Contribution ID: **153** Type: **Contributed Oral**

C3Or4A-06: Process simulation and techno-economic assessment of hydrogen liquefaction plants with integrated ortho-para conversion

Wednesday 21 May 2025 17:30 (15 minutes)

As the demand for climate-friendly mobility solutions increases, hydrogen stands out as a key enabler, especially in heavy-duty sectors like transportation and aviation. Liquid hydrogen, with its high energy density, holds significant promise for these industries. Many studies focus on the application of liquid hydrogen in these sectors. However, also the supporting infrastructure –including hydrogen generation, storage, transportation, and liquefaction –requires thorough investigation to enable large-scale adoption.

In this context, the HyNEAT project, funded by the German Federal Ministry of Education and Research (BMBF), investigates liquid hydrogen supply networks and their evolution for air transport. A crucial part of this infrastructure is the liquefaction process, which is energy-intensive and costly, but essential for building a CO2-emission-free hydrogen aviation sector. As the global demand for liquid hydrogen rises tremendously, particularly driven by the requirements of hydrogen-powered transportation, a fast scale-up of worldwide liquefaction capacities and the development of energy- and cost-wise optimized large-scale hydrogen liquefaction facilities are critical.

In hydrogen liquefaction plants, hydrogen is first precooled with either liquid nitrogen or mixed refrigerants, followed by cryogenic refrigeration and liquefaction. Additionally, the conversion of hydrogen from its ortho- to parahydrogen form plays a vital role. As hydrogen at ambient conditions consists of a mixture of 75% ortho- and 25% parahydrogen, while at cryogenic temperature, hydrogen consists almost entirely of its parahydrogen form, the conversion between ortho- and parahydrogen must take place within the liquefaction process. This exothermic conversion is catalytically driven and integrated continuously into the plate-fin heat exchangers within the cryogenic refrigeration process.

This study presents detailed steady-state simulations of small- and large-scale hydrogen liquefaction plants, developed in the process simulation tool UNISIM. Thereby, these models accurately consider the continuous ortho-para conversion and the corresponding conversion heat within the heat exchanger channels of the refrigeration process. Therefore, an approach is applied that utilizes the Boltzmann distribution to calculate the equilibrium parahydrogen fraction and the Van't Hoff equation to determine the conversion heat [1].

An integrated techno-economic analysis of the hydrogen liquefaction plants of different scales is performed to evaluate the cost-effectiveness and energy efficiency of the processes. The results are validated against industrial key performance indicators. By combining steady-state simulation with techno-economic evaluation, this study's results provide valuable insights into the performance and cost efficiency of hydrogen liquefaction processes and, therefore, contribute to advancing sustainable hydrogen infrastructure and improving the economic viability of hydrogen as a clean energy carrier.

[1] Kanz, B., Tafone, A., Stops, L., Massier, T. Klein, H. (2024). A Novel Approach to Simulate Ortho-Para Conversion in Hydrogen Liquefaction based on the van't Hoff Equation. Submitted for publication.

Author: STOPS, Laura (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany)

Co-authors: KANZ, Benjamin (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany; TUMCREATE Ltd., 1 Create Way, Singapore); DO, Khang (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany); Prof. ALEKSEEV, Alexander (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany; Linde GmbH, Clean Energy Technologies R&D, Pullach, Germany); REHFELDT, Sebastian (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany); KLEIN, Harald (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany)

Presenter: STOPS, Laura (Technical University of Munich, TUM School of Engineering and Design, Department of Energy and Process Engineering, Institute of Plant and Process Technology, Garching, Germany)

Session Classification: C3Or4A - LH2 and LNG II: Storage and Utilization