Computational fluid dynamic (CFD) of the Liquid organic hydrogen carrier (LOHC) dehydrogenation reactor and furnace

Nihal Rao[1*], Ashwin W Patwardhan[1]

1 ICT Mumbai, Nathalal Parekh Marg, Opposite Don Bosco, Maharashtra 400019

**Corresponding author: che20nu.rao@pg.ictmumbai.edu.in*

Highlights

- Validation of the steam cracking furnace design through CFD.
- CFD of the inhomogeneous Eularian two-phase LOHC dehydrogenation reactor.
- The temperature inside the LOHC dehydrogenation reactor ranges between 590 K -623 K.

1. Introduction

Transporting the hydrogen is quite expensive due to the low volumetric density. Therefore, lowering the transporting cost can reduce the cost per kilogram of hydrogen. Thus, hydrogen transportation can be beneficial when the existing transport infrastructure is utilized. Liquid organic hydrogen carrier (LOHC) can provide these benefits as they can transport hydrogen at atmospheric temperature and pressure, have a high hydrogen storage capacity and can be transported using the existing infrastructure. Designing the LOHC dehydrogenation reactor plays a key role in efficiently converting the hydrogenated compound to hydrogen and dehydrogenated compound. Previous studies were mainly focused on the dehydrogenation capacity and efficiency for various catalyst loading at different temperatures and pressures. Significantly, few papers were primarily on the flow and temperature distribution of the LOHC dehydrogenation system to understand the hydrogen release in the reactor. The LOHC dehydrogenation is an endothermic reaction, and temperature inside the reactor is essential in converting the dehydrogenated LOHC to hydrogen. Due to the complex nature of the dehydrogenation system, good predictive simulation models are required to achieve a good design LOHC dehydrogenation reactor and furnace. The furnace simulated by Habibi [1,2] for the steam cracker, an endothermic reaction similar to that of the LOHC dehydrogenation reaction, provides validation for the furnace box to be developed for the LOHC dehydrogenation reactor. The LOHC dehydrogenation reactor is also simulated to understand the flow and temperature distribution across the reactor for the constant wall temperature.

2. Methods.

2.1 Furnace modelling

The furnace modelling consists of the flow, combustion, and radiation models, which were calculated based on the Reynolds averaged Navier Stokes (RANS). The flow inside the furnace is modelled based on the continuity, momentum and turbulence model based on the RNG k-ϵ model. The combustion model uses a mix of the Finite rate and eddy dissipation model, which takes the minimum rate of the combustion based on finite rate and mixing. The radiation model is based on the P-1 radiation model. The combustion reaction is from methane and hydrogen combustion from the Westbrook and Dryer[3]. The pressure velocity is coupled using the SIMPLE algorithm. The mix of first-order and second-order upwind schemes discretizes the momentum, energy and species.

2.2 Reactor modeling

The reactor is modelled based on the two-phase model, consisting of the liquid phase (phase-1) containing the dibenzyltoluene - perhydrodibenzyltoluene and the gas phase of hydrogen (phase-2). The two-phase is simulated using the inhomogeneous Eularian model. The flow is laminar, and the energy equation is used for the heat used by the reaction and heat transfer between the wall and the fluid.

3. Results and discussion

The furnace model for the steam cracking furnace developed by Habibi et al.[1] is validated for the static temperature for the right-hand side of the burner in the furnace and the species concentration across the height of the reactor. The temperature contour of the steam cracking furnace and the centre of the dehydrogenation reactor across the length is given in **Figure 1,** and the validation of the static temperature and the species concentration across the right hand of the burner across the height of the furnace is given in **Figure 2.**

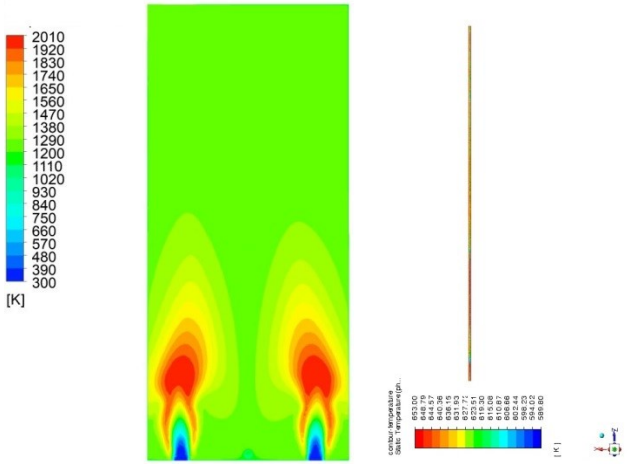

Figure 1. Temperature contour of the steam cracking furnace and phase -1 of the LOHC dehydrogenation reactor.

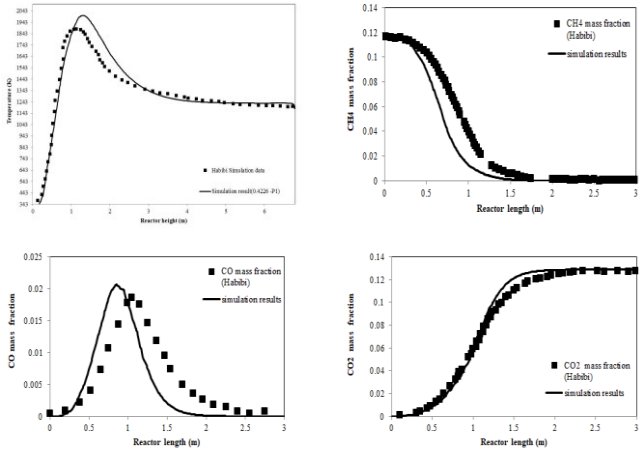

Figure 2. Static temperature and the species concentration for the right hand side burner across the height of the furnace.

There are recirculation zones that are formed in the furnace due to asymmetrical outlet design of the furnace The recirculation zone increases the residence time of the flue gas, and that region's temperature is reduced and uniform. The static temperature of the burner's right-hand side rises at the furnace's initial height, reaching adiabatic flame temperature, reduces and then remains constant along the length of the reactor, validating well with Habibi et al. [1].

4. Conclusion

Validation of the furnace design provides a design aspect for the LOHC dehydrogenation box proven by static temperature and species mass fraction across the furnace height. The simulation of the two-phase reaction of the LOHC dehydrogenation reactor was also performed, where, due to endothermicity, the temperature at the initial length of the reactor decreases and then increases due to heat transfer between the wall and the fluid.

References

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