


Retaining flavor while removing caffeine—a chemist explains the chemistry behind decaf coffee

July 23 2024, by Michael W. Crowder

THE CHEMISTRY OF DECAFFEINATED COFFEE



COFFEE & CAFFEINE

A typical cup of coffee contains between 70 to 140 milligrams of caffeine. Caffeine can influence the central nervous system, and can lead to sleep problems, restlessness and discomfort.

CAFFEINE

CN1C=NC2=C1C(=O)N(C)C2=O

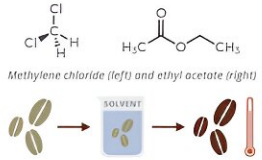
There are several processes used to decaffeinate coffee. In the U.S. decaffeination must remove 97% of the original caffeine content.

SOLVENT DECAFFEINATION


Solvent decaffeination uses solvents to selectively remove caffeine. Common solvents are methylene chloride and ethyl acetate.

ClC1=CC=CC=C1
CC(=O)OCC

Methylene chloride (left) and ethyl acetate (right)



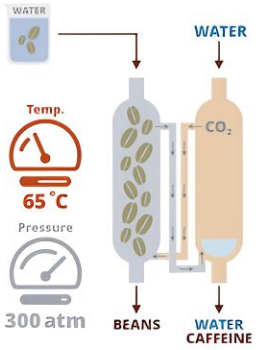
In direct solvent extraction (above) beans are steamed, then soaked in solvent to remove caffeine, before being steamed, dried, and roasted.



In indirect solvent extraction (above) beans are soaked in hot water. The water is then mixed with a solvent to remove caffeine, before flavours in the water are returned to the beans.

CO₂ DECAFFEINATION

Solvent decaffeination removes caffeine but can also remove other flavour compounds or precursors. Carbon dioxide is more selective.

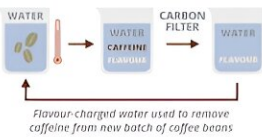


Temp. **65 °C**
Pressure **300 atm**

At high pressure carbon dioxide dissolves caffeine. The caffeine is removed from the carbon dioxide with water so it can be recirculated. The process lasts for up to 12 hours.


WATER DECAFFEINATION

'Swiss water decaffeination' soaks beans in hot water to remove caffeine and flavour compounds. Caffeine is removed from the water by filtration but flavour compounds remain. The flavour-saturated water removes caffeine from further bean batches without flavour loss.




Flavour-charged water used to remove caffeine from new batch of coffee beans

'French water decaffeination' soaks beans in hot water for 24 hours. The beans are removed and dried, and the water is filtered to remove caffeine. The caffeine-free water is added to the dried beans so that they reabsorb flavour compounds.



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A few chemical processes can remove the caffeine from coffee beans. Credit: [Andy Brunning/Compound Interest](https://www.compoundchem.com), [CC BY-NC](https://creativecommons.org/licenses/by-nc-nd/4.0/)

For many people, the aroma of freshly brewed coffee is the start of a great day. But [caffeine can cause headaches and jitters](#) in others. That's why many people reach for a decaffeinated cup instead.

[I'm a chemistry professor](#) who has taught lectures on why chemicals dissolve in some liquids but not in others. The processes of decaffeination offer great real-life examples of these chemistry concepts. Even the best decaffeination method, however, [does not remove all of the caffeine](#)—about 7 milligrams of caffeine usually remain in an 8-ounce cup.

Producers decaffeinating their [coffee](#) want to remove the caffeine while retaining all—or at least most—of the other chemical aroma and flavor compounds. Decaffeination [has a rich history](#), and now almost all coffee producers use [one of three common methods](#).

All these methods, [which are also used to make decaffeinated tea](#), [start with green, or unroasted, coffee beans](#) that have been premoistened. Using roasted [coffee beans](#) would result in a coffee with a very different aroma and taste because the [decaffeination steps would remove some flavor and odor compounds](#) produced during roasting.

The carbon dioxide method

In the relatively new carbon dioxide method, developed in the early 1970s, producers use high-pressure CO₂ to extract caffeine from moistened coffee beans. They pump the CO₂ into a sealed vessel containing the moistened coffee beans, and the caffeine molecules dissolve in the CO₂.

Once the caffeine-laden CO₂ is separated from the beans, producers pass the CO₂ mixture either through a container of water or over [a bed of activated carbon](#). Activated carbon is carbon that's been heated up to

high temperatures and exposed to steam and oxygen, which creates pores in the carbon. This step filters out the caffeine, and [most likely other chemical compounds](#), some of which affect the flavor of the coffee.

These compounds either bind in the pores of the activated carbon or they stay in the water. Producers dry the decaffeinated beans using heat. Under the heat, any remaining CO₂ evaporates. Producers can then repressurize and reuse the same CO₂.

This method [removes 96% to 98% of the caffeine](#), and the resulting coffee has only minimal CO₂ residue.

This method, which requires expensive equipment for making and handling the CO₂, is [extensively used](#) to decaffeinate commercial-grade, or supermarket, coffees.

Swiss water process

The Swiss water method, initially used [commercially in the early 1980s](#), uses hot water to decaffeinate coffee.

Initially, producers soak a batch of green coffee beans in hot water, which extracts both the caffeine and other chemical compounds from the beans.

It's kind of like what happens when you brew roasted coffee beans—you place dark beans in clear water, and the chemicals that cause the coffee's dark color leach out of the beans into the water. In a similar way, the hot water pulls the caffeine from not yet decaffeinated beans.

During the soaking, the caffeine concentration is higher in the coffee beans than in the water, so the caffeine moves into the water from the beans. Producers then take the beans out of the water and place them

into fresh water, which has no caffeine in it—so the process repeats, and more caffeine moves out of the beans and into the water. The producers repeat this process, up to 10 times, until [there's hardly any caffeine left](#) in the beans.

The resulting water, which now contains the caffeine and any flavor compounds that dissolved out from the beans, gets passed through activated charcoal filters. These trap caffeine and other similarly sized chemical compounds, such as sugars [and organic compounds called polyamines](#), while allowing most of the other chemical compounds to remain in the filtered water.

Producers then use the filtered water—saturated with flavor but devoid of most of the caffeine—to soak a new batch of coffee beans. This step lets the flavor compounds lost during the soaking process reenter the beans.

The [Swiss water process](#) is prized for its chemical-free approach and its ability to preserve most of the coffee's natural flavor. This method [has been shown to remove 94% to 96%](#) of the caffeine.

Solvent-based methods

This traditional and most common approach, [first done in the early 1900s](#), uses [organic solvents](#), which are liquids that dissolve organic chemical compounds such as caffeine. Ethyl acetate and methylene chloride are two common solvents used to extract caffeine from green coffee beans. There are two main solvent-based methods.

In the direct method, producers soak the moist beans directly in the solvent or in a water solution containing the solvent.

The solvent extracts most of the caffeine and other chemical compounds

with a similar solubility to caffeine from the coffee beans. The producers then remove the beans from the solvent after about 10 hours and dry them.

In the indirect method, producers soak the beans in hot water for a few hours and then take them out. They then treat the water with solvent to remove caffeine from the water. Methylene chloride, the most common solvent, does not dissolve in the water, so it forms a layer on top of the water. The caffeine dissolves better in methylene chloride than in water, so most of the caffeine stays up in the methylene chloride layer, which producers can separate from the water.

As in the Swiss water method, the producers can reuse the "caffeine-free" water, which may return some of the flavor compounds removed in the first step.

These methods remove [about 96% to 97% of the caffeine](#).

Is decaf coffee safe to drink?

One of the common solvents, [ethyl acetate](#), comes naturally in many foods and beverages. It's considered a [safe chemical for decaffeination](#) by the Food and Drug Administration.

The FDA and the Occupational Safety and Health Administration have deemed methylene chloride unsafe to consume at concentrations above 10 milligrams per kilogram of your body weight. However, the amount of residual methylene chloride found in roasted coffee beans is [very small—about 2 to 3 milligrams per kilogram](#). It's [well under the FDA's limits](#).

OSHA and its European counterparts have [strict workplace rules](#) to minimize methylene chloride exposure for workers involved in the

decaffeination process.

After producers decaffeinate coffee beans using methylene chloride, they steam the beans and dry them. Then the coffee beans are roasted at high temperatures. During the steaming and roasting process, the beans get hot enough that residual methylene chloride evaporates. The roasting step also produces new flavor chemicals from the breakdown of chemicals into other chemical compounds. These give coffee its distinctive flavor.

Plus, most people brew their coffee at [between 190°F to 212°F](#), which is another opportunity for methylene chloride to evaporate.

Retaining aroma and flavor

It's chemically impossible to dissolve out only the caffeine without also dissolving out other chemical compounds in the beans, so decaffeination inevitably removes some other compounds that contribute to the aroma and flavor of your cup of coffee.

But some techniques, like the Swiss water process and the indirect solvent method, have steps that may reintroduce some of these extracted compounds. These approaches probably can't return all the extra compounds back to the beans, but they may add some of the [flavor compounds](#) back.

Thanks to these processes, you can have that delicious cup of coffee without the [caffeine](#)—unless your waiter accidentally switches the pots.

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