Section: AM

## Modelling, numerical simulation, and optimization of new technologies related to hydrogen production (Zeppelin project)

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## Abstract:

The rising global energy demand, due to population growth, highlights the urgency for sustainable alternatives to fossil fuels. Hence, green Hydrogen (Green H2) is considered as a key energy solution for its ability to produce electricity, mechanical, and thermal energy without CO2 emissions. However, producing hydrogen from fossil fuels harms the environment, so we need to use circular economy ideas and manage waste better to minimize the impact and encourage industries to work together. Four types of technologies are considered for this purpose: catalytic technologies (bioethanol and biogas reforming reactors [1]), microbiological technologies (dark fermentation [2] and microbial electrolysis cell [4] reactors), thermochemical technologies (fluidized and fixed bed gasification reactors [5]), and storage technologies (inside porous materials [6] and in the form of ammonium [7]). Each individual technology or a network of technologies is modelled by a system of Differential Algebraic Equations (DAEs). In addition, to simulate and optimize it, a direct transcription approach is considered where the DAEs are discretized in a system of algebraical equations. This model is able to make decisions to turn on and off some of interconnected technologies by minimizing a cost function (and/or maximizing the hydrogen production). The final product of this research is a Python simulation and optimization package which can be used for designing and optimizing a network of hydrogen production and storage technologies based on minimizing the production and storage costs. Finally, some specific cases are solved and the results are discussed.

## **References:**

- Saidi, M. and Jahangiri, A., 2018. Theoretical study of hydrogen production by ethanol steam reforming: Technical evaluation and performance analysis of catalytic membrane reactor. International Journal of Hydrogen Energy, 43(32), pp.15306-15320.
- [2] Boshagh, F., Rostami, K. and Van Niel, E.W., 2022. Application of kinetic models in dark fermentative hydrogen production–A critical review. International Journal of Hydrogen Energy, 47(52), pp.21952-21968.
- [3] Asrul, M.A.M., Atan, M.F., Yun, H.A.H. and Lai, J.C.H., 2021. Mathematical model of biohydrogen production in microbial electrolysis cell: A review. International Journal of Hydrogen Energy, 46(75), pp.37174-37191.
- [4] Asrul, M.A.M., Atan, M.F., Yun, H.A.H. and Lai, J.C.H., 2021. Mathematical model of biohydrogen production in microbial electrolysis cell: A review. International Journal of Hydrogen Energy, 46(75), pp.37174-37191.
- [5] Agu, C.E., Pfeifer, C., Eikeland, M., Tokheim, L.A. and Moldestad, B.M., 2019. Detailed one-dimensional model for steam-biomass gasification in a bubbling fluidized bed. Energy & fuels, 33(8), pp.7385-7397.
- [6] Rahimi, M., Abbaspour-Fard, M.H. and Rohani, A., 2021. Machine learning approaches to rediscovery and optimization of hydrogen storage on porous bio-derived carbon. Journal of Cleaner Production, 329, p.129714.
- [7] Jorqueira, D.S.S., Neto, A.M.B. and Rodrigues, M.T.M., 2018. Modeling and numerical simulation of ammonia synthesis reactors using compositional approach. Advances in Chemical Engineering and Science, 8(3), pp.124-143.