Kirk-Othmer Encyclopedia of Chemical Technology.

ISOPROPYL ALCOHOL

Isopropyl alcohol [67-63-0], also known as isopropanol, 2-propanol, dimethylcarbinol, and *sec*-propyl alcohol, is a colorless, volatile, and flammable liquid, having a molecular weight of 60.09 and a slight odor resembling a mixture of ethyl alcohol [64-17-5] and acetone [67-64-1]. Isopropyl, the lowest member of the class of secondary alcohols, is generally known as the first petrochemical. Of the lower (C_1–C_5) alcohols, isopropyl alcohol is third in commercial production, behind methanol (qv) and ethyl alcohol. The 1993, U.S. production was 5.4×10^5 metric tons (1). Production of isopropyl alcohol has been declining at an average annual rate of 3% since 1980, mostly because of the declining use of isopropyl alcohol as an acetone (qv) feedstock. An estimated 50% of isopropyl alcohol was used in solvent applications in 1992 (see Solvents, industrial). Isopropyl alcohol is used for the manufacture of agricultural chemicals, pharmaceuticals (qv), process catalysts, and solvents. Properties, preparation, and uses of isopropyl alcohol have been discussed (2).

1. Physical Properties

Physical properties of isopropyl alcohol are characteristic of polar compounds because of the presence of the polar hydroxyl, –OH, group. Isopropyl alcohol is completely miscible in water and readily soluble in a number of common organic solvents such as acids, esters, and ketones. It has solubility properties similar to those of ethyl alcohol (qv). There is a competition between these two products for many solvent applications. Isopropyl alcohol has a slight, pleasant odor resembling a mixture of ethyl alcohol and acetone, but unlike ethyl alcohol, isopropyl alcohol has a bitter, unpotable taste.

Physical and chemical properties of isopropyl alcohol reflect its secondary hydroxyl functionality. For example, its boiling and flash points are lower than *n*-propyl alcohol [71-23-8], whereas its vapor pressure and freezing point are significantly higher. Isopropyl alcohol boils only 4°C higher than ethyl alcohol.

Anhydous and 91 vol % alcohol, the two main grades of isopropyl alcohol marketed in the United States, differ mainly in water content. The latter represents the azeotrope with water and is usually referred to as constant boiling mixture (CBM) isopropyl alcohol. A listing of some important physical constants of anhydrous and CBM isopropyl alcohol is given in Table 1. Because of its tendency to associate in solution, isopropyl alcohol forms azeotropes with compounds from a variety of classes, including hydrocarbons, esters, halocarbons, amines, ketones (qv), and aromatics. Examples of some binary azeotropes are given in Table 2. Isopropyl alcohol does not form binary azeotropes with acetone, ethyl alcohol, ethylbenzene [100-41-4], hexylamine [111-26-2], or methyl isobutyl ketone [108-10-1]. It does, however, form ternary systems with many of these and other compounds (2).

Table 1. Physical Properties of Isopropyl Alcohol[a]

Property	Anhydrous	91 Vol %
molecular weight	60.10	
boiling point, at 101.3 kPa[b], °C	82.3	80.4
freezing point, °C	−88.5	−50.0
specific gravity, 20/20	0.7864	0.8183
density, at 20°C, g/cm^3	0.7854	0.8173
surface tension, at 20°C, mN/m(= dyn/cm)	21.32	21.40[c]
specific heat, liquid at 20°C, J/(kg·K)[d]	2510.4	
refractive index, $n^{20}{}_{\mathrm{D}}$	1.3772	1.3769
heat of combustion, at 25°C, kJ/mol[d]	2005.8	
latent heat of vaporization, at 101.3 kPa[b], kJ/mol[d]	39.8	
vapor pressure, at 20°C, kPa[b]	4.4	4.5
critical temperature, °C	235.2	
critical pressure, at 20°C, kPa[b]	4764	
viscosity, mPa·s(= cP)		
at 0°C	4.6	
20°C	2.4	2.1[c]
40°C	1.4	
coefficient of expansion[e]	$V_t = V_0[1 + (1.0743 \times 10^{-3})t + (3.28 \times 10^{-7})t^2]$	
flammability limit in air, vol %[f]		
lower	2.5	
upper	12	
flash point, °C		
Tag open cup	17.2	21.7
closed cup	11.7	18.3
autoignition temperature, °C[g]	399	

[a] Refs. (3–5), except where noted.
[b] To convert kPa to mm Hg, multiply by 7.50.
[c] At 25°C.
[d] To convert J to cal, divide by 4.184.
[e] Ref. 6; t in °C.
[f] Ref. 7.
[g] Ref. 8.

Table 2. Azeotropes of Isopropyl Alcohol[a]

Component	CAS Registry Number	Bp[b], °C	Azeotrope bp[b], °C	Isopropyl alcohol composition, wt %
water		100	80.3	87.4
			120.5[c]	88.3
toluene	[108-88-3]	110.6	80.6	69
methyl propionate	[554-12-1]	79.6	77	28
methyl ethyl ketone	[78-93-3]	79.6	77.9	32
ethyl acetate	[141-78-6]	77.05	75.9	25
2-chlorobutane	[78-86-4]	68.25	64	18
hexane	[110-54-3]	68.9	62.7	23
cyclohexane	[110-82-7]	80.8	68.6	33
butylamine	[109-73-9]	77.8	84.7	60
diisopropyl ether	[108-20-3]	69	66.2	16.3

[a] Ref. 9.
[b] Determined at 101.3 kPa (1 atm), except where noted.
[c] At 411.5 kPa (4.06 atm).

2. Chemical Properties

Chemical properties of isopropyl alcohol are determined by its functional hydroxyl group in the secondary position. Except for the production of acetone, most isopropyl alcohol chemistry involves the introduction of the isopropyl or isopropoxy group into other organic molecules by the breaking of the C–OH or the O–H bond in the isopropyl alcohol molecule.

Isopropyl alcohol undergoes reactions typical of an active secondary alcohol. It can be dehydrogenated, oxidized, esterified, etherified, aminated, halogenated, or otherwise modified at the OH moiety more readily than primary alcohols such as *n*-propyl or ethyl alcohol. Manufacture of the commercially important aluminum isopropoxide [555-31-7] and isopropyl halides illustrates this reactivity. The aluminum isopropoxide reaction involves the aluminum replacement of the hydroxyl hydrogen atom and concomitant hydrogen evolution; the isopropyl halides reaction involves hydroxyl group displacement. Aluminum isopropoxide is produced in quantitative yield by refluxing isopropyl alcohol with aluminum turnings (10, 11).

$$6\ (\mathrm{CH_3})_2\,\mathrm{CHOH} + 2\ \mathrm{Al}^0 \longrightarrow 2\ ((\mathrm{CH_3})_2\,\mathrm{CHO})_3\,\mathrm{Al} + 3\ \mathrm{H_2}$$

Catalytic amounts of mercuric chloride are usually employed in this preparation. Aluminum isopropoxide is a useful Meerwein-Ponndorf-Verley reducing agent in certain ester-exchange reactions and is a precursor for aluminum glycinate, a buffering agent (see Alkoxides, metal).

Displacement of the hydroxyl group is exemplified by the production of isopropyl halides, eg, isopropyl bromide [75-26-3], by refluxing isopropyl alcohol with a halogen acid, eg, hydrobromic acid [10035-10-6] (12).

$$(\mathrm{CH_3})_2\,\mathrm{CHOH} + \mathrm{HBr} \longrightarrow (\mathrm{CH_3})_2\,\mathrm{CHBr} + \mathrm{H_2O}$$

The order of reactivity with acid is $\mathrm{HI} > \mathrm{HBr} > \mathrm{HCl}$. Reaction with hydrochloric acid [7647-01-0] to form isopropyl chloride [75-29-6] is facilitated by a zinc chloride catalyst.

2.1. Dehydrogenation

Before the large-scale availability of acetone as a co-product of phenol (qv) in some processes, dehydrogenation of isopropyl alcohol to acetone (qv) was the most widely practiced production method. A wide variety of catalysts can be used in this endothermic (66.5 kJ/mol (15.9 kcal/mol) at 327°C), vapor-phase process to achieve high (75–95 mol %) conversions. Operation at 300–500°C and moderate pressures (207 kPa (2.04 atm)) provides acetone in yields up to 90 mol %. The most useful catalysts contain Cu, Cr, Zn, and Ni, either alone, as oxides, or in combinations on inert supports (see Catalysts, supported) (13–16).

$$(\mathrm{CH_3})_2\,\mathrm{CHOH} \xrightarrow[\mathrm{ZnO\ catalyst}]{380^\circ\mathrm{C},100-200\ \mathrm{kPa}(1-2\ \mathrm{atm})} \mathrm{CH_3COCH_3} + \mathrm{H_2}$$

Although the selectivity is high, minor amounts of by-products can form by dehydration, condensation, and oxidation, eg, propylene [115-07-1], diisopropyl ether, mesityl oxide [141-79-7], acetaldehyde [75-07-0], and propionaldehyde [123-38-6]. Hydrotalcites having different Al/(Al + Mg) ratios have been used to describe a complete reaction network for dehydrogenation (17). This reaction can also be carried out in the liquid phase.

Dehydrogenation processes for acetone, methyl isobutyl ketone [108-10-1], and higher ketones (qv) utilizing, in one process, a copper-based catalyst have been disclosed (18, 19). Dehydrogenation reaction is used to study the acid–base character of catalytic sites on a series of oxides (20, 21).

2.2. Oxidation

Isopropyl alcohol can be catalytically oxidized using air or oxygen at high temperatures to give acetone and water.

$$(CH_3)_2\,CHOH + 0.5O_2 \xrightarrow[\text{catalyst}]{400\text{–}600^{\circ}C} CH_3COCH_3 + H_2O$$

The catalysts are of the same general type as those used for dehydrogenation processes. In contrast to dehydrogenation, oxidation is highly exothermic (180 kJ/mol (43 kcal/mol) at 295°C). Therefore, careful control of processing conditions is critical in order to minimize the formation of by-products, especially those of dehydration (22, 23). It is possible to run this oxidation and the dehydrogenation reactions simultaneously by proper choice of catalysts and conditions. Use of this technology for conversion of isopropyl alcohol to acetone is minimal compared to the dehydrogenation route.

Isopropyl alcohol can be partially oxidized by a noncatalytic, liquid-phase process at low temperatures and pressure to produce hydrogen peroxide [7722-84-1] and acetone (24–26).

$$(CH_3)_2\,CHOH + O_2 \xrightarrow[\text{253 kPa (2.5 atm)}]{\text{peroxide } 90\text{–}140^{\circ}C} CH_3COCH_3 + H_2O_2$$

Oxygen or air can be used with a peroxide initiator, eg, hydrogen peroxide (qv). The oxidation rate is sensitive to the quantity of by-product acetic acid [64-19-7] generated. The theoretical yield ratio of acetone to hydrogen peroxide produced is 1.7 by weight. This process is normally employed when hydrogen peroxide is desired, in which case acetone and unreacted isopropyl alcohol are recycled. The process is used by Shell, in which hydrogen peroxide is used for oxidation of allyl alcohol [107-18-6] to acrolein [107-02-8], and by Burmah Oil Company, in which hydrogen peroxide is converted to peracetic acid (26, 27).

Isopropyl alcohol can be oxidized by reaction of an α,β-unsaturated aldehyde or ketone at high temperature over metal oxide catalysts (28). In one Shell process for the manufacture of allyl alcohol, a vapor mixture of isopropyl alcohol and acrolein, which contains two to three moles of alcohol per mole of aldehyde, is passed over a bed of uncalcined magnesium oxide [1309-48-4] and zinc oxide [1314-13-2] at 400°C. The process yields about 77% allyl alcohol based on acrolein.

$$(CH_3)_2\,CHOH + CH_2{=}CHCHO \longrightarrow CH_3COCH_3 + CH_2{=}CHCH_2OH$$

2.3. Esterification

Isopropyl alcohol is esterified readily by treatment of carboxylic acids in the presence of an acidic catalyst, eg, *p*-toluenesulfonic acid [619252-5]. An equilibrium is established in the reaction typically carried out at 100–160°C and atmospheric pressure, using an excess of alcohol.

$$RCOOH + (CH_3)_2\,CHOH \rightleftarrows {}^{acid}RCOOCH\,(CH_3)_2 + H_2O$$

Energy is supplied to remove the water as an azeotrope, thus forcing the reaction in the desired direction. Excess alcohol is distilled and recycled, and yields of ester are nearly quantitative. For example, isopropyl acetate [108-21-4] can be prepared by the reaction of isopropyl alcohol and acetic acid in the presence of sulfuric acid catalyst and using toluene as the azeotroping agent. The kinetics of the esterification of isopropyl alcohol with some organic acids by sulfonated cation-exchange resins have been reported (29). Esterification of isopropyl alcohol with myristic acid [544-63-8] forms isopropyl myristate [110-27-0], an emollient and lubricant in various cosmetic products and topical medicinals (11, 30) (see Cosmetics). A jellied product is marketed as Estergel (30).

Xanthate esters are prepared by reaction of isopropyl alcohol and carbon disulfide [75-15-0]. Isopropyl xanthates have wide use in mineral flotation (qv) processes, and sodium isopropyl xanthate [140-93-2], $C_4H_7OS_2Na$, is a useful herbicide for bean and pea fields (see Herbicides) (30).

Phosphite esters are formed readily by the reaction of phosphorus halides and isopropyl alcohol. For example, triisopropyl phosphite [116-17-6] is prepared from phosphorus trichloride [7719-12-2] and isopropyl alcohol at low temperatures in the presence of an acid scavenger, eg, pyridine [110-86-1].

$$3\ (\mathrm{CH_3})_2\,\mathrm{CHOH} + \mathrm{PCl_3} \longrightarrow ((\mathrm{CH_3})_2\,\mathrm{CHO})_3\,\mathrm{P} + 3\ \mathrm{HCl}$$

Similarly, another important esterification reaction of isopropyl alcohol involves the production of tetraisopropyl titanate [546-68-9], a commercial polymerization catalyst, from titanium tetrachloride [7550-45-0] and isopropyl alcohol.

Isopropyl nitrate [1712-64-7] can be prepared by the reaction of isopropyl alcohol with nitric acid [52583-42-3].

$$(\mathrm{CH_3})_2\,\mathrm{CHOH} + \mathrm{HNO_3} \longrightarrow (\mathrm{CH_3})_2\,\mathrm{CHONO_2} + \mathrm{H_2O}$$

The reactants are fed separately into a still, from which the product is continuously removed by distillation (qv) (31). Isopropyl nitrate is a valuable engine-starter fuel and can be used in explosives (see Explosives and propellants) (32). The nitrite ester, isopropyl nitrite, can be prepared from the reaction of isopropyl alcohol and either nitrosyl chloride or nitrous acid at ambient temperature (33). The ester is used as a jet engine propellant (30).

2.4. Etherification

Isopropyl alcohol can be dehydrated in either the liquid phase over acidic catalysts, eg, sulfuric acid, or in the vapor phase over acidic aluminas to give diisopropyl ether (DIPE) and propylene(qv).

$$(\mathrm{CH_3})_2\,\mathrm{CHOH} \longrightarrow \mathrm{CH_3CH{=}CH_2} + \mathrm{H_2O}$$

$$2\ (\mathrm{CH_3})_2\,\mathrm{CHOH} \longrightarrow ((\mathrm{CH_3})_2\,\mathrm{CH})_2\,\mathrm{O} + \mathrm{H_2O}$$

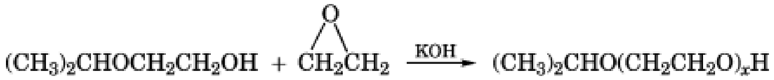
Either product can be favored over the other by proper selection of catalyst and reaction conditions. However, the principal source of DIPE is as a by-product from isopropyl alcohol production. Typically, excess DIPE is recycled over acidic catalysts in the alcohol process where it is hydrated to isopropyl alcohol. DIPE is used to a minor extent in industrial extraction and as a solvent.

The 1990 Clean Air Act mandates for blended oxygenates in gasoline created a potentially large new use for DIPE as a fuel oxygenate. Isopropyl alcohol can react with propylene over acidic ion-exchange (qv) catalysts at low temperatures, which favor high equilibrium conversions per pass to produce DIPE (34).

Glycol ethers can be prepared from isopropyl alcohol by reaction of olefin oxides, eg, ethylene oxide [75-21-8] (qv) or propylene oxide [75-56-9](qv). Reactions such as that to produce 2-isoproxyethanol [109-59-1] (isopropyl Cellosolve) are generally catalyzed by an alkali hydroxide.

$$(\mathrm{CH_3})_2\mathrm{CHOH} + \overset{\mathrm{O}}{\mathrm{CH_2CH_2}} \xrightarrow{\mathrm{KOH}} (\mathrm{CH_3})_2\mathrm{CHOCH_2CH_2OH}$$

Higher alkoxylated products, ie, oligomers, are formed by secondary reaction of oxide and the hydroxy group of the previous product.



$$(CH_3)_2CHOCH_2CH_2OH + \overset{O}{CH_2CH_2} \xrightarrow{KOH} (CH_3)_2CHO(CH_2CH_2O)_xH$$

This is a particularly troublesome competing reaction when the olefin oxide, eg, ethylene oxide, produces the more reactive terminal primary hydroxy group. Glycol ethers are used as solvents in lacquers, enamels, and waterborne coatings to improve gloss and flow.

2.5. Amination

Isopropyl alcohol can be aminated by either ammonolysis in the presence of dehydration catalysts or reductive ammonolysis using hydrogenation catalysts. Either method produces two amines: isopropylamine [75-31-0] and diisopropylamine [108-18-9]. Virtually no trisubstituted amine, ie, triisopropylamine [122-20-3], is produced. The ratio of mono- to diisopropylamine produced depends on the molar ratio of isopropyl alcohol and ammonia [7664-41-7] employed. Molar ratios of ammonia and hydrogen to alcohol range from 2:1–5:1 (35, 36).

$$(CH_3)_2\,CHOH + NH_3 \xrightarrow[\Delta,\ \text{pressure}]{\text{catalyst}} (CH_3)_2\,CHNH_2 + H_2O$$

$$(CH_3)_2\,CHOH + (CH_3)_2\,CHNH_2 \xrightarrow[\Delta,\ \text{pressure}]{\text{catalyst}} \left[(CH_3)_2\,CH\right]_2 NH + H_2O$$

In the reductive ammonolysis process, there is virtually no consumption of added hydrogen, which is used to increase catalyst life by inhibiting coking and tar formation. In this reaction, a gaseous mixture of the alcohol, ammonia, and hydrogen is fed to a fixed-bed reactor that contains a dehydrogenation catalyst, eg, Cu, Cr, or Ni, supported on alumina. Operating conditions are 150–250°C and 790–2860 kPa (100–400 psig) (35–40). The liquid hourly space velocity (LHSV) of isopropyl alcohol is about 0.5/h. Isopropyl alcohol conversions per pass are in excess of 85% and yields are $>90\%$. By-products, eg, nitrile (from dehydrogenation of the amine) and amide (from hydrolysis of the nitrile) are produced, but these are recycled to increase productivity.

Direct ammonolysis involving dehydration catalysts is generally run at higher temperatures (300–500°C) and at about the same pressure as reductive ammonolysis. Many catalysts are active, including aluminas, silica, titanium dioxide [13463-67-7], and aluminum phosphate [7784-30-7] (41–43). Yields are acceptable ($>80\%$), and coking and nitrile formation are negligible. However, little control is possible over the composition of the mixture of primary and secondary amines that can be obtained.

Isopropylamine is the most widely used of the propylamines. Most of it is consumed in herbicide manufacture, primarily in production of 2-chloro-4-ethyl-6-isopropylamino-*sym*-triazine. A smaller quantity is used for pesticide manufacture (40, 44). Diisopropylamine is used chiefly in pesticides (qv) and as a corrosion inhibitor, eg, diisopropylammonium nitrate (see Corrosion and corrosion control) (44, 45).

2.6. Halogenation

Normally, 2-halopropane derivatives are prepared from isopropyl alcohol most economically by reaction with the corresponding acid halide. However, under appropriate conditions, other reagents, eg, phosphorus halides and elemental halogen, also react by replacement of the hydroxyl group to give the halide (46).

$$3\ (CH_3)_2\,CHOH + PBr_3 \longrightarrow 3\ (CH_3)_2\,CHBr + H_3PO_3$$

Halogenation of isopropyl alcohol in aqueous solution results in concomitant oxidation. Thus, chlorination at 65°C produces a mixture of chloroacetone derivatives, chiefly 1,3-dichloroacetone [534-07-6] and 1,1,3-trichloroacetone [921-03-9] (47, 48). Further chlorination at 70–100°C provides nearly complete conversion of lower chloroacetones into 1,1,1,3,3-pentachloroacetone [1768-31-6] and hexachloroacetone [116-16-5] (48–52). Chlorination of isopropyl alcohol reportedly can be conducted to give 1,1,1,3-tetrachloroacetone [16995-35-0], which is converted to 1,1,1-trichloro-2,3-epoxypropane [3083-23-6], a useful intermediate for synthesis of agricultural and pharmaceutical chemicals and for the preparation of plastics having low flammability (53, 54). However, commercial processes to chloroacetones are believed to be based on chlorination of acetone rather than isopropyl alcohol, because of undesired by-products produced in the latter route. In addition to use as chemical intermediates, chloroacetones have excellent solvent properties, especially for plastics. However, toxicity may limit use.

Halogenated 2-propanol derivatives, eg, 1,3-dichloro-2-propanol [96-23-1], are generally prepared from glycerol [56-81-5] (qv). These materials are used in the preparation of halogen-containing phosphates to plasticize and lower the flammability of plastics, eg, polyurethanes and cellulosics.

2.7. Miscellaneous Reactions

Reactions of potential commercial significance include acylation by ketene [463-51-4]:

$$(CH_3)_2\,CHOH + CH_2{=}C{=}O \longrightarrow CH_3COOCH\,(CH_3)_2$$

and the Ritter reaction to prepare *N*-isopropylacrylamide [2210-25-5] from acrylonitrile [107-13-1] and isopropyl alcohol:

$$CH_2{=}CHCN + (CH_3)_2\,CHOH \longrightarrow CH_2{=}CHCONHCH\,(CH_3)_2$$

3. Manufacture

The first industrial quantities of isopropyl alcohol were produced in 1920 in the world's first petrochemical plant, owned by Standard Oil (Exxon) Company (Bayway, New Jersey). This was followed in 1921, by the start-up of isopropyl alcohol production in Clendenin, West Virginia, by the Carbide and Carbon Chemicals (Union Carbide) Corporation. The Shell Oil Company began production in the 1930s at Dominguez, California (55). These three companies are the principal domestic manufacturers as of the mid-1990s.

The indirect hydration, also called the sulfuric acid process, practiced by the three U.S. domestic producers, was the only process used worldwide until ICI started up the first commercial direct hydration process in 1951. Both processes use propylene and water as raw materials. Early problems of high corrosion, high energy costs, and air pollution using the indirect process led to the development of the direct hydration process in Europe. However, a high purity propylene feedstock is required. In the indirect hydration process, C_3-feedstock streams from refinery off-gases containing only 40–60 wt % propylene are often used in the United States.

Other potential synthetic methods include fermentation (qv) of certain carbohydrates (qv), oxidation of propane, hydrogenation of acetone, and hydrolysis of isopropyl acetate. The hydrogenation of by-product acetone is the only method practiced commercially.

3.1. Indirect Hydration

Indirect hydration is based on a two-step reaction of propylene and sulfuric acid. In the first step, mixed sulfate esters, primarily isopropyl hydrogen sulfate, but also diisopropyl sulfate, form. These are then hydrolyzed, forming the alcohol and sulfuric acid.

Step 1. Esterification:

$$CH_3CH{=}CH_2 + H_2SO_4 \rightleftarrows (CH_3)_2\,CHOSO_3H$$

$$(CH_3)_2\,CHOSO_3H + CH_3CH{=}CH_2 \rightleftarrows ((CH_3)_2\,CHO)_2\,SO_2$$

Step 2. Hydrolysis:

$$(CH_3)_2\,CHOSO_3H + H_2O \rightleftarrows (CH_3)_2\,CHOH + H_2SO_4$$

$$((CH_3)_2\,CHO)_2\,SO_2 + 2\ H_2O \rightleftarrows 2\ (CH_3)_2\,CHOH + H_2SO_4$$

3.1.1. By-Products

Diisopropyl ether is the principal by-product formed by reaction of the intermediate sulfate esters with isopropyl alcohol.

$$(CH_3)_2\,CHOSO_3H + (CH_3)_2\,CHOH \rightleftarrows ((CH_3)_2\,CH)_2\,O + H_2SO_4$$

$$((CH_3)_2\,CHO)_2\,SO_2 + (CH_3)_2\,CHOH \rightleftarrows (CH_3)_2\,CHOSO_3H + ((CH_3)_2\,CH)_2\,O$$

The principal reactions are reversible and a mixture of products and reactants is found in the crude sulfate. High propylene pressure, high sulfuric acid concentration, and low temperature shift the reaction toward diisopropyl sulfate. However, the reaction rate slows as products are formed, and practical reactors operate by using excess sulfuric acid. As the water content in the sulfuric acid feed is increased, more of the hydrolysis reaction (Step 2) occurs in the main reactor. At water concentrations near 20%, diisopropyl sulfate is not found in the reaction mixture. However, efforts to separate the isopropyl alcohol from the sulfuric acid suggest that it may be partially present in an ionic form (56, 57).

$$(CH_3)_2\,CHOH + H_2SO_4 \rightleftarrows (CH_3)_2\,CHOH^{+}{}_2 + HSO_3^-$$

Other by-products include acetone, carbonaceous material, and polymers of propylene. Minor contaminants arise from impurities in the feed. Ethylene and butylenes can form traces of ethyl alcohol and 2-butanol. Small amounts of *n*-propyl alcohol carried through into the refined isopropyl alcohol can originate from cyclopropane [75-19-4] in the propylene feed. Acetone, an oxidation product, also forms from thermal decomposition of the intermediate sulfate esters, eg,

$$(CH_3)_2\,CHOSO_3H \xrightarrow{\text{heat}} CH_3COCH_3 + SO_2 + H_2O$$

In addition to generating malodorous sulfur dioxide [7446-09-5], the acetone formed can undergo further condensation in the acidic medium to generate mesityl oxide [141-79-7], $(CH_3)_2C{=}CHCOCH_3$, and higher products.

High propylene concentrations in the presence of acids can form dimers, trimers, and higher homologues, which can polymerize or hydrate to C_6, C_9, or higher alcohols, and olefins. These derivatives can emit musty, woody, and camphoraceous odors, and their reaction products with sulfur-containing compounds can give a cat-like odor to the product (58). Odor can be improved by employing appropriate reaction conditions and by contacting isopropyl alcohol with various metals, eg, copper and nickel, or certain partially reduced metal oxides (59, 60).

3.1.2. Process

A typical indirect hydration process is presented in Figure 1. In the process, propylene reacts with sulfuric acid ($>$60 wt%) in agitated reactors or absorbers at moderate (0.7–2.8 MPa (100–400 psig)) pressure. The isopropyl sulfate esters form and are maintained in the liquid state at 20–80°C. Low propylene concentrations, ie, 50 wt %, can be tolerated, but concentrations of 65 wt % or higher are preferred to achieve high alcohol yields. Because the reaction is exothermic, internal cooling coils or external heat exchangers are used to control the temperature.

There are two general operational modes for conducting the reaction. In the two-step strong acid process, separate reactors are used for the propylene absorption and sulfate ester hydrolysis stages. The reaction occurs at high sulfuric acid concentration ($>$80 wt%), at 1–1.2 MPa (130–160 psig) pressure, and low (eg, 20–30°C) temperature. The weak acid process is conducted in a single stage at low acid (60–80 wt %) concentration and at higher (2.5 MPa (350 psig)) pressure and (60–65°C) temperature. Chemical selectivity to isopropyl alcohol and diisopropyl ether are above 98% for each process.

The sulfate ester hydrolysate is stripped to give a mixture of isopropyl alcohol, isopropyl ether, and water overhead, and dilute sulfuric acid bottoms. The overhead is neutralized using sodium hydroxide and refined in a two-column distillation system. Diisopropyl ether is taken overhead in the first, ie, ether, column. This stream is generally recycled to the reactors to produce additional isopropyl alcohol by the following equilibrium reaction:

$$((CH_3)_2CH)_2O + H_2SO_4 \rightleftharpoons (CH_3)_2CHOSO_3H + (CH_3)_2CHOH$$

Wet isopropyl alcohol (87 wt % and 91 vol %) is taken overhead in the second still. More than 93% of the charged propylene is converted to isopropyl alcohol in this system. If available, a propylene column may recover unreacted feedstock.

The bottoms from the stripper (40–60 wt % acid) are sent to an acid reconcentration unit for upgrading to the proper acid strength and recycling to the reactor. Because of the associated high energy requirements, reconcentration of the diluted sulfuric acid is a costly operation. However, a propylene gas stripping process, which utilizes only a small amount of added water for hydrolysis, has been described (63). In this modification, the equilibrium quantity of isopropyl alcohol is stripped so that acid is recycled without reconcentration. Equilibrium is attained rapidly at 50°C and isopropyl alcohol is removed from the hydrolysis mixture. Similarly, the weak sulfuric acid process minimizes the reconcentration of the acid and its associated corrosion and pollution problems.

The 91 vol % alcohol is sold as such or is dehydrated by azeotropic distillation using either diisopropyl ether or cyclohexane to produce an anhydrous product (see Table 2) (see Distillation, azeotropic and extractive) (64). Wet isopropyl alcohol is fed at about the center of a dehydrating column, and the azeotroping agent is fed near the top. As the ternary azeotrope forms, it is taken overhead, condensed, and the layers are separated. The upper layer, which is mainly azeotroping agent and alcohol, is returned to the top of the column as reflux. Anhydrous isopropyl alcohol is removed from the base of the column. The lower layer is mostly water. It is fed

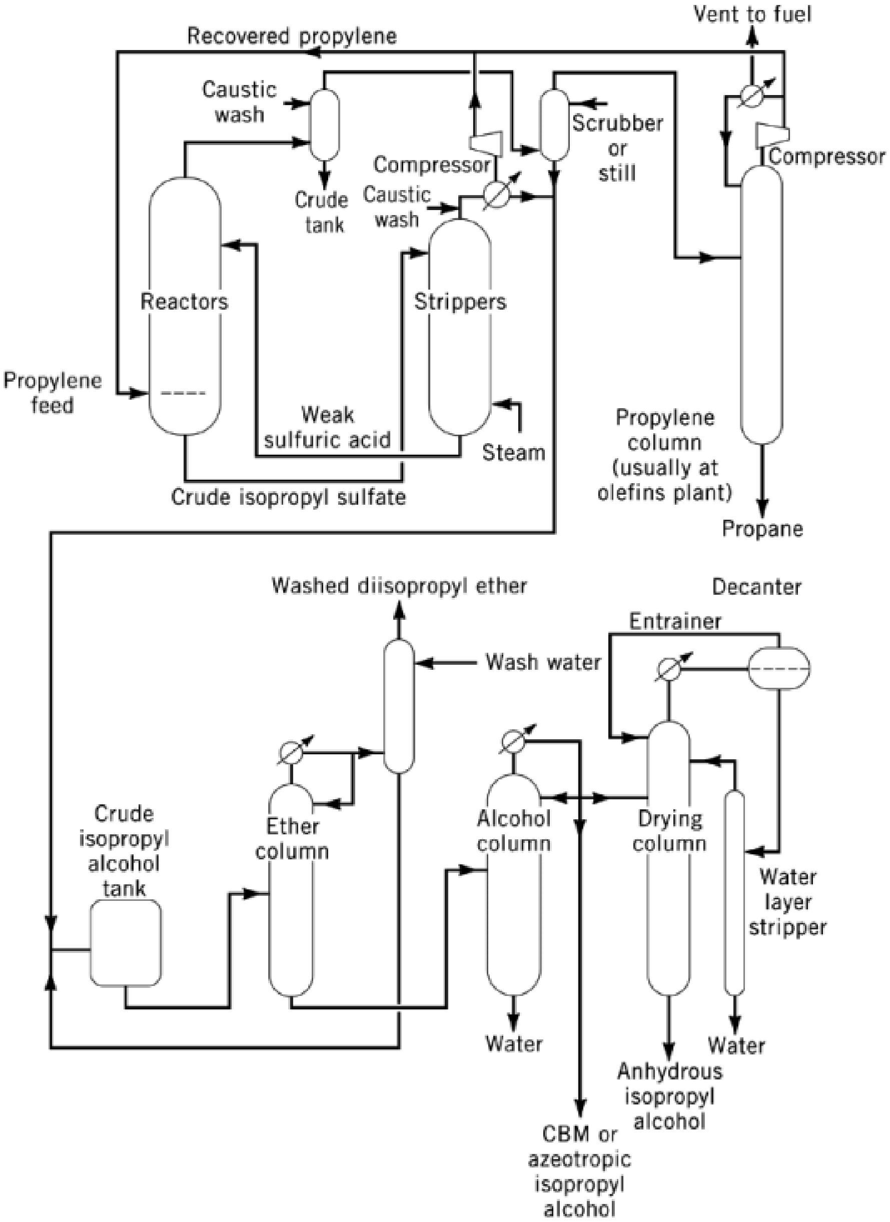


Fig. 1. Indirect hydration process for the manufacture of isopropyl alcohol; CBM=constant boiling mixture (61, 62).

to a stripping column for recovery of isopropyl alcohol and azeotroping agent. A purge may be taken to remove by-products such as acetone.

Acid corrosion presents a problem in isopropyl alcohol factories. Steel (qv) is a satisfactory material of construction for tanks, lines, and columns where concentrated (>65 wt%) acid and moderate ($<60°C$) temperatures are employed. For dilute acid and higher temperatures, however, stainless steel, tantalum, Hastelloy, and the like are required for corrosion resistance and to ensure product purity (65).

The extent of purification depends on the use requirements. Generally, either intense aqueous extractive distillation, or post-treatment by fixed-bed absorption (qv) using activated carbon, molecular sieves (qv), and certain metals on carriers, is employed to improve odor and to remove minor impurities. Essence grade is produced by final distillation in nonferrous, eg, copper, equipment (66).

Manufacturing plants in the United States are believed to use solely indirect propylene hydration. Several European companies, eg, British Petroleum, Shell, and Deutsche Texaco, also employ this older technology in plants in Europe and Japan (67).

3.2. Direct Hydration

The acid-catalyzed direct hydration of propylene is exothermic and resembles the preparation of ethyl alcohol from ethylene(qv).

$$CH_3CH{=}CH_2 + H_2O \xrightleftharpoons{} {}^{\text{catalyst}} (CH_3)_2\,CHOH \qquad \Delta H = -50\ \text{kJ/mol}\ (-12\ \text{kcal/mol})$$

The equilibrium can be controlled to favor product alcohol if high pressures and low temperatures are applied. The advantage of low temperature is difficult to utilize, however, because most known catalysts require high or moderate temperatures to be effective.

3.2.1. Process

There are three basic processes in commercial operation: (*1*) vapor-phase hydration over a fixed-bed catalyst of supported phosphoric acid (Veba-Chemie) (68–71), or silica-supported tungsten oxide with zinc oxide promoter (ICI) (66, 67, 72); (*2*) mixed vapor–liquid-phase hydration at low (150°C) temperature and high (10.13 MPa (100 atm)) pressure using a strongly acidic cation-exchange resin catalyst (Deutsche Texaco AG) (73–77); and (*3*) liquid-phase hydration at high (270°C) temperature and high (20.3 MPa (200 atm)) pressure in the presence of a soluble tungsten catalyst (Tokuyama Soda) (78–80).

A typical process scheme for the direct hydration of propylene is shown in Figure 2. Turnkey plants based on this technology are available (71, 81). The principal difference between the direct and indirect processes is the much higher pressures needed to react propylene directly with water. Products and by-products are also similar, and refining systems are essentially the same. Under some conditions, the high pressures of the direct process can increase the production of propylene polymers.

The first direct hydration plant (ICI, 1951) used a WO_3–ZnO catalyst supported on SiO_2, high (230–290°C) temperature, and high (20.3–25.3 MPa (200–250 atm)) pressure. Similarly, in the Veba-Chemie process (see Fig. 2), a vaporized stream of propylene and water is passed through an acidic catalyst bed (H_3PO_4 supported on SiO_2) at 240–260°C and 2.5–6.6 MPa (25–65 atm) (69). The gas stream from the reactor is cooled and fed to a scrubber where the remaining isopropyl alcohol is removed. Isopropyl alcohol selectivity is ca 96% for the gas-phase process. Owing to equilibrium limitations in the gas phase at high temperature and low pressure, a low propylene conversion (5–6%) results and thus a large amount of unreacted propylene is recycled. Both processes involve high plant costs owing to high pressure requirements, gas recycles, and the requirement for high purity propylene (ca 99 wt %).

Deutsche Texaco developed a trickle-bed process to avoid the disadvantages of the gas-phase process. In the trickle-bed process, a mixture of liquid water and propylene gas in a molar ratio of 12 to 15:1 is introduced at the top of a fixed-bed reactor and allowed to trickle down over a sulfonic acid ion-exchange resin. Reaction between the liquid and gas phases takes place at 130–160°C and 8–10 MPa (80–100 atm), forming aqueous isopropyl alcohol. Propylene conversions per pass are greater than 75%, and isopropyl alcohol selectivity is 93%. Only 92 wt % propylene purity is needed for this process. Approximately 5% diisopropyl ether and some alcohols of the higher oligomers form as by-products. The life of the cation-exchange resin is at least eight months.

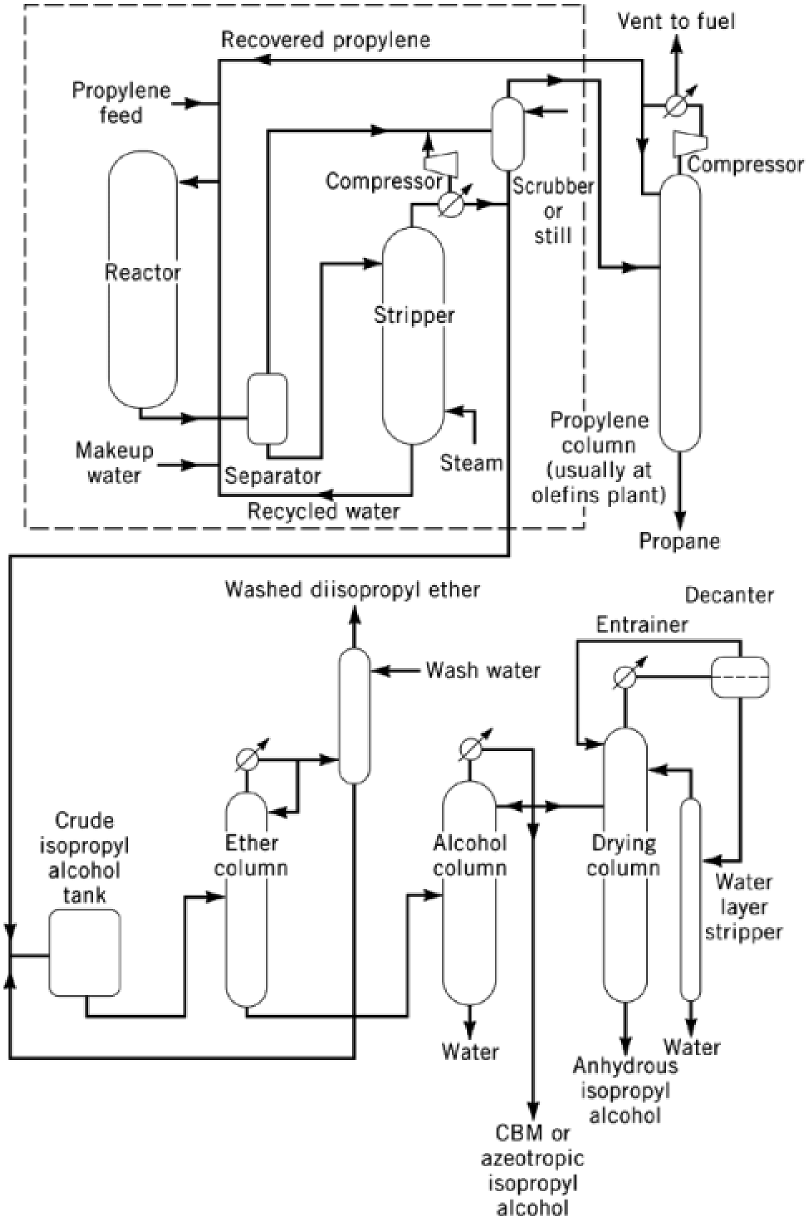


Fig. 2. Direct hydration process for the manufacture of isopropyl alcohol. The steps within the dashed box differentiate the direct from the indirect processes (see Fig. 1).

A liquid-phase variation of the direct hydration was developed by Tokuyama Soda (78). The disadvantages of the gas-phase processes are largely avoided by employing a weakly acidic aqueous catalyst solution of a silicotungstate (82). Preheated propylene, water, and recycled aqueous catalyst solution are pressurized and fed into a reaction chamber where they react in the liquid state at 270°C and 20.3 MPa (200 atm) and form aqueous isopropyl alcohol. Propylene conversions of 60–70% per pass are obtained, and selectivity to isopropyl alcohol is 98–99 mol % of converted propylene. The catalyst is recycled and requires little replenishment compared to other processes. Corrosion and environmental problems are also minimized because the catalyst is a weak acid and because the system is completely closed. On account of the low gas recycle ratio, regular commercial propylene of 95% purity can be used as feedstock.

After flashing the propylene, the aqueous solution from the separator is sent to the purification section where the catalyst is separated by azeotropic distillation; 88 wt % isopropyl alcohol is obtained overhead. The bottoms containing aqueous catalyst solution are recycled to the reactor, and the light ends are stripped of low boiling impurities, eg, diisopropyl ether and acetone. Azeotropic distillation yields dry isopropyl alcohol, and the final distillation column yields a product of more than 99.99% purity.

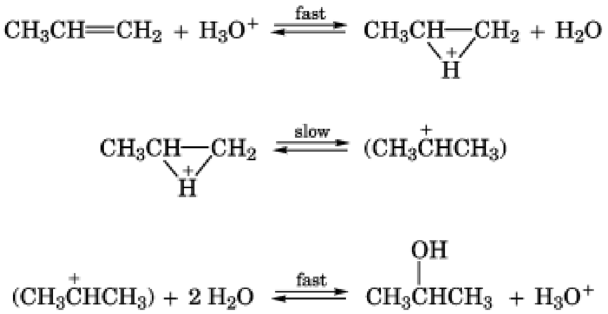
3.2.2. Catalysts

Because low temperature and high pressure favor product formation in propylene hydration, one of the earliest efforts in developing the isopropyl alcohol process technology was a search for a catalyst that maximizes alcohol productivity at low temperatures within a reasonable time. Patents issued in the early 1950s involved various tungsten compounds (83–87). Studies of acidic supports and of acids adsorbed on various porous supports were conducted at about the same time (88–99). Since that time, many other acidic materials have been claimed, including cation-exchange resins (100–105), molybdophosphoric acid [51429-74-4] (106), titanium and zinc oxides (107), tungsten and zirconium oxides (108), silicotungstates (82, 109), molybdenum oxalate [24958-46-1] (110), and zeolites (111).

Improved versions of acid ion-exchange resin catalysts have been offered by Universal Oil Products (112–114), where increased activity allowing lower temperature operation and higher equilibrium conversions per pass is claimed. When used in a variation of the Deutsche Texaco process with reduced water feed, the trickle-bed process becomes a single liquid-phase process that simplifies reactor design. By refeeding the isopropyl alcohol as shown in Figure 3, the final product is diisopropyl ether. The ether process is offered as a means of making oxygenates for reformulated gasoline.

3.2.3. Reaction Mechanism

Propylene hydration in dilute acid solution probably proceeds according to the rate-determining formation of propyl carbonium ion (115).



$$CH_3CH{=}CH_2 + H_3O^+ \xrightleftharpoons{\text{fast}} CH_3CH\overset{+}{\underset{H}{—}}CH_2 + H_2O$$

$$CH_3CH\overset{+}{\underset{H}{—}}CH_2 \xrightleftharpoons{\text{slow}} (CH_3\overset{+}{C}HCH_3)$$

$$(CH_3\overset{+}{C}HCH_3) + 2\,H_2O \xrightleftharpoons{\text{fast}} CH_3\overset{OH}{\overset{|}{C}}HCH_3 + H_3O^+$$

According to this mechanism, the reaction rate is proportional to the concentration of hydronium ion and is independent of the associated anion, ie, rate = $k[CH_3H_6][H_3O^+]$. However, the acid anion may play a marked role in hydration rate, eg, phosphomolybdate and phosphotungstate anions exhibit hydration rates two or three times that of sulfate or phosphate (78). Association of the polyacid anion with the propyl carbonium ion is suggested. Protonation of propylene occurs more readily than that of ethylene as a result of the formation of a more stable secondary carbonium ion. Thus higher conversions are achieved in propylene hydration.

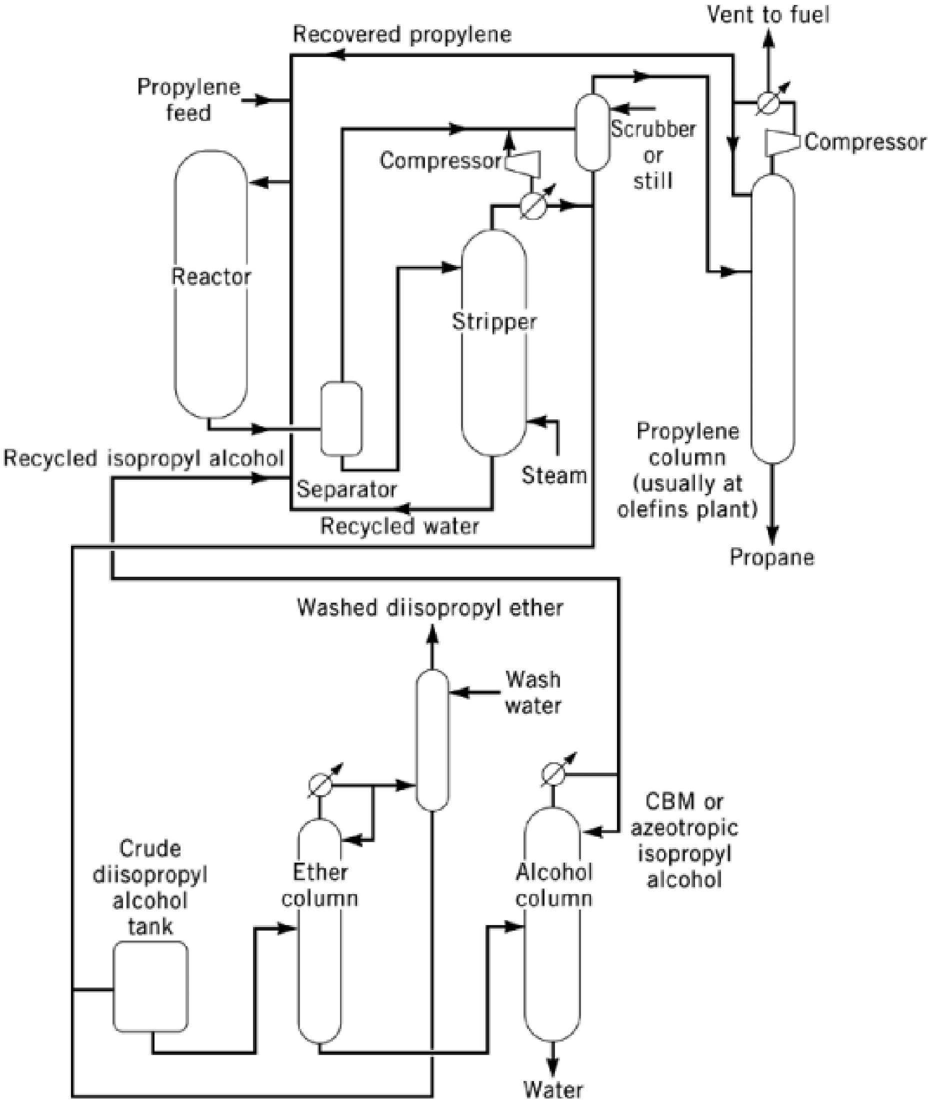


Fig. 3. Direct hydration process where the product is isolated as diisopropyl ether.

3.3. Thermochemical Data

Equilibrium considerations significantly limit alcohol yield at low pressures in the vapor-phase process (116). Consequently, conditions controlling equilibrium constants have been determined and give the following relation, where T is in K (116, 117):

$$\log K = 2624/T - 7.584$$

Table 3. Calculated Vapor–Liquid Equilibrium Composition for Propylene Hydration[a]

		Concentrations in vapor phase, mol %			
Pressure, MPa[b]	Alcohol concentration in liquid phase, mol %	Isopropyl alcohol	Water	Propylene	Isopropyl ether
		Temperature of 200°C			
10.13	3.8	17.3	23.3	54.8	4.6
20.26	5.5	24.0	18.9	48.8	8.3
30.39	6.2	28.3	18.2	43.6	9.9
40.52	6.3	31.2	18.8	37.6	12.4
50.65	5.7	35.3	19.8	31.9	13.0
		Temperature of 250°C			
10.13	1.2	7.9	49.3	42.5	0.3
20.26	2.1	13.0	37.6	48.6	0.8
30.39	2.6	14.5	36.1	48.5	0.9
40.52	3.2	15.3	36.1	47.5	1.1
50.65	3.7	15.2	37.8	45.7	1.3
		Temperature of 275°C			
10.13	0.9	3.9	69.7	26.3	0.1
20.26	1.6	8.1	52.0	39.7	0.2
30.39	2.0	9.5	49.2	41.0	0.3
40.52	2.3	9.8	48.5	41.3	0.4
50.65	2.4	9.7	51.0	38.9	0.4

[a] Ref. 116.

[b] To convert MPa to psi, multiply by 145.

Likewise, hydration in the liquid phase can be expressed by the free-energy (ΔF°) equation:

$$\Delta F^\circ = 23.25T - 9352$$

The effects of pressure and temperature on the equilibrium concentration of alcohol in both phases of hydration of propylene when both liquid and vapor phases are present have been calculated and are presented in Table 3. Low temperature reduces by-product diisopropyl ether.

3.4. Other Processes

Isopropyl alcohol can be prepared by the liquid-phase oxidation of propane (118). It is produced incidentally by the reductive condensation of acetone, and is partly recovered from fermentation (119). Large-scale commercial biological production of isopropyl alcohol from carbohydrate raw materials has also been studied (120–123).

4. Storage and Shipping

Anhydrous isopropyl alcohol is typically shipped in plain steel railroad tank cars, tank trucks, 3.8-L (1-gal) glass jugs, and 19- and 208-L (5- and 55-gal) DOT 17E phenolic-lined steel pails and drums, respectively. Plain steel is not suitable for isopropyl alcohol containing water because rusting can result. Instead, baked phenolic-lined steel tanks are used. Aluminum is also unsuitable. It is attacked by isopropyl alcohol, especially the anhydrous grade, resulting in the formation of aluminum isopropoxide. Containers must comply with DOT specifications. Tanks, piping, and equipment can be made of similar material.

The U.S. domestic shipping name of isopropyl alcohol is UN No. 1219 Isopropanol. Anhydrous as well as water solutions to 91 vol % alcohol are considered flammable liquid materials by the DOT. Both have flash points below 37.8°C by the Tag closed-cup method. Acceptable modes of transportation include air, rail, road, and water (124). For international air and water shipments, the International Maritime Organization (IMO) class is 3.2, the packaging group is II, and the primary hazard label required is "Flammable Liquid."

5. Economic Aspects

Economic comparisons of the indirect and direct hydration processes show a cost savings for use of the latter technology (79, 125). The largest savings are in capital investment, processing, and maintenance (qv), all of which are necessitated by the troublesome sulfuric acid reconcentration of the indirect process. Greater corrosion and pollution problems are also associated with indirect hydration. However, drawbacks of direct hydration are its high energy usage and the need for highly concentrated propylene feedstock. Economics of the various direct hydration processes are roughly comparable (79).

5.1. Price and Demand

In terms of production volume, isopropyl alcohol is about the fourth largest chemical produced from propylene (66). Total 1993 U.S. nameplate capacity for isopropyl alcohol production was 8.48×10^5 metric tons. The total world capacity is about 2.0×10^9 metric tons (Table 4) (126–128). The 1995 U.S. prices were $0.55/L ($2.10/gal) for refined 91 vol % and $0.62/L ($2.36/gal) for anhydrous alcohol (129), an increase from the $0.18/L ($0.70/gal) average price of 1977. The price of isopropyl alcohol is driven by the price of propylene, the primary feedstock, and by the price of ethyl alcohol, a competing solvent.

U.S. production of isopropyl alcohol declined by 3%/yr from 1983 through the mid-1990s (130). 1993 demand was 5.5×10^5 metric tons, including exports, which have been growing at a 3–5% annual rate. The biggest factor contributing to the decline in demand is the decrease in use for acetone production. Only 8% of the isopropyl alcohol produced in 1993 was used for acetone feedstock, compared to 38% in 1977. Most acetone is produced as a co-product of cumene [98-82-8] oxidation to phenol (qv).

The future demand for isopropyl alcohol is expected either to remain flat or to grow slightly. Its main use as a chemical intermediate is growing, and this should offset the pressure on use as a solvent from tighter volatile organic chemicals (VOC) regulations.

6. Specifications

Typical specifications for the two basic grades of isopropyl alcohol are shown in Table 5. Other grades that are marketed include a cosmetic grade (91 vol % and anhydrous) containing perfume, and an electronic grade of low conductivity. Other more restrictive specifications for special grades are shown in Table 6.

7. Analytical and Test Methods

Purity of commercial aqueous isopropyl alcohol mixtures is most simply determined by specific gravity measurement. However, this technique, based on the assumption that impurities are not present in significant quantities, does not provide a positive identification of isopropyl alcohol. Gas chromatography, which overcomes the disadvantages of the specific gravity method, is an excellent technique for determining isopropyl alcohol in the presence of other organic substances, eg, ethyl alcohol, methyl alcohol, and acetones (131).

Table 4. Isopropyl Alcohol Capacities

Producer	Plant location	Capacity, t × 10^3
	United States[a]	
ARCO Chemical Co.	Channelview, Tex.	30
Exxon Chemical Co.	Baton Rouge, La.	295
Shell Chemical Co.	Deer Park, Tex.	273
Union Carbide Corp.	Texas City, Tex.	250
Total		*848*
	Europe[b]	
Shell Chimie, SA	Berre-l'Etang, France	120
Hüls Aktiengesellschaft	Herne, Germany	75
RWE–DEA AG für Mineralöl und Chemie	Moers, Germany	140
Shell Nederland Chemie BV	Rotterdam-Pernis, the Netherlands	250
Industrias Quimicas Associadas, SA	Tarragona, Spain	36
BP Chemicals, Ltd.	Port Talbot, U.K.	85
Shell Chemicals U.K., Ltd.	Ellesmere Port, U.K.	105
Total		*811*
	Asia[c]	
Jinzou Petrochemical Corp.	China	60
Mitsui Toatsu Chemicals Inc.	Takaishi, Japan	33
Nippon Petrochemicals Co., Ltd.	Kawasaki, Japan	60
Tokuyama Soda Co., Ltd.	Tokuyama, Japan	38
Shell Eastern Chemicals (Pte.) Ltd.	Pulau Ular, Singapore	70
Lucky Ltd.	Yeochon, S. Korea	30
Yukong Ltd.	Ulsan, S. Korea	35
Lee Chang Yung Chemical Industry Corp.	Linyuan City, Taiwan	45
Total		*371*

[a] Ref. 126.
[b] Ref. 127.
[c] Ref. 128.

Table 5. Typical Specifications for Isopropyl Alcohol

Test	Anhydrous	Azeotropic, 91–93 vol %
isopropyl alcohol, wt %	99.8, min	85, min
acidity, wt %[a]	0.002	0.005
dilution	clear	clear
alkalinity, meq/mL	0.0001	
water, wt %	0.1, max	
nonvolatile, g/100 mL	0.0008, max	
color, Pt–Co units	5, max	10, max
odor	nonresidual	
sulfur/chlorides, ppm		3
specific gravity, 20/20	0.7861–0.7866	0.8246, max
refractive index, at 20°C	1.3763–1.3780	
appearance	no visible/settled matter	some suspended matter
distillation, °C	0.5, max[b]	
permanganate time test, minutes	45, min	
copper corrosion test	no pitting or black stain	

[a] As acetic acid.
[b] Including 82.3 ± 0.1.

Table 6. Special Specifications for Isopropyl Alcohol

Test	ACS reagent 1987	1990 USP XXII Anhydrous[a]	ASTM D770-85
isopropyl alcohol, %[b]		99.0	
acidity, meq/mL	0.0001[c]	0.00028	0.002[d]
dilution	clear		no turbidity
alkalinity, meq/g	0.0001		
water, wt %	0.2, max		0.2, max
nonvolatile, mg/100 mL	1, max	2.5, max[e]	5, max
color, Pt–Co units	10, max		10, max
odor			nonresidual
specific gravity[f]			
20/20	0.7883		0.785–0.787
25/25		0.783–0.787	
refractive index, at 20°C		1.376–1.378	
infrared	identification		
distillation, °C[g]	1.0, max		1.5, max
ultraviolet scan absorbance, max			
330–400	0.01		
300	0.02		
275	0.03		
260	0.04		
245	0.08		
230	0.2		
220	0.4		
210	1		

[a] Values of acidity, nonvolatility, and refractive index for 1990 *U.S. Pharmacopeia* XXII azeotropic (91–93 vol %) isopropyl alcohol are equal to those of 1990 USP XXII anhydrous.

[b] By gas chromatography, area %. For USP XXII azeotropic, % of organics.

[c] Value is meq/g.

[d] Value is percent as acetic acid.

[e] Per 50 mL.

[f] For ASTM D310-86 (91 vol %) at 20°C, value is 0.8180 ± 0.0005; for USP XXII azeotropic at 25°C, value is 0.815–0.810.

[g] Including 82.3; for ASTM D1310-86, value is 1.0°C, max, including 80.4.

Colorimetric methods can be used to determine trace amounts of ethyl alcohol upon the addition of specific compounds known to form complexes with alcohols (132). In the case of isopropyl alcohol, some of the colorimetric methods make use of its facile oxidation to acetone, which can provide highly colored complexes. Trace amounts of isopropyl alcohol can also be determined photometrically in the presence of acetone and acetic acid (133). A conductometric method has been developed for isopropyl alcohol–water mixtures (134).

8. Health and Safety Factors

Alcohols as a class have low toxicity. Isopropyl alcohol, however, is about twice as toxic as ethyl alcohol (135), but less toxic than methyl alcohol. There is no known systematic investigation of the effects of inhalation, eg, from aerosols, of isopropyl alcohol in humans. The known human toxicity is based on numerous cases of accidental ingestion or topical application. Toxic doses of ingested isopropyl alcohol, usually as rubbing alcohol, may produce narcosis, anesthesia, coma, and death. The single lethal dose for humans is about 250 mL, although as little as 100 mL can be fatal. Death occurs from paralysis of the central nervous system. Approximately 70–90% of ingested isopropyl alcohol is oxidized to acetone in the body, thus it is not a cumulative poison

(136). Acetone appears on the breath within 15 minutes after ingestion. There is no fixed relationship between blood and urine isopropyl alcohol concentrations. NIOSH has published an extensive review of the toxicology of isopropyl alcohol (137).

Use of isopropyl alcohol in industrial applications does not present a health hazard. The alcohol produces anesthetic effects in high vapor concentration. Consequently, the OSHA permissible exposure limit (PEL) and the ACGIH threshold limit value (TLV) have been established at 400 ppm (0.098 mg/L) for an 8-h exposure (TWA) (138). This level causes a mild irritation of the eyes, nose, and throat (139). However, the TLV level does not produce symptoms of anesthesia (140). The OSHA and ACGIH short-term exposure limits (STELs) are 500 ppm. The odor threshold for isopropyl alcohol ranges from 3 to 200 ppm, which is the minimum concentration having identifiable odor (141).

An EPA–TSCA Section 4 Test Rule (142) requires manufacturers of isopropyl alcohol to test the alcohol for health and environmental effects. The Chemical Manufacturers Association (CMA) formed a panel to oversee the required testing. Rodent studies were designed to assess hazards for systemic effects (rats and mice) as evaluated by subchronic (90 d) inhalation exposure; adult neurotoxicity (rats) evaluated in a subchronic inhalation exposure; developmental toxicity (rats and rabbits) evaluated in an oral, gavage study; developmental neurotoxicity (rats) evaluated in an oral, gavage study; reproductive toxicity (rats) evaluated in a two-generation, oral, gavage study; and oncogenicity (rats and mice) evaluated in a two year inhalation study. Testing was completed in 1994. No adverse effects were found. As of this writing (1996), the test results are under review by the U.S. EPA.

9. Uses

Uses of isopropyl alcohol are chemical, solvent, and medical. Estimated U.S. uses in 1993 were as chemical intermediates, 34%; personal care and household products, 24%; coatings and ink solvent, 15%; processing solvent, 12%; pharmaceuticals, 10%; and miscellaneous uses, 5% (143).

9.1. Chemical

The use of isopropyl alcohol as a feedstock for the production of acetone is expected to remain stable, as the dominant process for acetone is cumene oxidation. Isopropyl alcohol is also consumed in the production of other chemicals such as methyl isobutyl ketone, methyl isobutyl carbinol [108-11-2], isopropylamine, and isopropyl acetate. The use of diisopropyl ether as a fuel ether may become a significant outlet for isopropyl alcohol.

9.2. Solvent

Because of its balance between alcohol, water, and hydrocarbon-like characteristics, isopropyl alcohol is an excellent, low cost solvent free from government regulations and taxes that apply to ethyl alcohol. The lower toxicity of isopropyl alcohol favors its use over methyl alcohol, even though the former is somewhat higher in cost. Consequently, isopropyl alcohol is used as a solvent in many consumer products as well as industrial products and procedures, eg, gasification and extractions. It is a good solvent for a variety of oils, gums, waxes (qv), resins, and alkaloids, and consequently is used for preparing cements, primers, varnishes, paints, printing inks, etc.

Isopropyl alcohol is also employed widely as a solvent for cosmetics (qv), eg, lotions, perfumes, shampoos, skin cleansers, nail polishes, makeup removers, deodorants, body oils, and skin lotions. In cosmetic applications, the acetone-like odor of isopropyl alcohol is masked by the addition of fragrance (144).

Over 68 aerosol products containing isopropyl alcohol solvent have been reported (145). Aerosol formulations include hair sprays (146), floor detergents (147), shoe polishes (148), insecticides (149, 150), burn ointments (151), window cleaners, waxes and polishes, paints, automotive products (eg, windshield deicer), insect repellents, flea and tick spray, air refreshers, disinfectants, veterinary wound and pinkeye spray, first-aid spray, foot fungicide, and fabric-wrinkle remover (152) (see Aerosols).

9.3. Medical Usage

Isopropyl alcohol is also used as an antiseptic and disinfectant for home, hospital, and industry (see Disinfectants and antiseptics). It is about twice as effective as ethyl alcohol in these applications (153, 154). Rubbing alcohol, a popular 70 vol % isopropyl alcohol-in-water mixture, exemplifies the medicinal use of isopropyl alcohol. Other examples include 30 vol % isopropyl alcohol solutions for medicinal liniments, tinctures of green soap, scalp tonics, and tincture of mercurophen. It is contained in pharmaceuticals, eg, local anesthetics, tincture of iodine, and bathing solutions for surgical sutures and dressings. Over 200 uses of isopropyl alcohol have been tabulated (2).

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