# CONCEPTUAL DESIGN OF A SPECIALTY CHEMICAL PRODUCTION PLANT

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## Abstract

This study presents the conceptual design of a continuous plant to produce 5,000 tonnes per year of a speciality pharmaceutical intermediate at 99.9% molar purity via catalytic hydrogenation over a supported metal catalyst. The process involves two consecutive irreversible reactions described by a Langmuir-Hinshelwood kinetic model, where the desired intermediate product is susceptible to further hydrogenation to yield an undesired by-product. 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 recycle 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) with a cooling jacket, and a gas recycle loop with a compressor; optimal hydrogen partial pressure and catalyst concentration are determined through simulation. 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 vacuum distillation columns to handle thermally sensitive organic components and achieve the target product purity. The optimal operating point is identified through sensitivity analysis, balancing conversion and recycle purge composition. A comprehensive profitability analysis confirms economic feasibility over a 20-year operational life, with positive Net Present Value and Internal Rate of Return exceeding typical hurdle rates.

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