

A comparison of *Agent-based Simulation of Ecological Alcohol Systems* (Dissertation by Yasmin H Said), p. 6-10
and *Chemical of the Week: Ethanol* (web page by Bassam Z. Shakhashiri)

Regular font indicates substantially close wording between the two sources, *italic* represent paraphrased sections, **bold** represents significant departures of Wegman et al from sources, and **bold underline** represent points of outright contradiction. Paragraphs have been reformatted for easy comparison. Within sections of close wording, identical phrases (ID) are highlighted in cyan, trivial changes (TC) with yellow. Changes resulting in issues are underlined.

Said - 1.1 Ethanol, Ethyl, Grain Alcohol, Alcohol

p.6

Ethanol is a clear liquid with a fairly sweet taste in dilute solutions, but can result in a burning taste at higher concentrations. Ethanol, $\text{CH}_3\text{CH}_2\text{OH}$, is classified as an alcohol, which is characterized by a hydroxyl group attached to a carbon atom. Although the term alcohol originates from the Arabic al-kuhul, or a fine powder used as eye makeup, medieval alchemists later applied the word to products of distillations, which is where the current term gets its usage (Petrucci, 2001; Shakhashiri, 2005).

Physical properties of ethanol include a melting point of -114.1°C , a boiling point of 78.5°C , and a density of 0.789 grams/milliliter at 20°C . Relative to mercury with a freezing point of -40°C , alcohol is the fluid of choice in thermometers with low temperature readings and for use as antifreeze in automobile radiators (Petrucci, 2001; Shakhashiri, 2005).

From ancient times through today, ethanol has been produced through the fermentation process of sugars. The enzyme that provides the force in the conversion of simple sugars to ethanol and carbon dioxide is zymase, which is derived from yeast, through the following reaction:



Said p. 7

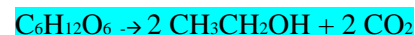
Although the production of ethanol through this fermentation reaction with the use of impure yeast cultures results in impurities such as glycerine and other organic acids, it is precisely these impurities that provide the flavors for beverage alcohol.

Shakhashari - Chemical of the Week: Ethanol

Ethanol (ethyl alcohol, grain alcohol) is a clear, colorless liquid with a characteristic, agreeable odor. In dilute aqueous solution, it has a somewhat sweet flavor, but in more concentrated solutions it has a burning taste. Ethanol, $\text{CH}_3\text{CH}_2\text{OH}$, is an alcohol, a group of chemical compounds whose molecules contain a hydroxyl group, $-\text{OH}$, bonded to a carbon atom. The word *alcohol* derives from Arabic *al-kuhul*, which denotes a fine powder of antimony used as an eye makeup. *Alcohol* originally referred to any fine powder, but medieval alchemists later applied the term to the refined products of distillation, and this led to the current usage.

Ethanol melts at -114.1°C , boils at 78.5°C , and has a density of 0.789 g/mL at 20°C . Its low freezing point has made it useful as the fluid in thermometers for temperatures below -40°C , the freezing point of mercury, and for other low-temperature purposes, such as for antifreeze in automobile radiators.

Ethanol has been made since ancient times by the fermentation of sugars. All beverage ethanol and more than half of industrial ethanol is still made by this process. Simple sugars are the raw material. Zymase, an enzyme from yeast, changes the simple sugars into ethanol and carbon dioxide. The fermentation reaction, represented by the simple equation



is actually very complex, and impure cultures of yeast produce varying amounts of other substances, including glycerine and various organic acids. In the production of beverages, such as whiskey and brandy, the impurities supply the flavor.

Said p.7 – cont.

Starches supplied from corn, potatoes, and other wheat plants including barley can also yield ethanol through fermentation, although starches must be broken down into simple sugars before the fermentation process can begin through the naturally occurring enzyme diastase. This enzyme is released through the germination of barley, which is therefore required to be the first step in producing alcohol from starchy plants (Petrucci, 2001; Shakhshiri, 2005).

Zymase is only active as an enzyme in ethanol concentrations up to 14 percent, at which point the enzyme is destroyed and fermentation is ceased. Pure ethanol cannot be produced by distillation because although ethanol is normally concentrated by the distillation of aqueous solutions, the constitution of vapor from aqueous ethanol results in four percent of the solution being water. To produce pure ethanol, dehydrating agents can be used to absorb any excess water, however, commercial ethanol is sold as 95 percent by volume ethanol, with the remaining five percent as water.

Said p. 7-8

To prevent its consumption, industrial ethanol is often denatured and small amounts of poisonous or unpleasant substances are added to it. The price industrial corporations would have to pay in order to remove these substances would exceed the federal excise tax on alcoholic beverages, however, because some industries require undenatured ethanol, federal supervision in such cases is mandatory.

Said p. 8

After swallowing an alcoholic beverage, ethanol is rapidly absorbed in the small intestine and distributed throughout the body entering body tissues in direct proportion with their water content. This results in more ethanol being distributed to the blood and brains rather than muscles or fat tissue. Because ethanol is significantly diluted by body fluids, a one-ounce shot of 100 proof distilled spirits, which is composed of a half of an ounce of ethanol, is diluted by a factor of 5000 in a 150-pound human, resulting in an approximate blood alcohol concentration of 0.02 percent.

Shakashari – cont.

Starches from potatoes, corn, wheat, and other plants can also be used in the production of ethanol by fermentation. However, the starches must first be broken down into simple sugars. An enzyme released by germinating barley, diastase, converts starches into sugars. Thus, the germination of barley, called malting, is the first step in brewing beer from starchy plants, such as corn and wheat.

The ethanol produced by fermentation ranges in concentration from a few percent up to about 14 percent. Above about 14 percent, ethanol destroys the zymase enzyme and fermentation stops. Ethanol is normally concentrated by distillation of aqueous solutions, but the composition of the vapor from aqueous ethanol is 96 percent ethanol and 4 percent water. Therefore, pure ethanol cannot be obtained by distillation. Commercial ethanol contains 95 percent by volume of ethanol and 5 percent of water. Dehydrating agents can be used to remove the remaining water and produce absolute ethanol.

...

Most industrial ethanol is denatured to prevent its use as a beverage.

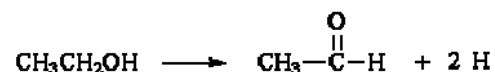
Denatured ethanol contains small amounts, 1 or 2 percent each, of several different unpleasant or poisonous substances. The removal of all these substances would involve a series of treatments more expensive than the federal excise tax on alcoholic beverages (currently about \$20 per gallon). These denaturants render ethanol unfit for some industrial uses. In such industries undenatured ethanol is used under close federal supervision.

When an alcoholic beverage is swallowed, it passes through the stomach into the small intestine where the ethanol is rapidly absorbed and distributed throughout the body. The ethanol enters body tissues in proportion to their water content. Therefore, more ethanol is found in the blood and the brain than in muscle or fat tissue. The ethanol is greatly diluted by body fluids. For example, a 1-ounce shot of 100-proof whiskey, which contains 0.5 fluid ounces of ethanol (about 15 mL), is diluted 5000-fold in a 150-pound human, producing a 0.02% blood alcohol concentration.

Said p. 8 (cont.)

As ethanol is a toxic substance, upon its consumption the body disposes of it immediately through alcohol dehydrogenase in the liver. Alcohol dehydrogenase converts ethanol into acetaldehyde. As acetaldehyde is also a toxic substance,

aldehyde dehydrogenase immediately converts acetaldehyde into acetate ions.



Said p. 9

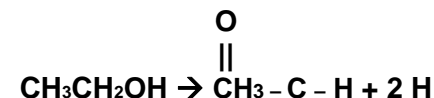
Hydrogen atoms in the above equations become bound to nicotinamide-adenine dinucleotide (NAD) and results in the generation of NADH.

In order for ethanol elimination to continue, NADH must constantly be converted back to NAD.

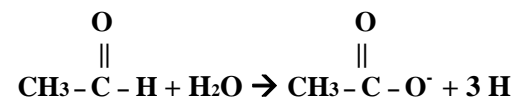
As shown in the figure, blood alcohol levels change over time depending on the amount of ethanol consumed, with lower amounts of ethanol being cleared from the body more quickly (Petrucci, 2001; Shakhshiri, 2005).

Shakhshari – cont.

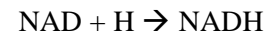
Ethanol is toxic, and the body begins to dispose of it immediately upon its consumption. ... In the liver, the alcohol dehydrogenase enzyme converts ethanol into acetaldehyde, which is itself toxic.



Acetaldehyde is destroyed almost immediately by the aldehyde dehydrogenase enzyme, which converts it to acetate ions.



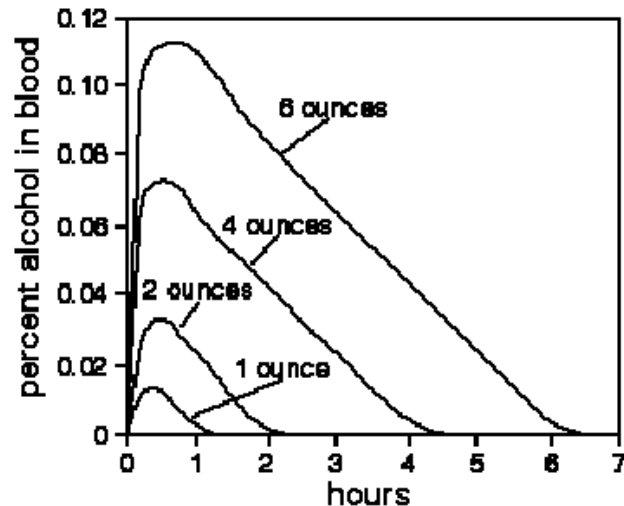
The hydrogen atoms represented by these equations are not unattached, but are picked up by another biologically important compound, nicotinamide-adenine dinucleotide (NAD), whose function is to carry hydrogen atoms. NAD is involved in both of the above processes, being converted to NADH.



NADH must be recycled to NAD for the disposal of ethanol to continue. ...

The figure shows how the blood alcohol level changes with time for various doses of ethanol.

Said p. 9 (cont.)



Source: <http://scifun.chem.wisc.edu/CHEMWEEK/ETHANOL/ethanol.html>

Figure 1: A response curve showing how the body clears different amounts of alcohol in the blood.

The central nervous system is significantly affected by the consumption of ethanol. Instead of affecting muscles of the body, ethanol's effects are directed at the brain.

Ethanol can serve as a depressant or general anesthetic because of its suppression of certain brain functions.

Said p. 10

However, ethanol consumed at low doses can suppress some inhibitory brain functions and can therefore act as a stimulant. With higher concentrations of ethanol, more brain functions are suppressed and reaction time becomes slowed down along with slurred speech, and other symptoms of intoxication. At especially high concentrations within the body, ethanol serves as a general anesthetic.

Shakashari – cont.

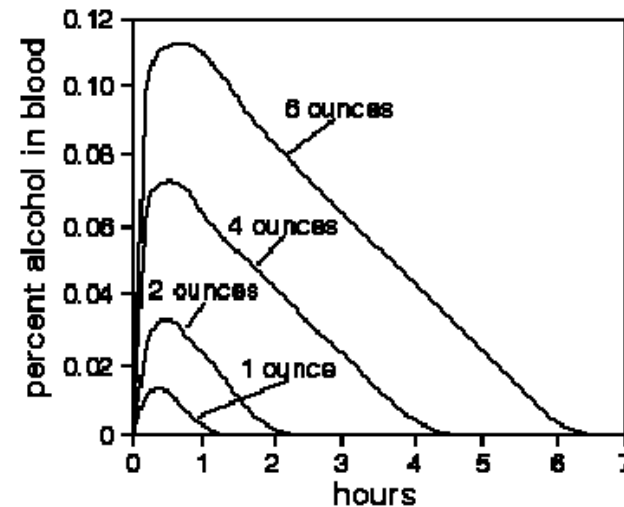


Figure. Blood alcohol content versus time after consumption of 1, 2, 4, and 6 ounces of ethanol.

Ethanol acts as a drug affecting the central nervous system. Its behavioral effects stem from its effects on the brain and not on the muscles or senses themselves.

It is a depressant, and depending on dose, can be a mild tranquilizer or a general anesthetic. It suppresses certain brain functions.

At very low doses, it can appear to be a stimulant by suppressing certain inhibitory brain functions. However, as concentration increases, further suppression of brain functions produce the classic symptoms of intoxication: slurred speech, unsteady walk, disturbed sensory perceptions, and inability to react quickly. At very high concentrations, ethanol produces general anesthesia; ...

Said p. 10 (cont.)

Because directly measuring alcohol levels in the brain is rather difficult, monitoring of blood alcohol level serves as a good substitute.

Impairment of brain functions for most people begin to become noticed at around a blood alcohol percentage of 0.05,

while clearly noticeable physical impediments become visible at around a percentage of 0.10, and slurred speech becomes evident at 0.15 percent.

Most people lose consciousness at a blood alcohol level of 0.4 percent,

and at a level of 0.5 percent the brain's breathing center and the pumping of the heart can become anesthetized resulting in their impediment.

While reaching such an extreme degree of intoxication is quite improbable, a 150 pound human may attain this level after the quick ingestion of a fifth of a gallon of 100 proof alcohol.

Shakashari – cont.

Alcohol levels in the brain are difficult to measure, and so blood alcohol levels are used to assess degree of intoxication.

Most people begin to show measurable mental impairment at around 0.05 percent blood alcohol.

At around 0.10 percent, mental impairment will show obvious physical signs, such as an unsteady walk. Slurred speech shows up at around 0.15 percent.

Unconsciousness results by 0.4 percent.

Above 0.5 percent, the breathing center of the brain or the beating action of the heart can be anesthetized, resulting in death.

Reaching this level of blood alcohol by ingestion is unlikely, however. In a 150-pound human, it would require rapid consumption of a fifth gallon of a 100-proof spirit.

Agent-based Simulation of Ecological Alcohol Systems (PhD Dissertation by **Yasmin H Said**), p. 6-10

The dissertation was removed from the George Mason University website in August, 2010. However it may be found at:
<http://web.archive.org/web/20060905150733/http://www.galaxy.gmu.edu/stats/syllabi/IT871/MasterCopyDissertation.pdf>

Chemical of the Week: Ethanol (web page by **Bassam Z. Shakhshiri**)

<http://scifun.chem.wisc.edu/CHEMWEEK/PDF/Ethanol.pdf> (revised 2009)

<http://web.archive.org/web/20050609031831/http://scifun.chem.wisc.edu/CHEMWEEK/ETHANOL/ethanol.html> (2005-6 version)

Identical Words (ID): 46%

Nearly identical (NI): 67% (synonyms, change of tense, number, person, voice).

Average “identical block”: 2.0 words.