TURTON DESIGN FOR PRODUCTION OF ACETONE VIA DEHYDROGENATION OF ISOPROPANOL

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❑ ACETONE :

1. Acetone is a colourless, volatile, flammable liquid, and is the simplest and smallest ketone.
2. It is miscible with water and serves as an important solvent in its own right, typically for cleaning purposes in laboratories.
3. Acetone is produced and disposed of in the human body through normal metabolic processes.
4. It is normally present in blood and urine. People with diabetes produce it in larger amounts.
5. Reproductive toxicity tests show that it has low potential to cause reproductive problems

❖ DESCRIPTION :

The production of acetone involves the dehydrogenation of IPA in a high-temperature gas-phase reactor.

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$$

Turton et al6 assumed the reaction to be irreversible and specify that the per-pass conversion of IPA is 90% to prevent side reactions. The reaction occurs in the vapour phase in the presence of a solid catalyst

Using the reactor size and kinetics given in Turton et al as shown in Table 1 gave the 90% conversion specified by the authors if the presence of the solid catalyst was neglected. Of course, the catalyst is present, so a bigger reactor would have to be used to give the same conversion.

The kinetics used by Turton et al are also unrealistic in that the reaction cannot be irreversible. If it were irreversible, we could operate at high pressure, which would raise the concentration of IPA and drive the reaction toward the products. But LeChatier's principle tells us that raising pressure should drive the reaction toward the reactant since there are two moles of product generated from one mole of reactant. In an attempt to modify the kinetics so as to capture these realistic effects, an RGIBBS reactor was run in Aspen Plus to find the effect of pressure on conversion. At 623 K (the temperature in the Turton flowsheet), the RGIBBS equilibrium conversion is 97.1% at 2 atm. This should be compared with the 90% conversion in the Turton design. As pressures are raised to 5, 10, and 15 atm, the equilibrium conversions decrease to 93.3, 87.8, and 83.2%. Clearly the effect of pressure must be considered.

The kinetics were modified to assume a reversible reaction:

(CH3)2CHOH <-> (CH3)2CO + H2

The activation energy of the forward reaction used is the value given in Turton et al (72 380 kJ/kmol). The activation energy of the reverse reaction was calculated using the heat of reaction (+62 900 kJ/kmol).

$$\lambda = EF - ER$$

An empirical trial-and-error procedure was employed to find the unknown values of the pre-exponential factors kF and kR that satisfied two conditions. First, they should give approximately the same pressure dependence of conversion in a large tubular reactor as predicted by RGIBBS. Second, they should give 90% conversion when used in the Turton tubular reactor (including the presence of catalyst). Table 1 shows the parameters used in the rest of this study. To be consistent with the assumption made by Turton, the conversion in the reactor is held at 90% as other design parameters are changed.

REFERENCE :

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