CONCEPTUAL DESIGN OF A 1-(4-ISOBUTYLPHENYL) ETHANOL PLANT

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Abstract

This study presents the conceptual design of a continuous plant for the production of 5,000 tonnes per year of 1-(4-isobutylphenyl) ethanol (IBPE) at 99.9% molar purity, via catalytic hydrogenation of 4-isobutylacetophenone (IBAP) over a palladium-on-silica catalyst. The process involves two consecutive irreversible reactions described by a Langmuir-Hinshelwood kinetic model, where the desired intermediate IBPE is susceptible to further hydrogenation to yield the by-product 4-isobutylethylbenzene (IBEB). The design follows a four-level hierarchical approach with increasing detail. At Level 1, continuous operation is selected over batch processing based on the required production scale. At Level 2, material balances and economic potential are evaluated as functions of single-pass conversion and hydrogen purge composition, incorporating a derived ordinary differential equation relating selectivity to conversion. At Level 3, the reactor is identified as an isothermal continuous stirred-tank reactor (CSTR) operating at 373 K, equipped with a cooling jacket and a gas recycle loop with compressor. The optimal hydrogen partial pressure and catalyst concentration are set at 10 bar and 0.78 g/L respectively. At Level 4, the separation system is designed and simulated in Aspen Plus, comprising a flash vessel for gas-liquid separation and a sequence of three vacuum distillation columns to handle the thermally sensitive organic components while achieving the target product purity. The optimal operating point is identified as 50% single-pass conversion with 70% hydrogen composition in the gas purge. A comprehensive profitability analysis yields a Total Capital Investment of €1.72 million, a Net Present Value of €0.66 million over a 20-year operational life, an Internal Rate of Return of 20%, and a discounted payback period of approximately 11 years, confirming the economic feasibility of the proposed process.

Keywords: Conceptual Design; Hydrogenation; IBPE; Hierarchical Approach; Vacuum Distillation; Aspen Plus; Profitability Analysis