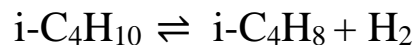


Heterogeneous Catalyst Design for Efficient Isobutane Dehydrogenation to Isobutene

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Background & Description:

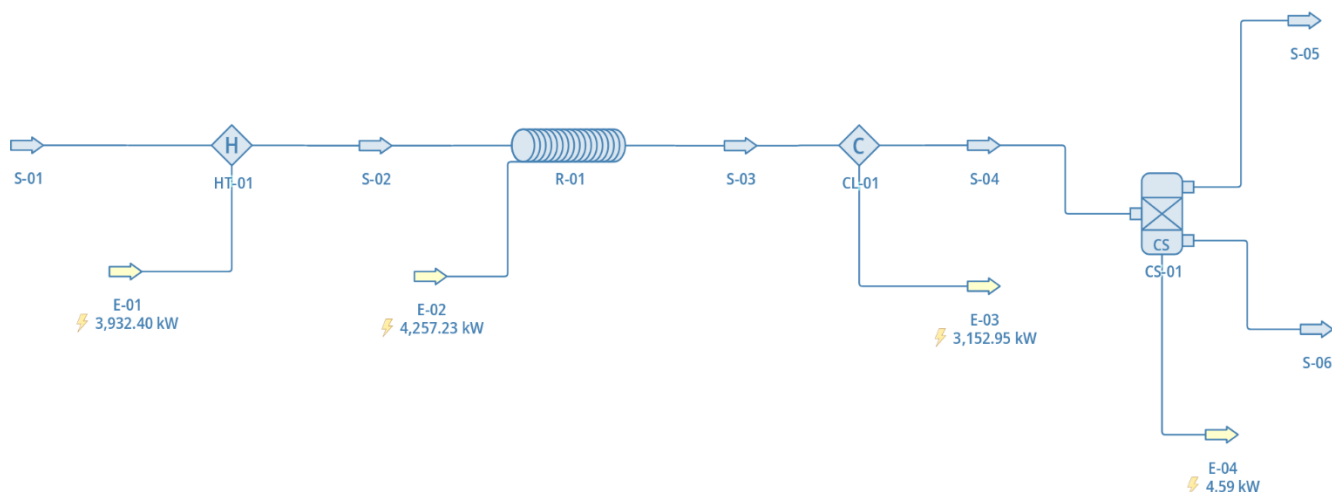
Isobutene is one flexible hydrocarbon used in the petrochemical sector somewhat extensively. It is a monomer used for the synthesis process of polyisobutylene an elastomer used in adhesives, sealants, and lubricants. Because of its gas impermeability, this monomer's polymerization generates butyl rubber—used in tire manufacture. Moreover, mixing isobutene with methanol produces tert-butyl ether (MTBE), a fuel additive improving the octane rating of gasoline. The study investigates using a plug flow reactor to turn isobutane into isobutene over a catalytic surface in order to get the most isobutene and hydrogen as a byproduct. The process starts with an isobutane stream at 25 °C and 5 bar pressure with a molar flow rate of 125 kmol/hr. Applying a 2-bar pressure drop, a heater heats the stream to 600 °C. The PFR is utilized for the main dehydrogenation reaction in isobutane into isobutene by using the optimum catalyst and reaction kinetics. Once chilled to 85 °C, a compound separator produces a stream of 99.99% pure isobutene and another stream of 100% hydrogen.



The results can be verified from the master property table: the product yields 7013.3 kg/hr of isobutene and 251.98 kg/hr of hydrogen; the initial mass flow rate of 7265.27 kg/hr is mostly converted into isobutene. Moreover, by the mole fraction, it is clear that both the desired isobutene stream and by-product hydrogen stream are pure at 99.99% and 100% purity, respectively, in their mixture forms; both the streams showcase approximately 125 kmol/hr molar flow rates with 85 °C and 2.37 bar pressure at the outlet.

Thermodynamic Package: Peng-Robinson (PR) Equation of State

Flowsheet:



Results:

Master Property Table				
Object	Isobutene	Isobutane	Hydrogen	
Temperature	85	25	85	C
Pressure	2.37928	5	2.37928	bar
Mass Flow	7013.3	7265.27	251.98	kg/h
Molar Flow	125	125	124.997	kmol/h
Molar Fraction (Mixture) / Isobutane	2.08893E-05	1	0	
Molar Fraction (Mixture) / Isobutene	0.999979	0	0	
Molar Fraction (Mixture) / Hydrogen	0	0	1	

Reference:

1. Sun G, Wang Q, Huang S, Huang Q, Li H, Liu H, Zhang X, Wang J. Intrinsic kinetics of dehydrogenation of isobutane over $K_2O-CuO-Cr_2O_3/Al_2O_3$ catalyst. Proceedings of the 2015 International Conference on Advanced Engineering Materials and Technology. Atlantis Press; 2015. p. 760–767. Available from: <https://doi.org/10.2991/icaemt-15.2015.144>
2. Aspen Plus® simulation software - a basic course for beginners-NPTEL