**Conceptual and Basic Design of an Innovative Catalytic Reactor for Dehydrogenation of Liquid Organic Hydrogen Carriers**

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**Highlights**

* Most of existing LOHC dehydrogenation models suffer from a low reaction yield.
* Followed concept promises an efficiency enhancement, modularity & scalability.
* The optimized basic design is achieved by series of analyses & simulations.

**1. Introduction**

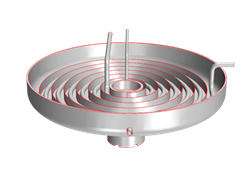
The greatest hurdles in terms of traditional energy storage are the improvement of efficiency and the minimization of final costs, whereby sustainable resources are both seasonal and daylight-dependent. The storage of energy in the form of liquid organic hydrogen carriers, the so-called LOHC, is a new, progressive trend. LOHC are hetero- or homocyclic aromatic hydrocarbons and because of their unsaturated chemical structure, they are able to store additional hydrogens (as energy carrier) in a chemically bonded form. In addition, these energy-carrying materials will not be consumed during their utilization, but instead will be recycled for further loading and unloading cycles. A whole storage system includes a water-electrolyze unit, a water reservoir, a hydrogenation reactor, two LOHC tanks, a dehydrogenation reactor and a hydrogen-burning unit. The division into sector steps is a significant benefit of this new system, e.g. the division into hydrogenation unit and dehydrogenation unit. The dehydrogenation side is highly endothermic (70 kJ/mol H2) and its thermal efficiency is very crucial in the energy aspects of the overall system. We have developed a concept, which is positively remarked in the evaluations. This concept is inspired by helical heat exchangers, which benefit from a high thermal efficiency and relatively lower pumping energy [1].

**2. Conceptual design**

The existing reactor models are based on horizontal shell-and-tube heat exchangers in which the bottom halves of the tubes are filled with catalyst pellets. The loaded LOHC is pumping through the reaction tubes, which are heating to the reaction temperature and after passing the residence time, the hydrogen will release on the surface of the catalyst and can leave the reaction zone via empty top halves of the tubes [2]. The heat transfer values are in the expected range. Nevertheless, the overall performance of the reactor is not satisfactory. This is probably due to the large volume of hydrogen released (9 mol H2/mol LOHC), which pushes the LOHC out of the reactor, reducing the residence time.

Our new concept solves the problems of the large volume increase during the reaction and poor heat transfer. The Figure 1 shows the general structure of this concept. The idea here is to run the hydrogenated LOHC (loaded form) on an open plate, where a semi-helical heat exchanger provides the necessary temperature and heat flux for the dehydrogenation reaction. The hydrogen releases by bringing the reactants in contact with the heating coils along an open coiled channel filled by catalyst pellets or granules, which are small enough to cover all the empty spaces.

Being modular and scalable in this particular concept is very advantageous. The basic components of reaction plate are designed for a simple modification or extension. This makes the concept unique and it eases to reconstruct the reactor plate on different capacities or stack-on more parallel plates in a pressure vessel for any demanded purposes and power-outputs.



heating coils

loaded LOHC inlet tube

unloaded LOHC outlet tube

coiled channels

reaction plate

**Figure 1.** General schematics of a single internal plate of the reactor

**3. Basic design**

In the next step, mathematical & theoretical analyses, simulations and experimental investigations are concerned. The reaction kinetics of perhydro-dibenzyltoluene are studied and verified [2]. Maintaining the residence time and heat of reaction are the key parameters, which are followed as the functionality basics of any concepts, and in addition to developing a reasonable and functional dehydrogenation reactor, finding the essential influencing parameters on thermal efficiency and reaction progress are mainly in focus. Optimization of the thermal efficiency addresses mainly the reaction zone inside the plate and channel geometries. Here the channel size and paired heating-coil measures must be optimized. Regarding plate’s outside, the inlet temperatures, flow directions, vessel’s pressure must be studied and optimized. In case of stacked-on plates, the plates’ gaps and similarity for the even heat and flow regulations are particularly important. As an example, the temperature profiles by three different channel widths are shown in Figure 2.

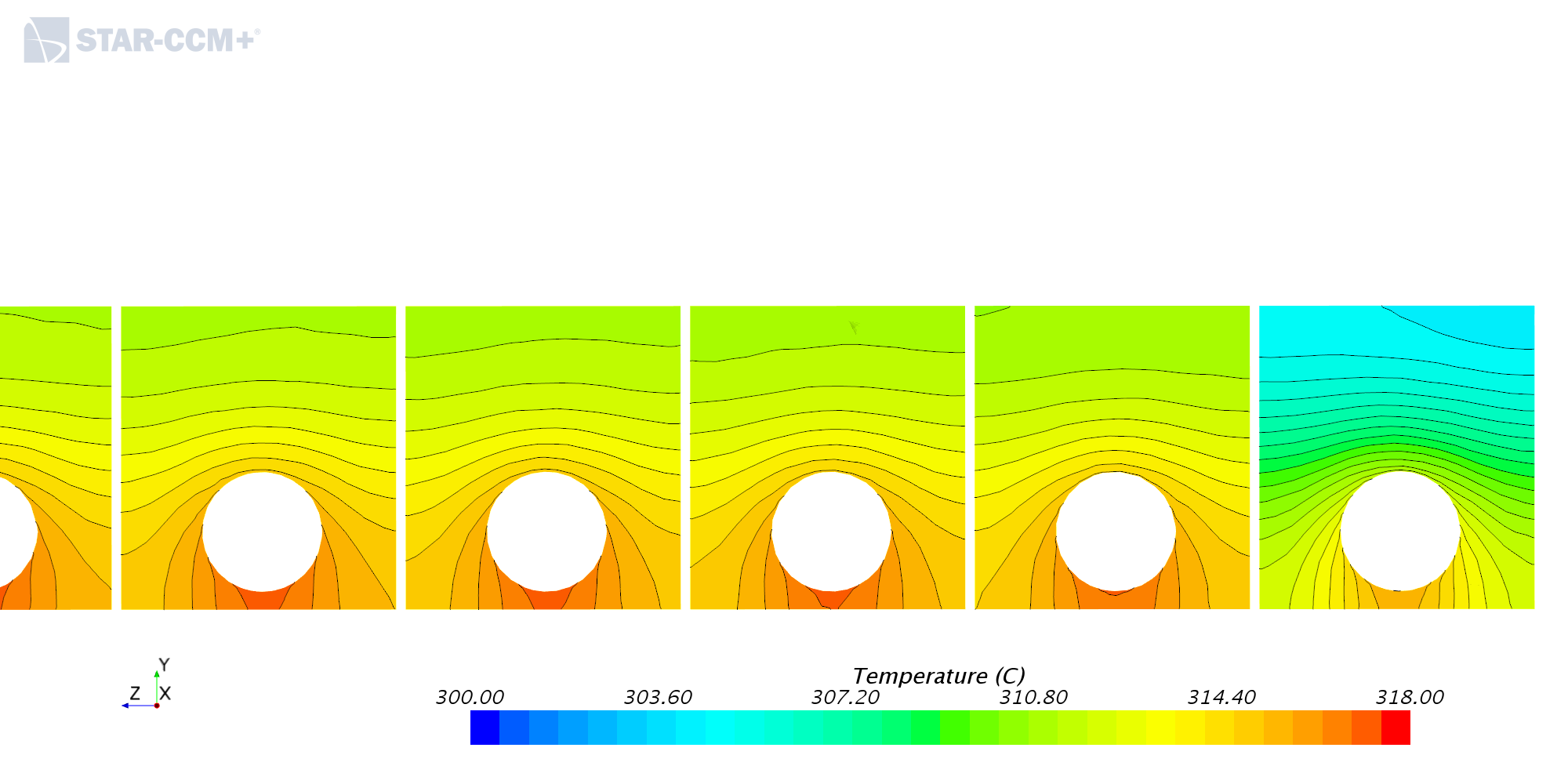
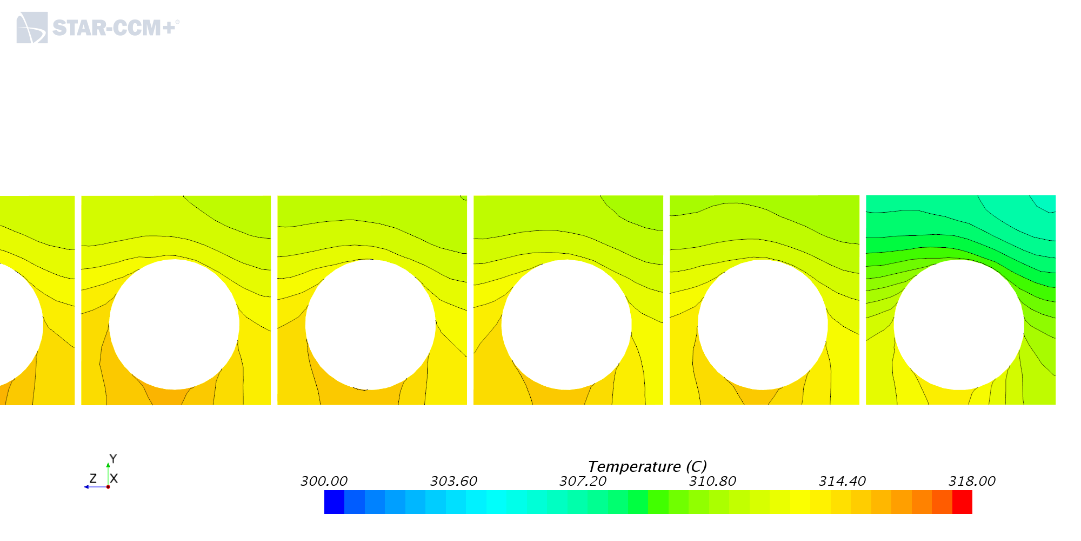
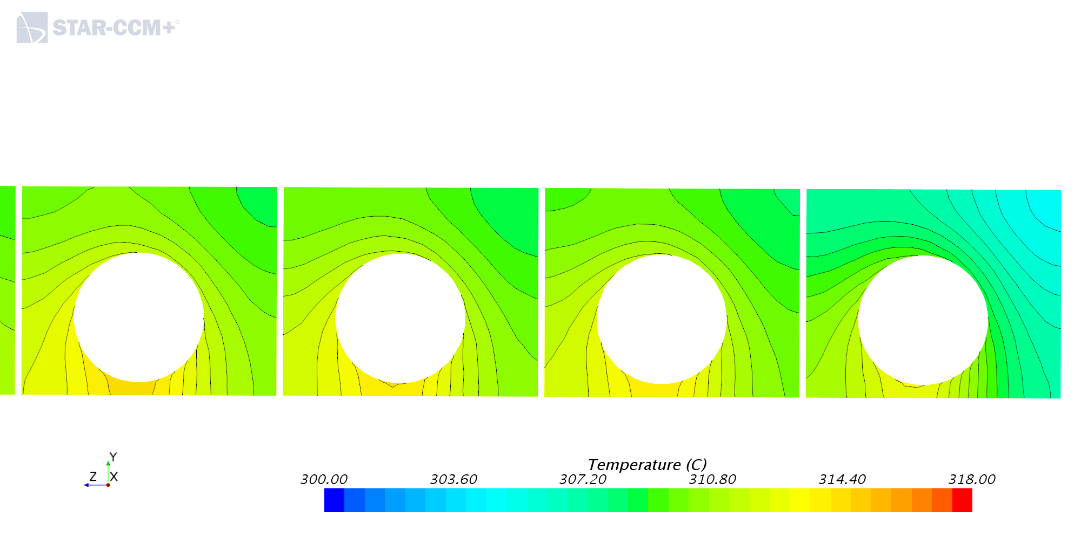
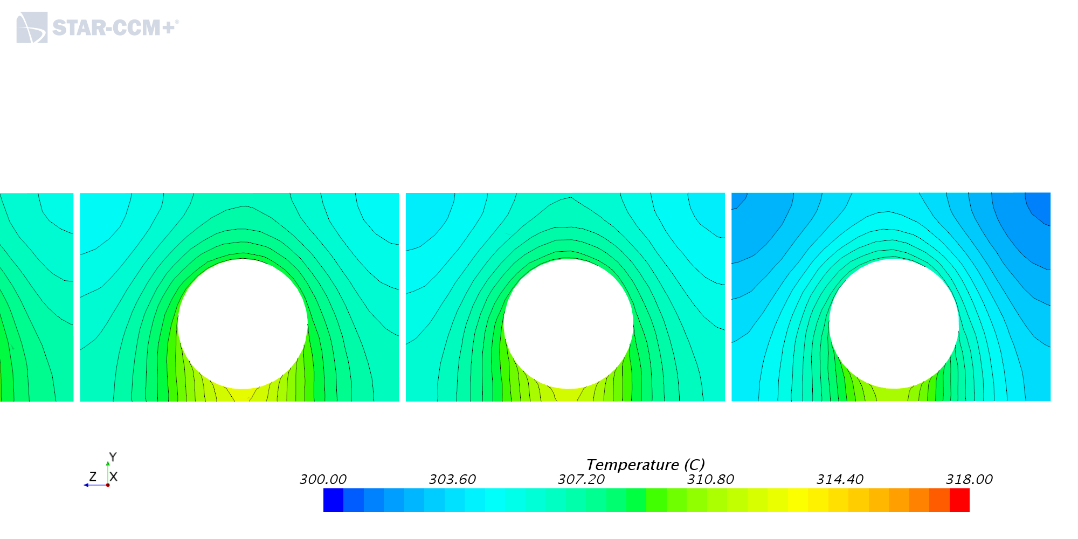


Figure 2. Temperature profiles in cross section of channel with 3 widths

**4. Conclusions**

Currently, the semi-helical structure reports to be known as the most promising concept for dehydrogenation of LOHC. Very less limitation concerning released amount of hydrogen gas makes this concept already attractive in the conceptual design step, in addition to notable improvements on heat transfer and residence time in the optimized basic design. After experimental verification of optimized parameters in series of empirical studies, the detailed engineering step follows.

**References**

1. S.E. Emamjomeh, E. Schlücker, Book of Abstracts: 10th World Congress of Chem. Eng. (2017) p. 469.
2. P.K.E. Preuster, Development of a reactor for the dehydrogenation of chemical hydrogen carriers as part of a decentralized, stationary energy storage system, Doctoral Thesis, Erlangen 2017.