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Numerical Model of Crude Glycerol Autothermal Reforming to Hydrogen-Rich Syngas

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Abstract : Hydrogen is a clean source of energy for power production and transportation. The main source of hydrogen in this research is biodiesel. Glycerol also called glycerine is a by-product of biodiesel production by transesterification of vegetable oils and methanol. This is a reliable and environmentally-friendly source of hydrogen production than fossil fuels. A typical composition of crude glycerol comprises of glycerol, water, organic and inorganic salts, soap, methanol and small amounts of glycerides. Crude glycerol has limited industrial application due to its low purity thus, the usage of crude glycerol can significantly enhance the sustainability and production of biodiesel. Reforming techniques is an approach for hydrogen production mainly Steam Reforming (SR), Autothermal Reforming (ATR) and Partial Oxidation Reforming (POR). SR produces high hydrogen conversions and yield but is highly endothermic whereas POR is exothermic. On the downside, PO yields lower hydrogen as well as large amount of side reactions. ATR which is a fusion of partial oxidation reforming and steam reforming is thermally neutral because net reactor heat duty is zero. It has relatively high hydrogen yield, selectivity as well as limits coke formation. The complex chemical processes that take place during the production phases makes it relatively difficult to construct a reliable and robust numerical model. Numerical model is a tool to mimic reality and provide insight into the influence of the parameters. In this work, we introduce a finite volume numerical study for an 'in-house' lab-scale experiment of ATR. Previous numerical studies on this process have considered either using Comsol or nodal finite difference analysis. Since Comsol is a commercial package which is not readily available everywhere and lab-scale experiment can be considered well mixed in the radial direction. One spatial dimension suffices to capture the essential feature of ATR, in this work, we consider developing our own numerical approach using MATLAB. A continuum fixed bed reactor is modelled using MATLAB with both pseudo homogeneous and heterogeneous models. The drawback of nodal finite difference formulation is that it is not locally conservative which means that materials and momenta can be generated inside the domain as an artifact of the discretization. Control volume, on the other hand, is locally conservative and suites very well problems where materials are generated and consumed inside the domain. In this work, species mass balance, Darcy’s equation and energy equations are solved using operator splitting technique. Therefore, diffusion-like terms are discretized implicitly while advection-like terms are discretized explicitly. An upwind scheme is adapted for the advection term to ensure accuracy and positivity. Comparisons with the experimental data show very good agreements which build confidence in our modeling approach. The models obtained were validated and optimized for better results.

Keywords : autothermal reforming, crude glycerol, hydrogen, numerical model
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