عنوان مقاله:

CFD model for evalution of palladium membrane reactorperformance during propane dehydrogenation process

محل انتشار:

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خلاصه مقاله:

This study presents a 2D-axisymmetric computational fluid dynamic (CFD) model to investigate the performance propane dehydrogenation process (PDH) for hydrogen production. The proposed CFD model provided the local information of temperature and component concentration for the driving force analysis. After investigation of mesh independency of CFD model, the validation of dehydrogenationduring PDH reaction was carried out by modeling data and a good agreement between CFD model results and theoretical data was achieved. In the present model, a tubular reactor with length of 150 mm was considered, in which the Pt-Sn-K/Al2O3 as catalyst were filled in reaction zone. Hence, the effects of the important operating parameter (reaction temperature) on the performances of membrane reactor(MR) were studied in terms of propane conversion and hydrogen yield. The CFD results showed that the suggested system during PDH reaction presents higher performance with respect to once obtained in the conventional reactor. The model results have indicate the higher efficiency of the MR in comparison with the tubular one which is achieved due to removal of hydrogen from reactionary zone through themembrane to shift the reaction equilibrium towards formation of products. The use of membrane was found to cause the propane conversion increase from 41% to 67%. The highest value of propane conversion (X = 96%) was reached in case of additional oxidation of the removed hydrogen (conjugated dehydrogenation). The maximum value of propylene selectivity S = 98% can be as well reached in case ofconjugated dehydrogenation in the MR at the reaction temperature of 500 ∘C. The oxidation of hydrogen in conjugated dehydrogenation process gives the increase of propylene yield from 65% (the tubular reactor) to 95%. The maximum propylene yield corresponds to T = 525 ∘C. It was also established that the gas space velocity in both internal and external parts of the MR is to be the one of the most importantfactors defining efficiency of the conjugated dehydrogenation process.

کلمات کلیدی:

Hydrogen production, CFD, Modeling, propane dehydrogenation

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