remains the main intermediate to produce fertilizers. Ammonia synthesis, decomposition, and oxidation are all industrially-relevant reactions that require heterogeneous catalysts. In this project, the students will obtain a hands-on experience with applying Temporal Analysis of Products (TAP) kinetic measurements to investigate a challenging high-temperature NH_3 oxidation reactions.

In industry, ammonia oxidation is the first step in the Ostwald process for the production of nitric acid. NH_3 is oxidized with oxygen on bimetallic Pt-Rh gauze catalysts at 900 °C. The main challenge at these conditions is Pt volatility, which is partially alleviated by alloying Pt with Rh. However, the exact mechanisms of the promotional effect and its influence on the reaction mechanism remain poorly understood.

Herein, Temporal Analysis of Products (TAP) reactor will be used to study the interaction of O_2 and NH_3 with the surface of Pt-Rh gauze with sub-second temporal resolution. TAP is a transient technique for kinetic measurements, in which the transport of gas through the reactor packing occurs at low pressure conditions (10^{-8} mbar) by means of Knudsen diffusion. This well-defined transport regime provides a reliable process against which the reaction kinetics can be assessed with high precision and temporal resolution for gaining in depth insights into the reaction mechanism. The Catalysis section at UiO operates the only TAP facility in the Nordics, one of only ca. 20 such instruments in the World.

Typically, TAP experiments are conducted at moderate temperatures up to 600 °C. Researchers at UiO are collaborating with Yara Int., the leading fertilizer producer who operate nitric acid production industrially, on developing a high-temperature TAP reactor for studying ammonia oxidation. Students in the project will have a unique opportunity:

- to learn about physico-chemical principles of kinetic measurements, in general, and TAP technique in particular
- to educate themselves about the fascinating subject of ammonia chemistry and materials science of metallic surfaces
- to participate in the commissioning of the new high-temperature reactor, including trial experiments with inert and reactive gases
- to perform mathematical analysis of preliminary data
- to learn about the industrial perspective on R&D and innovation for “green transition” (via collaboration with Yara)

Depending on the background of the candidate(s), the following two scopes of work will be executed, in tandem or separately.

Scope 1 – Experiments

- Learn (hands-on) the basics of operating the TAP reactor
- Conduct temperature calibration of the reactor up to 900 °C
- Perform pulsing of neon, oxygen, and ammonia at several temperatures between 800-900 °C
- Plot and discuss experimental data

Scope 2 – Modeling

- Learn (hands-on) the basics of modeling data from the TAP reactor
- Participate in selected high-temperature experiments to gain appreciation of experimental work and place the modeling efforts in perspective
- Model the transport of Ne, O_2, and NH_3 through the reactor at 800-900 °C

The main expected outcomes of the project are two-fold: educational and practical. On the one side, students will learn new skills (experiments or modeling) related to advanced research in materials science and catalysis. They will also gain a holistic perspective on the role of science in industrial innovation. On the other hand, the project will advance the technical capabilities of the TAP instrument which will be used in full-scale MSc and PhD projects.

Deliverables:

- Research findings will be presented as a poster, in the context of the “green” transition of the ammonia supply chain
- In the medium-term future, students will participate in the preparation of a research manuscript based on the follow-up experiments with the commissioned high-temperature TAP reactor