Isopropyl Alcohol synthesis from propylene and Water adapted

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Introduction:

Isopropyl alcohol (IPA), also known as isopropanol or 2-propanol, is a secondary alcohol with the chemical formula of C_3H_7OH and molecular mass of 60.09502 kg/kmol. It is widely used as a solvent in many industries and finds applications in food processing, coatings to reduce flammability, as thinner and additive in paints, as well as disinfectants such as alcohol wipes in household products and medical applications. With water, IPA forms an azeotrope of 87.4 wt % alcohol, having a boiling point of 80.3°C at atmospheric pressure.

IPA is manufactured by two major commercial processes: indirect and direct hydration of propylene, of which the latter is common due to less corrosion in unit operations. Direct hydration of propylene is an exothermic, reversible reaction carried out with an acid catalyst, which could be cation-exchange resins such as molybdophosphoric acid, titanium and zinc oxides. The main reaction is

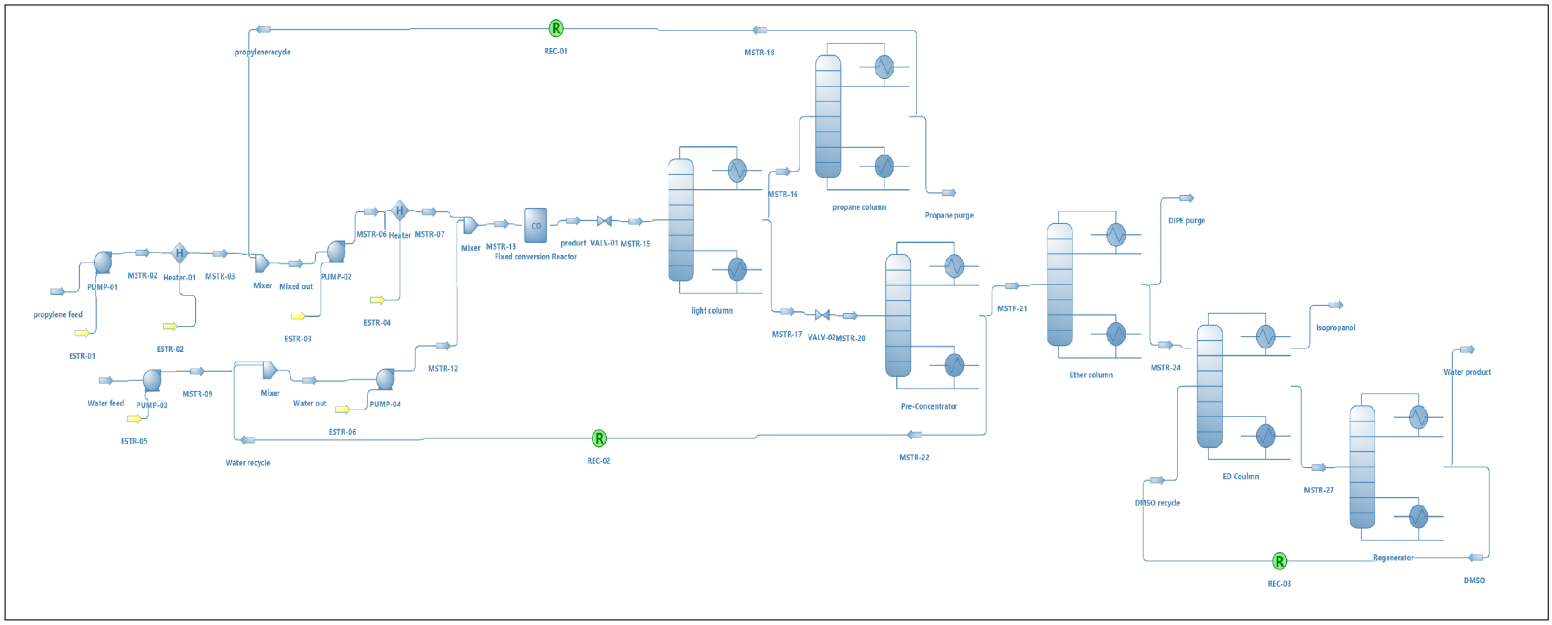
$$\mathbf{CH_3-CH=CH_2 + H_2O \longrightarrow (CH_3)_2CHOH}$$

The main side product, diisopropyl ether (DIPE) forms after the etherification reaction:

$$\mathbf{2\,(CH_3)_2CHOH \longrightarrow H_2O + [(CH_3)_2CH]_2O}$$

The most popular propylene direct hydration is the trickled bed process‘

Flowsheet;



Description;

fresh propylene (at 47.6°C and 101.325 kPa) and recycled propylene are mixed in a molar ratio of 4.65:1, pressurized, and preheated before feeding into the trickle bed reactor. Meanwhile, another reactant water (fresh/recycled = 1:7.63) is pressurized to 7500 kPa and also fed into the reactor. The product stream from the bottom of the reactor is depressurized to 902 kPa and sent to the lights column to strip the dissolved propylene and propane. The gaseous mixture leaving the top of the lights column is transferred to the propane column to remove propane (in order to avoid its accumulation in the process) from propylene as the latter is recycled to the reactor.

Heavier components from the bottoms of the propane column are depressurized to 120 kPa, mixed with recycled IPA and then sent to the pre-concentrator, where more than 90% of water is removed in the bottoms stream; this water stream is recycled to the reactor.The distillate stream of the preconcentrator contains mainly water, IPA, and DIPE. In this mixture, the DIPE mole fraction is only 0.043, and its boiling point is lower than that of water and IPA; therefore, it is removed in the ether column before separation of IPA and water. DIPE leaves the process from the top of the ether column, while the IPA and water mixture is collected from the bottom and fed to the extractive distillation (ED) column. As mentioned above, IPA and water form an azeotrope; to break this azeotrope, dimethyl sulfoxide (DMSO) is introduced as the entrainer.30 After ED, IPA with a molar purity of 0.9999 is collected from the column top as the main product, whereas the bottoms stream is sent to the regenerator to recover the entrainer. DMSO is concentrated to 0.99999 (mole fraction) in the bottoms of the regenerator.

Master Property Table:

Objects	Propylene feed	Propylene recycle	Water feed	Water recycle	Propane purge	DIPE purge	Isopropanol	DMSO recycle
Temperature[°C]	-49	13	25	104	26.1322	81.5162	80	197
Pressure[kPa]	101.325	850	101.325	120	954.3	120	105	125
mass flow[kg/hr]	16872.2	3664	11785	61734	970.79	1270	21236.	3600
molar flow[kmol/hr]	400	87	654.2	3476	20.9804	18.2	347	46
Volumetric flow[m^3/hr]	27.45	6.95	11	64.65	1.94726	448	29.47	3.93
Molar fraction/propylen	0.95	0.99	0	0	$2.03e^{-06}$	0.000374974	0	0
Molar fraction/propane	0.05	0.0027	0	$6.64e^{-23}$	0.95708	0.000524874	$7.79e^{-22}$	$3.69e^{-21}$
Molar fraction/Iso propanol	0	0	0	$6.87e^{-05}$	0.00058	0.7702	0.97	$6.960e^{-14}$
Molar fraction/DIPE	0	0	0	$7.81e^{-21}$	0.0388574	0.227146	0.025	$6.96e^{-14}$
Molar fraction/water	0	0	1	0.999	0.00346976	0.00168568	$4.30e^{-07}$	0.0001
Molar fraction/Dimethyl sulfoxide	0	0	0	0	0	0	$1.04e^{-08}$	0.999

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