

High pressure, high purity, dry hydrogen

Publieke samenvatting / Public summary

Aanleiding

One of the prime ways of utilizing renewable electricity is by using hydrogen as renewable source for transportation fuel and as renewable feedstock for petrochemical industries (e.g. refineries and the production of chemicals). Providing an economically viable technology for hydrogen compression (and temporary storage), at industrial relevant scales, and so to work towards the aims of TKI Nieuw Gas and the TKI Energie program Systeemintegratie, is at the heart of the motivation for this project. There are various emerging green hydrogen applications, and a detailed and comprehensive description of the phase behavior and mass transport of systems with hydrogen is crucial, because of the wide range of possible applications and process conditions. Typical applications will include adsorption and membrane processes for hydrogen purification, development of transport networks and transmission of hydrogen, decentral generation of hydrogen from water electrolysis, high pressure storage of hydrogen and the use of hydrogen in fuel cells to generate electricity. All these systems are in need for an accurate description of the thermodynamic and transport properties of hydrogen.

Doelstelling

Development of new drying technology and molecular models relevant for the processing of compressed hydrogen up to 875 bar. High purity, dry hydrogen is required for hydrogen fueling stations and for optimal working of hydrogen fuel cells. Both 'systems' should comply with the ISO specification of a maximum water fraction of 5 ppm. However, during the electrochemical hydrogen

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compression water is required for optimal performance, and as a result the high pressure hydrogen will be saturated (with an unknown) amount of water. The main objective is to improve the physical-chemical understanding of the thermodynamics, mass transport, and the kinetic phenomena taking place on (and in) the membrane electrode assembly (MEA) during compression of hydrogen up to high pressures (around 875 bar) to optimize the hydrogen production. The hydrogen output (in terms of maximum pressure, amount, and purity) is a function of a range of conditions, like the water vapor partial pressure, current density, operating temperature, and hydrogen back diffusion as a result of the pressure gradient over the MEA.

Korte omschrijving

There are two main thrusts of activity in this project: experimental testing and molecular simulations, both in an effort to understand how to further optimize the process of electrochemical compression of hydrogen. The main focus will be on the relation between the membrane electrode assembly, the core of the electrochemical compressor, and the specifications of the high pressure hydrogen. We will start with a holistic approach of developing a detailed molecular simulation model for water-hydrogen mixtures. Subsequently, this model will be used to calculate and predict the specific properties of the MEA, in particular various thermodynamic properties of hydrogen-water mixtures at elevated pressures (vapor-liquid equilibrium, relative humidity of the hydrogen, mass transport properties). These results will serve as an input for the design of a high pressure, bench-scale hydrogen dryer, based on the concept of heat-exchangers. The high-pressure dryer will be connected to the electrochemical compressor to remove excess water.

Resultaat

The different results of this project will comprise of an experimental data set, a high-pressure device for drying of hydrogen, computational (molecular simulation and equation-based), models, and an overall economic analysis. One of the main results

will be an optimized high-pressure hydrogen dryer that can be coupled with the electrochemical compressor stack. Furthermore, comprehensive molecular simulation software, a molecular simulation model based on Monte Carlo and Molecular Dynamics simulations, and verification of the molecular simulation results with experimental data. An important result of the project is also an experimental data set with accurate thermophysical properties of hydrogen (with water) at high pressures, which is currently lacking.

De data in deze applicatie is afkomstig van de Rijksdienst voor Ondernemend Nederland (RVO) en wordt in samenwerking met de Topsector Energie ontsloten.

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