

# Integrated Fuel Cell Systems for Rail Transport: Design and Optimisation

Maria Portarapillo\*, Augusto Bellucci Sessa, Almerinda Di Benedetto

*Department of Chemical, Materials and Production Engineering, University of Naples Federico II, P.le Tecchio  
80, 80125, Naples, Italy*

*\*Corresponding author: maria.portarapillo@unina.it*

## **Highlights**

- Design of integrated systems for hydrogen production and fuel cells for rail transport
- Different hydrogen storage medium were analysed such as methanol, ethanol glycerol and ammonia.
- Alternative hydrogen storage results feasible in terms of weight and volume and safer.

## **1. Introduction**

Due to the depletion of fossil fuels and the deterioration of environmental conditions, global attention is increasingly focussing on the use of renewable energy sources and the improvement of energy efficiency. The use of hydrogen-based technologies requires infrastructures for production, transport, storage and distribution on a small, medium and large scale. The main focus is on optimising technical performance. However, when developing hydrogen infrastructure, safety must be considered first and foremost. In this context, the proton exchange membrane fuel cell (PEMFC), which can efficiently convert hydrogen into electricity, is becoming increasingly important, especially in mobile systems (e.g. vehicles). The HT-PEMFC in particular is very promising thanks to the typical operating temperatures (120-200 °C) and the resulting CO tolerance (4-5 % at 200 °C). In addition, the improvement in reaction kinetics, catalysts tolerance, heat dissipation and water management due to the temperature increase also leads to higher energy efficiency of the HT-PEMFC. For the development of safe hydrogen storage, the in-situ production of hydrogen from "safer" chemicals was proposed as an alternative.

The aim of this work is to investigate the feasibility of an integrated railway traction system in terms of volume and weight based on hydrogen storage in the form of liquid methanol, ethanol, glycerol or ammonia, hydrogen production by oxidative steam reforming (OSR) or decomposition and HT-PEMFC. The calculations were performed for configurations optimised for energy self-sufficiency. The results were compared with those obtained for a configuration with on-board hydrogen storage at 350 bar. For the comparison of the different fuels, a train was used that was to be equipped with two three-phase asynchronous electric motors driven by inverters, each with an output of 314 kW (total output 628 kW). It was assumed that the entire traction system is housed in a single carriage (traction unit), the centre carriage, as developed, for example, as part of the HydroFlex project in the UK.

## **2. Methods**

The energy self-sufficiency assessment of the integrated system was carried out using AspenPlus<sup>®</sup>. This assessment took into account the presence of a first stage to preheat the reactants, the reaction phase and the cooling phase of the outlet stream to reduce the temperature to a level acceptable for HT-PEM. The heat emitted by the fuel cell was compared with the heat required in the heating phase. The heat emitted by the cooling phase was also taken into account in order to achieve the autothermal state of the system. In the preliminary design of the system, an electrical output of 628 kW was assumed, which is also supported by ad hoc dimensioned Li-ion batteries. In accordance with literature data, the efficiency of the HT-PEMFC was assumed to be 50 %. The volume and mass of the catalyst were calculated on the basis of kinetic data given in the literature ([1]–[3]). The calculated volume was multiplied by a factor of 10 to take into account the necessary catalyst dilution to ensure quasi-isothermal operating conditions. The reactor volume is assumed to be 2 to 3 times the volume of the already assessed catalyst bed, taking into account the void fraction, heat exchanger and auxiliary equipment. Some commercial data is taken into account for the volume of the HT-PEMFC. The volumes of the alcohol/water or ammonia tanks were determined taking into account the hydrogen production yields given in the literature ([1]–[3]).

### 3. Results and discussion

The electrical system, consisting of high-temperature PEM fuel cells and batteries, was dimensioned by simulating the Brescia-Edolo line (Italy) and evaluating the required electrical power, motor traction and travelling speed using conventional train kinematics equations [4]. The battery used has a capacity of 400 kWh, the power is based on the maximum instantaneous power and the fuel cells correspond to the electrical power of the motors. For the reference case, where hydrogen is stored at 350 bar, the total weight of the traction system is 20 tonnes, of which about 50% is the weight of the Type IV containers used for gas storage at this high pressure and 437 kg is the weight of the hydrogen alone. In the case of methanol and ethanol, the total weight of the traction system is less than in the reference case and amounts to 14 and 17 tonnes respectively. Both alcohols are stored under liquid conditions at room temperature and pressure and with water under stoichiometric conditions, which ensures much safer conditions than storing H<sub>2</sub> under high pressure.

In the case of glycerol, the optimum operating temperature of the reactor is 600 °C. Under these conditions, a system weight of around 22 tonnes was determined. In the case of ammonia, liquid storage at room temperature and 9 bar as well as a reactor operating temperature of 300 °C are required. Under these conditions, the system has a weight of 14 tonnes. All volumes are compatible with the size of a railway wagon and the weights are below those permitted on railway lines such as the Brescia-Edolo line. In the chemical storage of H<sub>2</sub>, the influence of by-products such as N<sub>2</sub>, CO, CO<sub>2</sub> and CH<sub>4</sub> produced during reforming or cracking should be considered. In fact, the presence of CO<sub>2</sub> in the reformat can lead to a drop in stack voltage, but the presence of CO<sub>2</sub> in the reformat can lead to a drop in stack voltage, but it has a limited effect on the electrical efficiency of the stack [5]. In general, hydrogen-rich reformat with a purity of >50 % can be utilised directly by HT-PEMFCs without further purification processes. The reduction in hydrogen utilisation and PEM efficiency was taken into account, and the storage volumes were also updated and discussed.

### 4. Conclusions

The sizing of the proposed integrated systems with high-temperature PEM fuel cells, batteries and H<sub>2</sub> production step in the Brescia-Edolo route simulation has provided valuable insights into the potential application of different and safe hydrogen storage solutions. The comparison of hydrogen storage methods, including storage at high pressure, under liquid conditions and chemical processes such as reforming or cracking, revealed clear trade-offs in terms of weight, operating temperatures and efficiency. These results highlight the complexity of selecting an optimal hydrogen storage solution, with factors such as weight, operating conditions and by-product management playing a crucial role. The results contribute to ongoing efforts to develop sustainable and efficient electrical systems for train traction and have potential implications for future developments in this area.

### References

- [1] S. J. Kim, T. S. Nguyen, J. Mahmood, and C. T. Yavuz, *Chem. Eng. J.*, 463 (2023) 142474
- [2] S. Bac, S. Keskin, and A. K. Avci, *Int. J. Hydrogen Energy*, 45 (2020) 34888–34917
- [3] L. Selva Roselin and H. W. Chiu, *J. Saudi Chem. Soc.*, 22 (2018) 692–704
- [4] Joshua Peli, “APPLICAZIONE DELLE FUEL CELL PER L’ALIMENTAZIONE DI VEICOLI FERROVIARI,” Politecnico Milano, 2018.
- [5] T. Guan, P. Alvfors, and G. Lindbergh, *Appl. Energy*, 130 (2014) 685–691

### Keywords

Alcohols Oxidative Steam Reforming, Ammonia Cracking, Fuel Cell, Energy Self-Sustainability in railway Systems.

This study was carried out within the MOST – Sustainable Mobility National Research Center and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1033 17/06/2022, CN00000023). This manuscript reflects only the authors’ views and opinions, neither the European Union nor the European Commission can be considered responsible for them.