

Master Thesis

Thermodynamics of energy storage reactions

Project location: Paul Scherrer Institut (PSI), Villigen, Switzerland
Laboratory for Thermal Processes and Combustion
Energy and Environment Research Division

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Time frame: Available from August 2020. Can be undertaken as a 4 or 6 month project.

Research background and context:

The increased production of renewable energy brings the need for a seasonal storage. In fact, energy production with renewable sources is possible only in certain periods of time (mainly in summer), while the energy demand takes mostly place in other phases. To avoid this mismatch, energy must be seasonally stored in an appropriate form. As batteries are too expensive for large scale applications, the storage in chemical bonds, i.e. in synthetic fuels is considered as an optimal solution. Several possible fuels can be formed from the reaction of CO₂ (from localized emissions or other sources) and H₂ (from water electrolysis performed with excess energy).

Objectives of the research project:

The thesis focuses on identifying the most suitable products to use as energy storage molecule. Among the various possible routes, a quantitative analysis will be conducted, with appropriate modelling tools to identify the necessary process integration to efficiently perform the reaction and to identify the most suitable synthesis routes. The study will move from a simple thermodynamic/stoichiometric analysis, to more complex thermodynamic and rate-based models. This will allow determining the boundary conditions that make every class of storage materials suitable for this task.

Tasks:

- Analyze literature to verify the available technologies for energy storage in chemical bonds.
- Derive an appropriate thermodynamic model to forecast the storage efficiency of the synthetic fuels and verify the possibilities for process integration
- Study with appropriate rate-based model the most promising solutions

Benefits for the student:

- Development of modelling skills in the context of energy storage materials
- Possibility to work remotely, with flexible working time
- Learning to write scientific reports and communicate results, including at webinars and/or workshops with national and international collaborators and stakeholders.

References:

- [1] Moioli, E., Mutschler, R., & Züttel, A. (2019). Renewable energy storage via CO₂ and H₂ conversion to methane and methanol: Assessment for small scale applications. *Renewable and Sustainable Energy Reviews*, 107, 497–506.
<https://doi.org/10.1016/j.rser.2019.03.022>