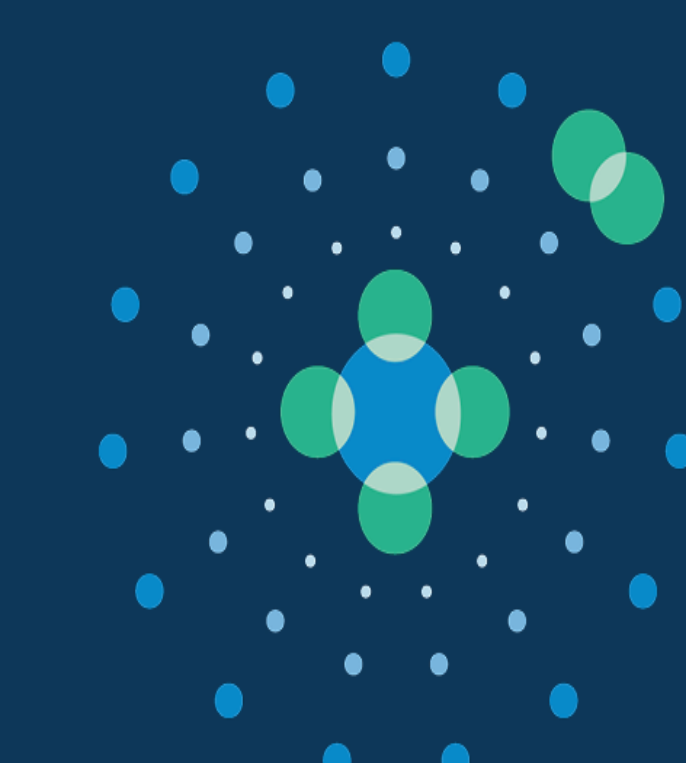


Industrial-Scale Quantum Mechanics: Online Sensing and Catalyst Kinetics for Ortho-Para Hydrogen Conversion



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Background and Aim

To prevent boil-off losses from exothermic *ortho-para* (*o-p*) hydrogen conversion, hydrogen liquefaction processes must control *o-p* composition to its cryogenic equilibrium state. This is achieved using purpose-designed *o-p* catalysts. However, despite their critical role, there is limited cryogenic kinetic data available, and the effects of catalyst activation and impurity-driven deactivation remain poorly understood.

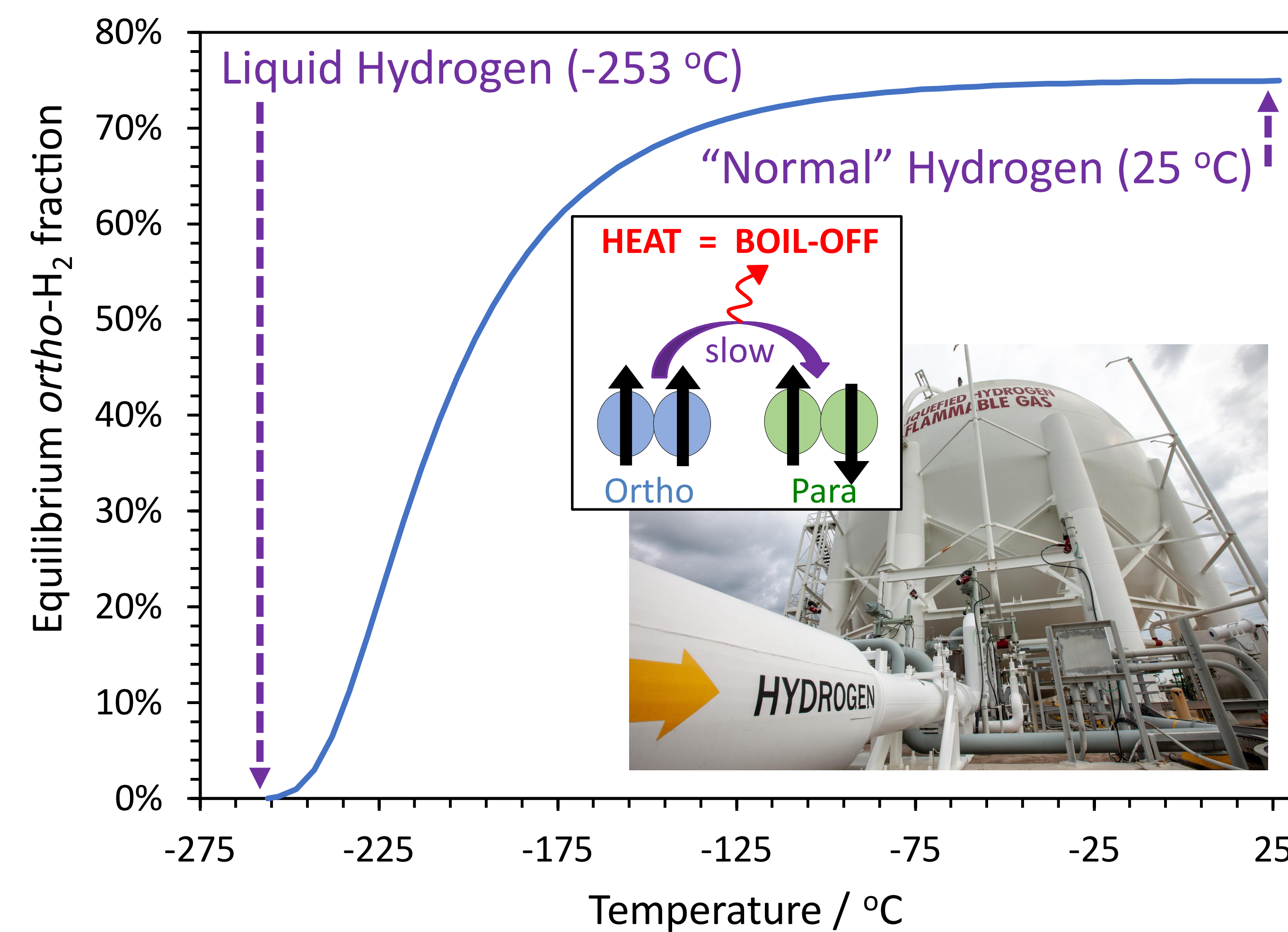


Figure 1. Calculated equilibrium *ortho*-hydrogen fraction versus temperature, highlighting exothermic *o-p* conversion risks for liquid hydrogen storage (NASA Kennedy Space Centre).

Methodology

A cryogenic hydrogen flow system was developed based around a pulsetube cryocooler (-228 – -196 °C) with online Raman spectroscopy to monitor *o-p* composition. A cryogenic tube reactor was used to study methods for catalyst activation and mechanisms of catalyst deactivation, by measuring the *o-p* hydrogen conversion kinetics under controlled cryogenic conditions. Reaction kinetics were modelled assuming first-order behaviour relative to space velocity.

Activation methods:

- Vacuum activation (150 °C under vacuum)
- Nitrogen activation (150 °C under warm N₂ flow)

Deactivation studies:

- Continuous monitoring under different moisture impurity levels in the hydrogen process stream to assess catalyst stability and performance loss over time

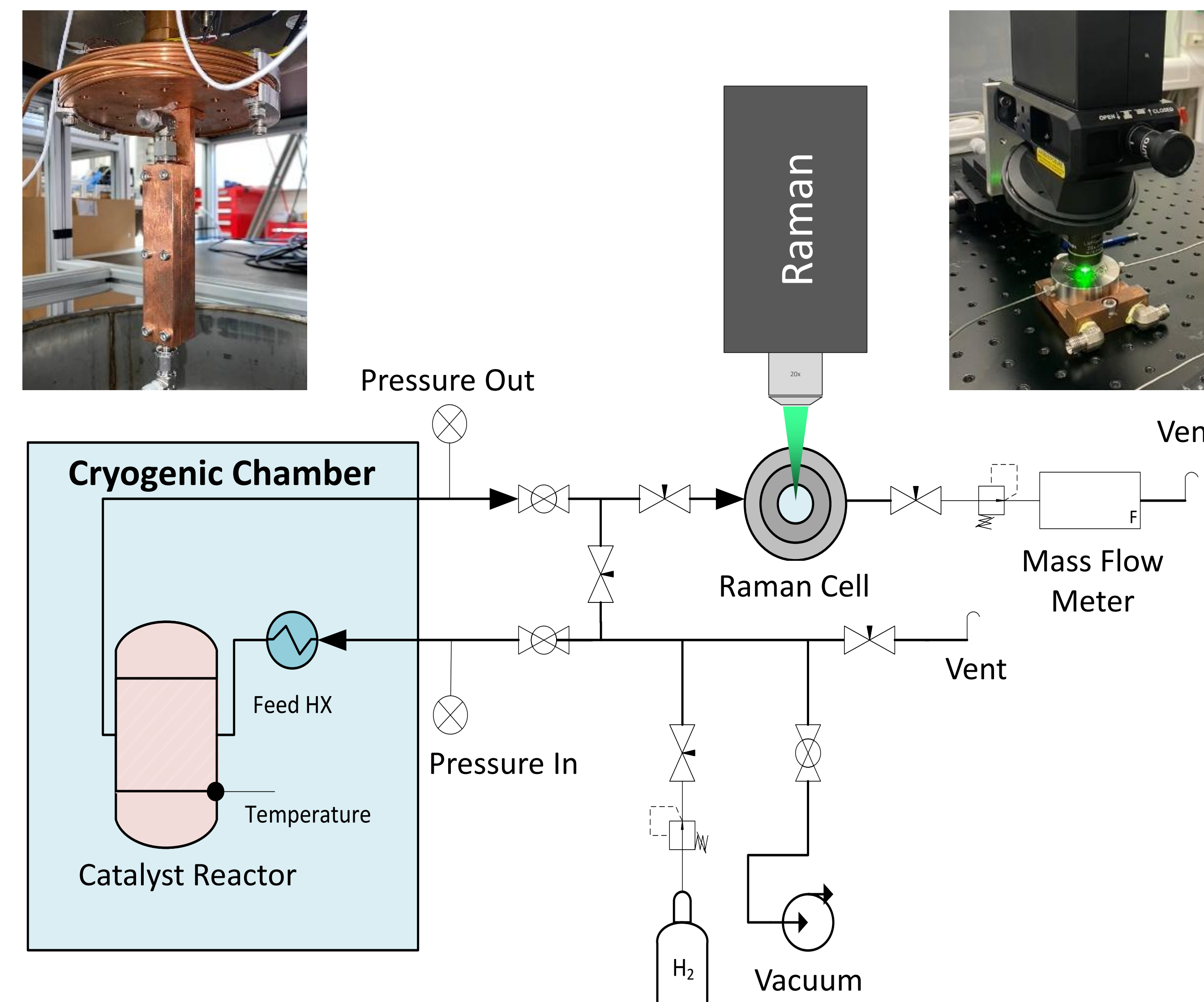


Figure 2. Schematic of experimental setup for conducting kinetics measurements including picture of tube reactor in conductive bracket and in-situ Raman cell and laser.

Results

- Kinetics data (*k*) were collected across a broad range of conditions between -228 and -196 °C and 1 to 4 MPa
- Nitrogen activation achieved comparable catalyst activity to vacuum activation with sufficient hydrogen flushing
- Moisture impurities caused significant catalyst deactivation, leading to rapid loss of conversion efficiency

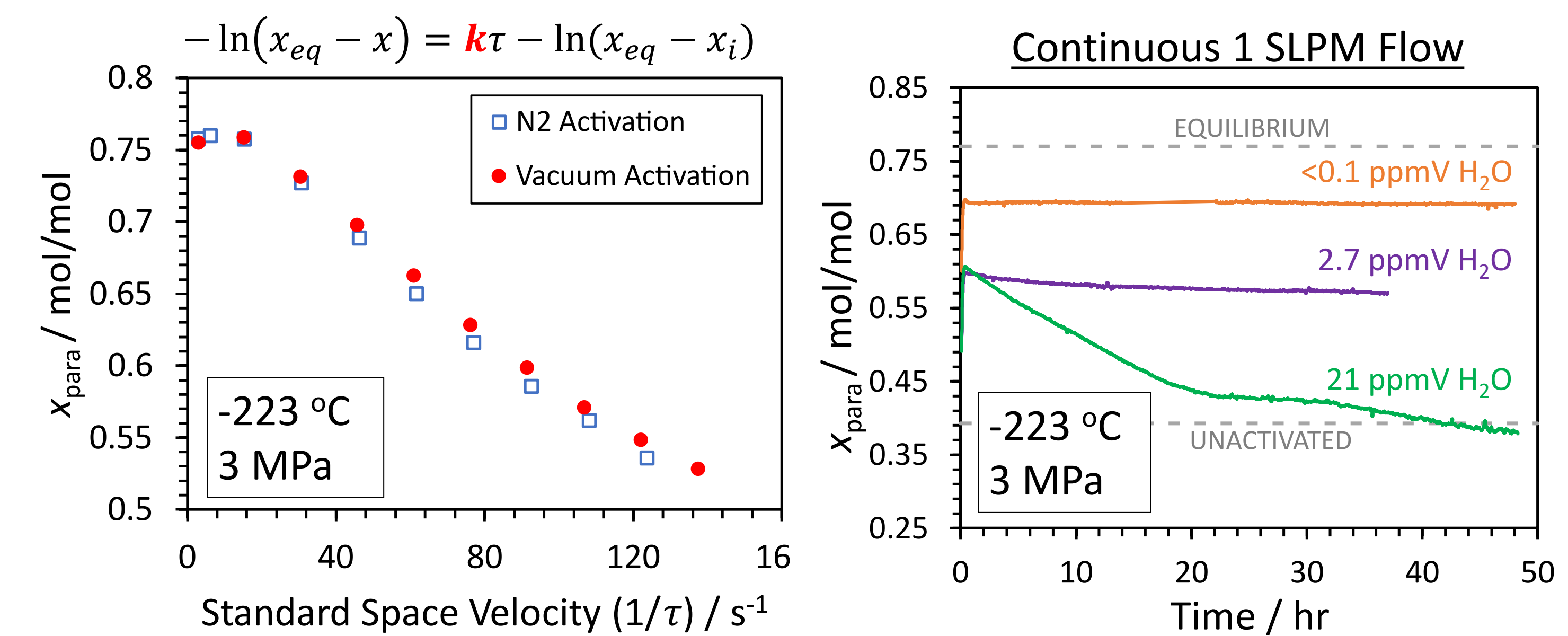


Figure 3. Left: Comparison of nitrogen and vacuum activated catalyst kinetics. Right: Continuous flow moisture impurity enabled catalyst deactivation over time.

Outcomes and Impact

- Established a new **cryogenic kinetics database**
- Evaluated the performance and limitations of **nitrogen activation**
- Identified **gas impurity management** as critical to preventing catalyst deactivation and blockage formation
- Validated **Raman analysis for *o-p* composition sensing**
- Highlighted the value of **real-time *o-p* sensing** for catalyst quality assurance

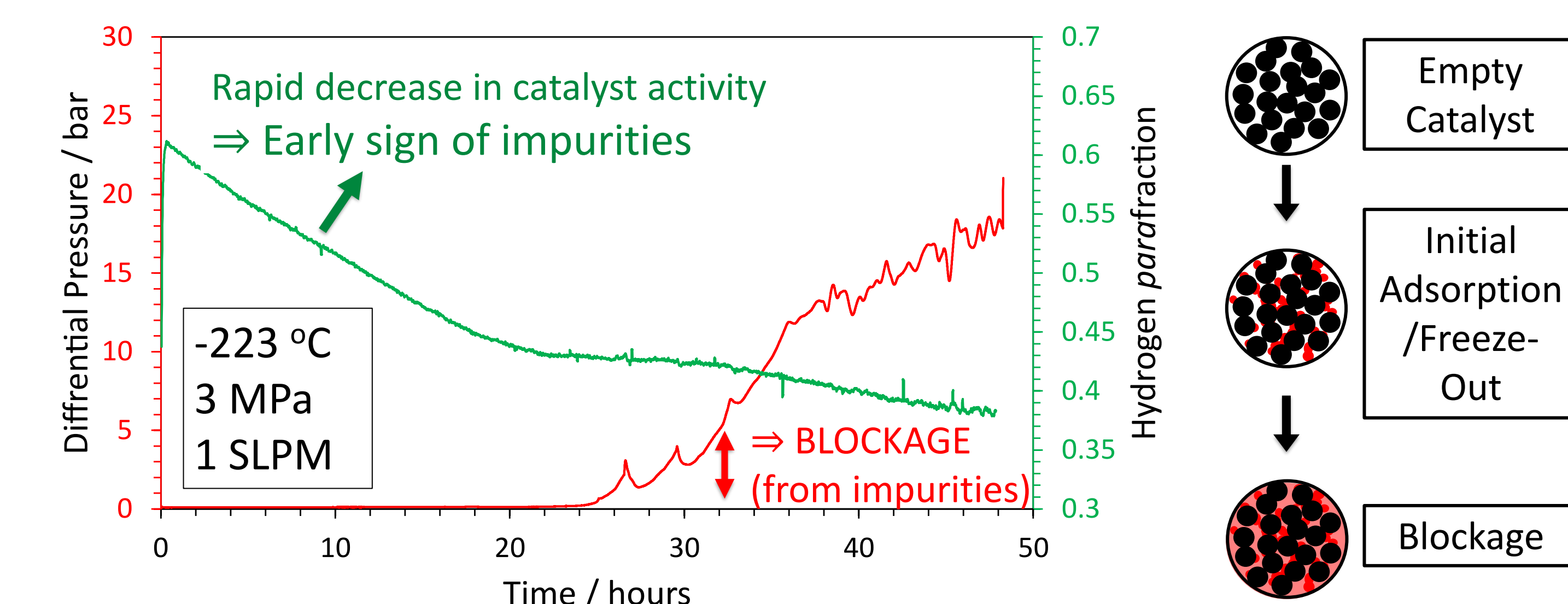


Figure 4. Representation of the importance of online *o-p* sensing to identify impurities in hydrogen liquefaction as opposed to traditional pressure differential sensing methods.

Aim: Develop an experimental platform to:

- measure *o-p* hydrogen conversion at industrial conditions
- study activation / deactivation of *o-p* conversion catalysts
- validate online sensing techniques



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