DEVELOPMENT OF A MATHEMATICAL MODEL FOR A FLUIDIZED BED REACTION VESSEL

By

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SUMMARY

Ethylene oxychlorination in fluidized bed reactor is considered one of the most selective and economical processes for large scale production of 1,2 dichloroethane in the balanced vinyl chloride monomer (VCM) plants. The reactor normally consists of a cylindrical vessel with internal cooling coils for heat removal and cyclones to minimize catalyst losses. This type of reactor is well suited for good temperature control of the highly exothermic oxychlorination reaction because the fluidization of the catalyst provides intimate contact between reactants, catalysts, and heat transfer surface. In the present study, a steady-state mathematical model based on the two-phase theory of fluidization is developed for the gas fluidized bed reactor using Wachi and Asai kinetics. The model is verified by comparing the calculated values of ethylene conversion and reactor temperature with the industrial ones at different loads. The model predictions agree well with the industrial data and the percentage error is very small. Different parameters such as cross-sectional area of the bubble phase, bubble velocity, fraction of bed consisting of bubbles, void fraction, molar flow rate of ethylene in bubble phase, inlet molar flow rate of ethylene in bubble phase, molar flow rate of ethylene in the dense phase, inlet molar flow rate of ethylene in the dense phase, volumetric flow rate in the bubble phase, volumetric flow rate in the dense phase, inlet volumetric flow rate in the dense phase, volumetric flow rate of the gas in the feed, initial concentration of ethylene, molar heat capacity of gas, cooling surface heat transfer coefficient, interphase heat transfer coefficient between bubble and dense phase based on bubble phase volume, interphase mass transfer coefficient between the bubble and dense phases based on the bubble phase volume, dense phase temperature, feed gas temperature, cooling medium temperature, and heat of reaction have been studied for different loads to determine their effects on the reactor performance. It is found that the calculated values of ethylene conversion and reaction temperature at 85% load (obtained by mass balance equations and heat balance equations) are the closest ones to the industrial data with the least percentage error in both ethylene conversion and reaction temperature. The error in case of applying the mass balance equations is less than the one obtained by applying the heat balance equations for the loads investigated. The most effective parameter on ethylene conversion for the studied loads (in case of applying mass balance equations) is the volumetric flow rate in the dense phase (Q_d) and the least effective one is the initial concentration of ethylene gas. On the other hand, the most effective parameter on ethylene conversion for the studied loads (in case of applying heat balance equations) is the cooling surface heat transfer coefficient (h_w) and the least effective ones are gas feed temperature (T_f), gas density, and bubble velocity.