ENCONTRO COM A CIÊNCIA E TECNOLOGIA EM PORTUGAL

28 a 30 JUNHO 2021

#ciencia2021PT

Fundação para a Ciência e a Tecnologia

MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

Recovery of Green Hydrogen from Natural Gas Grids

Lucas F. A. S. Zafanelli[1,2], Alírio E. Rodrigues[2] and José A. C. Silva[1*]

[1] Grupo de Processos e Produtos Sustentáveis, Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal

[2] Laboratory of Separation and Reaction Engineering (LSRE), Associate Laboratory LSRE/LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, S/N, 4099-002, Porto, Portugal

*(*jsilva@ipb.pt)*

Introduction

Hydrogen (H_2) can play an important role as a clean energy in a sustainable future. For example, H_2 can store surplus renewables power when the grid cannot soak it, help to decarbonize heavy industry and long-distance transport, and replace fossil fuels as a zero-carbon feedstock in chemicals and fuel production. [1] However, H_2 as an energy source is only sustainable if its production is free of carbon emissions. In this sense, green hydrogen produced via electrolysis of water powered by renewable energy sources (solar, wind, hydroelectricity, or biomass) is an important strategy to reduce CO_2 emissions levels (Figure 1). The global concern to replace fossil fuels is reflected by a forecast of more than $ 300 billion in H_2 investments through 2030, motivating studies to enable its use. [2]

One of the main barriers to set-up the use of green hydrogen produced from renewables is its transportation to the end-users. To surpass this issue, the use of the existing natural gas networks has been proposed for distributing green hydrogen. There is at least three main advantages by using the existing natural gas pipelines, namely: (i) the use of existing ones avoid large investments to build new ones, (ii) H_2 can be transported by long distance cheaply ($0.1/kg for up to 500 km), and (iii) H_2 can be used directly without chemical conversion required. [2] However, a new technology to recover green hydrogen from natural gas grids needs to be developed to allow the pure distribution of H_2 and CH_4. In this context, the present work seeks to identify strategies to develop a new separation technology based on adsorption processes to recover green hydrogen from natural gas grids.

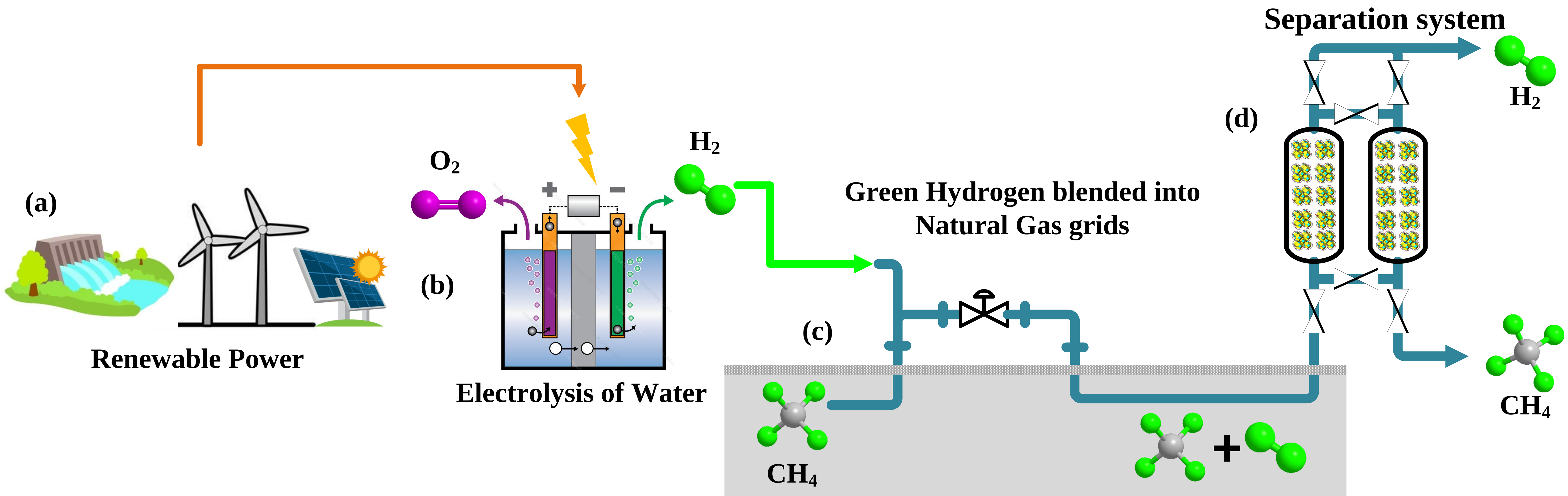

Figure 1. Overview of green hydrogen production, transportation, and distribution to the end-users. (a) renewable source of energy as hydroelectric, wind, and solar; (b) electrolysis of water powered by renewable energy to produce green hydrogen; (c) transportation of green hydrogen blended in the natural gas grids; (d) Adsorption separation technology to separate green hydrogen from methane before reach to the end-users.

Methodology

A key factor to develop a suitable adsorption separation process is to select a specific adsorbent material able to adsorb reasonable quantities of H_2 (>1wt.%) and to reject CH_4 (Figure 2). Among a large options of adsorbents, the Metal-Organic Frameworks (MOFs) can be considered as prime candidates to address this issue due to their versatility, which allows their synthesis and upgrade for specific targets. For example, MOFs-based mesh-adjustable molecular sieve fits perfectly into gas adsorption when it is desired to separate molecules with a small difference in their kinetic size. [3] The kinetic difference between CH_4 and H_2 is very small (~0.92 Å) but large enough to design a framework that allows the H_2 access through the small aperture and excludes CH_4 by the sieving effect.

Thus, in the initial stage of this project, we have identified three MOFs-based materials able to address this separation by screening considering three criteria, namely (i) very narrow pore aperture (allowing the diffusion of H_2 only), connecting, if possible, (ii) larger cavities (for higher loading) and (iii) showing high affinity to H_2 (for better confinement and higher loading). These materials will be tested by fixed bed adsorption to access separation dynamic information and to evaluate their sieving effect. According to the preliminary results, new frameworks will be synthesized to improve the separation performance. Additionally, an adsorption mathematical model will be implemented to optimize a Pressure Swing Adsorption system by using the most suitable adsorbent materials develop in the first stage, seeking high recovery and economic factors.

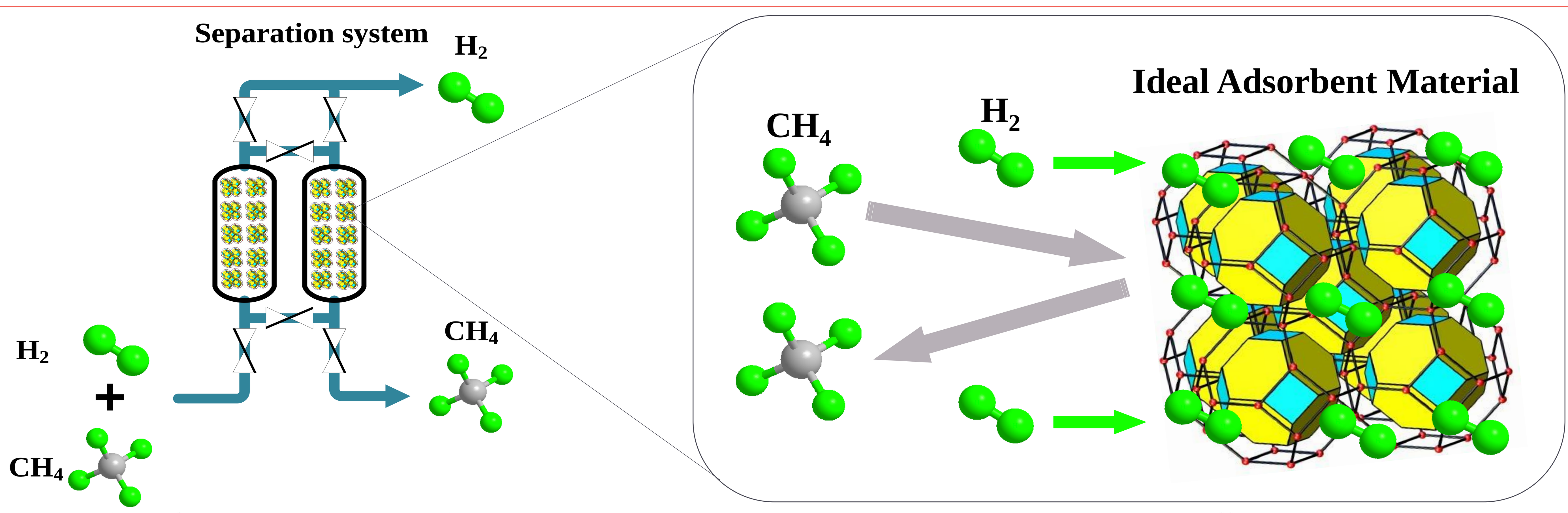

Figure 2. An ideal adsorbent framework to address the separation between green hydrogen and methane by sieving effect at nearly atmospheric conditions. The framework represented belongs to the ZIF-8 [4] that has large cavities not suitable for this proposal. Its use here is merely illustrative.

References and Acknowledgements

[1] Van Renssen, S. *Nature Climate Change* **2020**, *10*, 799–801.
[2] Council, H.; McKinsey. Hydrogen Insights; tech. rep.; *Hydrogen Council*, **2021**.
[3] Ma, S.; Sun, D.; Wang, X.-S.; Zhou, H.-C. *Microporous Materials* **2007**, *46*, 2458–2462.
[4] Park, K. S.; Ni, Z.; Côté, A. P.; Choi, J. Y.; Huang, R.; Uribe-Romo, F. J.; Chae, H. K.; O'Keeffe, M.; Yaghi, O. M. *Proceedings of the National Academy of Sciences* **2006**, *103*, 10186–10191.

The authors would like to acknowledge Foundation for Science and Technology (FCT), through the individual research grant 2020.07925.BD of Lucas F. A. S. Zafanelli.