Acetone

Acetone (M.P = -94.6°C, B.P at 101.3 kPa = 56.29 °C) is the first and most important member of the homologous series of aliphatic ketones. It is a colorless, mobile liquid widely used as a solvent for various polymers. Its largest application, however, is as an intermediate in the synthesis of methyl methacrylate, bisphenol A, diacetone alcohol, and other products. Acetone is an excellent solvent for a wide range of gums, waxes, resins, fats, greases, oils, dyestuffs, and cellulosics. It is used as a carrier for acetylene, in the manufacture of a variety of coatings and plastics.

Most of the world's manufactured acetone is obtained as a coproduct in the process for phenol from cumene and most of the remainder from the dehydrogenation of isopropyl alcohol.

Manufacture:

1) Cumene Hydroperoxide Process for Phenol and Acetone

Benzene is alkylated to cumene, and then is in oxidized to cumene hydroperoxide, which in turn is cleaved to phenol and acetone. One kilogram of phenol production results in ≈ 0.6 kg of acetone or about ≈ 0.40–0.45 kg of acetone per kilogram of cumene used.

$$C_6H_5CH(CH_3)_2 \xrightarrow[\text{oxygen}]{\text{air or}} C_6H_5\overset{\overset{OOH}{|}}{C}(CH_3)_2 \xrightarrow[\text{heat}]{\text{acid}} C_6H_5OH + (CH_3)_2C{=}O$$

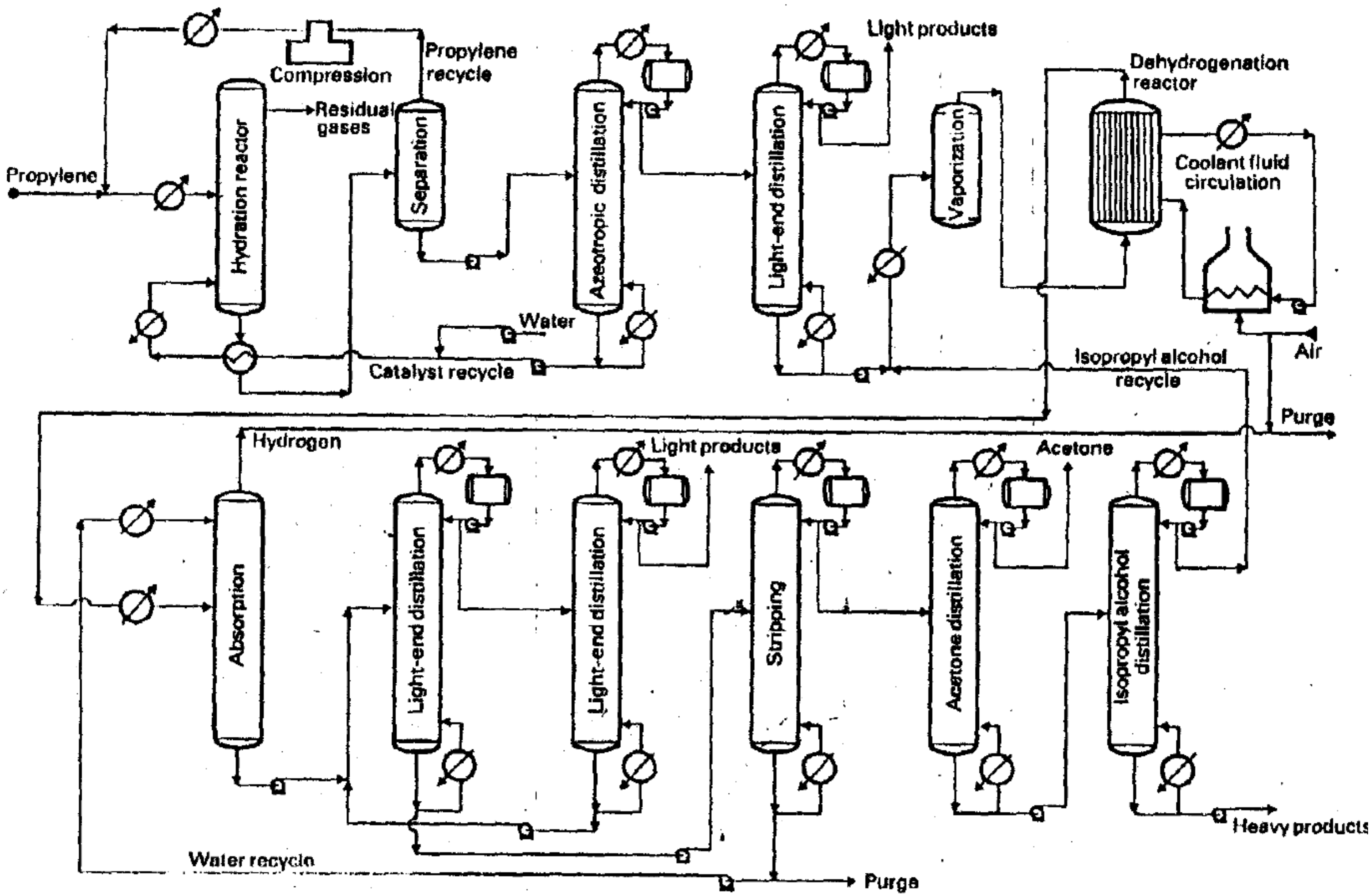
2) Dehydrogenation of Isopropyl Alcohol

Isopropyl alcohol is dehydrogenated in an endothermic reaction.

$$CH_3CHOHCH_3 + 66.5\ \text{kJ/mol (at 327°C)} \longrightarrow CH_3COCH_3 + H_2$$

The equilibrium is more favorable to acetone at higher temperatures. At 325°C, 97% conversion is theoretically possible. A large number of catalysts have been investigated, including copper, silver, platinum, and palladium metals, as well as sulfides of transition metals of groups 4(IVB), 5(VB), and (VIB)6 of the periodic table. These catalysts are made with inert supports and are used at 400–600°C. Lower temperature reactions (315–482°C) have been successfully conducted using zinc oxide zirconium oxide combinations, and combinations of copper–chromium oxide and of copper and silicon dioxide.

The main side reaction is the dehydration of 2-propanol to propene. Other competing reactions are the self-condensation of acetone to diacetone alcohol, which leads to further condensation products. All catalysts gradually lose activity because of a buildup of carbon deposits, so the operating temperature is increased as the catalyst ages.



Acetone manufacture by vapor phase dehydrogenation of isopropyl alcohol.

Vapor phase processes

In this type of technology, the reaction is conducted between 350 and 400°C, and 0.3 . 10^6 Pa absolute, in tubular units featuring the flow of a heat transfer fluid (steam, preheated air etc) on the shell side, designed to compensate for the endothermicity of the reaction, and the catalyst on the tube side. Good performance has been achieved with systems containing 7 to 8 per cent weight zinc oxide, promoted by zirconium oxide (0.5 per cent weight) and deposited on a pumice carrier. Isopropyl alcohol and hydrogen in a molar ratio of 1/1 are sent at 380°C on the catalytic bed operating with a LHSV of about 1.5 h^{-1}. Once-through conversion, as high as 98 per cent at the beginning of the runs, drops rapidly to less than 90 per cent owing to organic deposits which reduce the activity of the catalyst. Its regeneration by combustion at 500°C using a mixture of oxygen and nitrogen (2 and 98 per cent volume respectively) must be carried out at ten-day intervals. To guarantee continued production, it is therefore necessary to have several reactors in parallel, with a staggered operating schedule.

The operation presents a number of drawbacks, including the difficulty of temperature control in the neighborhood of 400°C. In the earliest versions, yields also failed to exceed 75 to 85 molar per cent. The latest technologies (*BP, Standard Oil* in particular) claim total yields approaching 98 molar per cent, with average once-through conversions above 90 per cent, for a reaction temperature ranging between 450 and 550°C.

The reactor output is first cooled and then scrubbed with water to rid the hydrogen of entrained reactants and products, followed by light and heavy ends separation in a series of three distillation columns, the second producing acetone to specifications at the top, with the third column designed to recover unconverted isopropanol to be recycled. If the feed consists of the azeotrope containing 87 per cent weight alcohol, three additional columns are required for the purification of the acetone and the recycling of isopropanol in a sufficient concentration.