Multiphysics Numerical Model of Short Contact Time Catalytic Plate Diesel Reformer

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Reforming of diesel fuel is an attractive option for hydrogen production because of its wide distribution and high energy density. Remote communities in northern Canada are facing serious challenges in electrical energy production at the cost of environment. Communities in north Canada produce electrical power using diesel generators. This has a number of negative impacts, e.g. health problems from particulates, NO_x and SO_x emissions, and water pollution from diesel spillage. An alternative is to reform the fuel to produce hydrogen-rich stream and feed it to a fuel cell system that can efficiently produce on-demand clean electrical power. However, this alternative solution poses technological challenges. One of the challenges is the development of a cost effective and efficient reformer for the production of hydrogen.

The design of a diesel reformer presents number of challenges such as maximizing heat transfer, minimizing pressure drop, maximizing utilization of expensive catalyst and achieving proper mixing of the reactants, etc. This is feasible by employing compact hydrogen generators (reformer). To this aim, a newly designed experimental Catalytic Plate Diesel Reformer (Figure 1) with laminar flow could lead to the development of improved design for compact reformer.

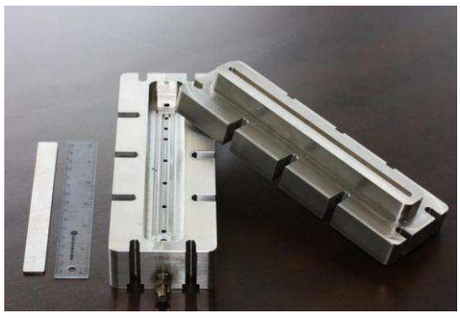

Figure 1. Catalytic Plate Diesel Reformer (CPDR)

Catalytic plate reactors (CPRs) are attractive because they can achieve high throughput with much smaller size than their conventional fixed bed counterpart. A CPR is a simple but elegant reactor concept consisting of a thin metal plate coated with appropriate catalyst to support an endothermic reaction on one side and an exothermic reaction on the other side. To drive an endothermic process on one side of the plate, the necessary heat can be provided by the exothermic process (i.e., by combustion of part of the fuel) or high temperature exhaust stream from fuel cell on the other side of the plate (Zanfir and Gavriilidis, 2003).

Multiphysics Numerical Model

A detailed two dimensional steady-state multiphysics numerical model consisting of heat and mass transfer and fluid dynamics both in flow channel and in coated catalyst is developed for the Catalytic Plate Diesel Reformer (CPDR). For an accurate prediction of the performance of CPDR, one should need to solve the flow equations through the channels and the porous structure of the catalyst layers on the plate. The flow equations include the continuity equation and the Navier-Stokes equations. The problem becomes very complex in the case of reactive flows where fluid dynamics and momentum transfer is coupled with reactions of chemical species. Further to this complexity, temperature gradients will develop inside the reactor due to generation or consumption of heat of reaction. For the species transfer, the Stefan-Maxwell diffusion model along with convective mass transfer is implemented in flow channel and in coated catalyst. Heat transfer effects are captured by implementing the heat source term in coated catalyst in the convection-conduction equation. Hexadecane is considered to act as a diesel surrogate. To account for the reactions in coated catalyst, two types of surface kinetics namely the LHHW (developed by Parmar et al., 2010) and the microkinetics (developed by Thormann et al., 2009) are used as a source term for the species mass transfer.

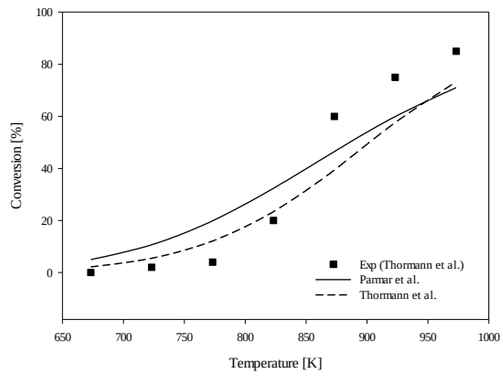

Figure 2. Hexadecane conversion and hydrogen yield

The model predictions for hexadecane conversion using microkinetics of Thormann et al. and LHHW kinetics of Parmar et al. gave good agreement with the experimental results of Thormann et al. (see Figure 2). It should be noted here that the Parmar et al. model is developed for Pt/Al_2O_3 catalyst. Further parameter optimization of the model could result in much better predictions. Also the microkinetics model, although gives detailed surface reaction information, is found to be computationally intensive and hence poses problems for optimization of reformer design.

References

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