*Technically Speaking – by Dr. John Nordin*

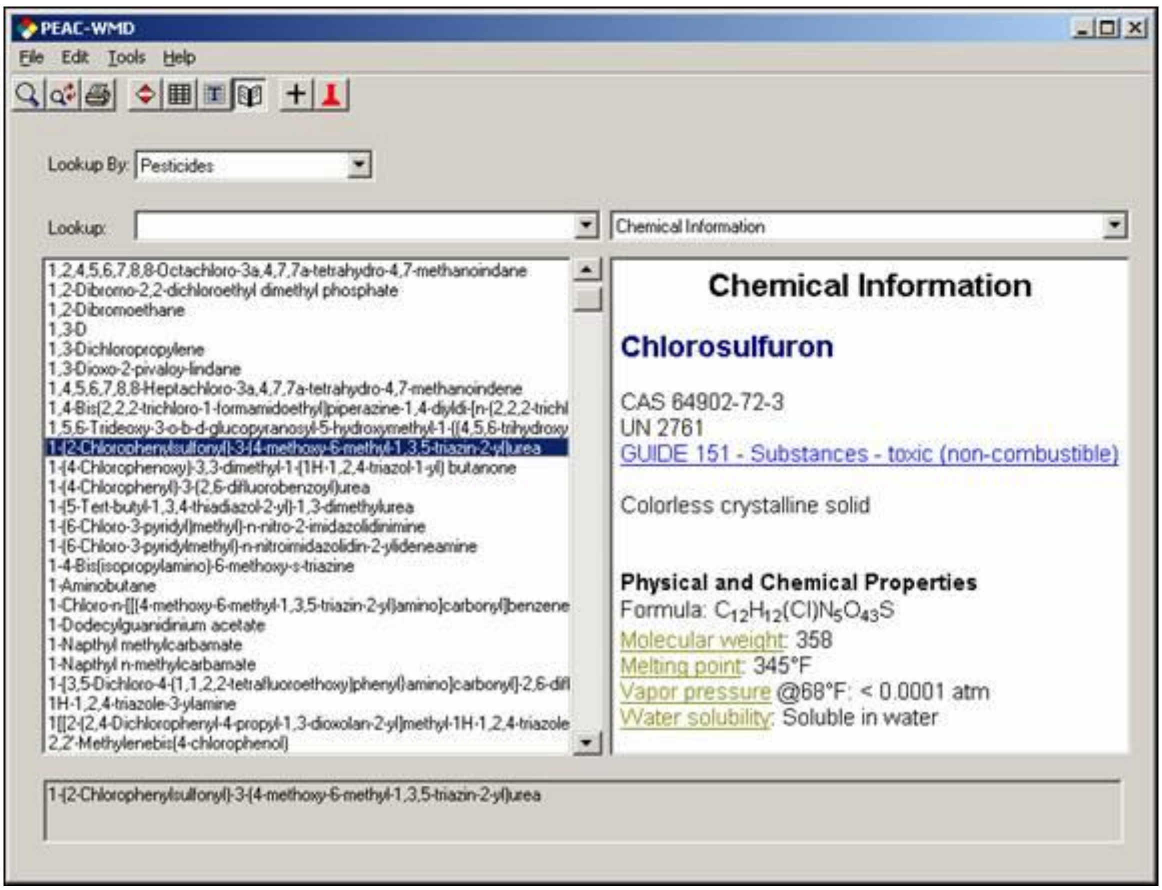
## Figuring Out Information on Chemicals Can Be Frustrating

We have all run into the problem of researching information on chemicals. Do we have the right chemical? Is Phenylenediamine the same as n-Phenylenediamine? Is Isopropyl methylphosphoniofluoridate another name for Sarin? Is Mercury chloride the same as mercuric chloride? What is the difference between 5 ppm chlorine and 5 mg/$m^3$ chlorine? If an organic chemical has a vapor pressure of 30 torr, what does this mean? What is a KPa? What is the difference between open cup and closed cup flash points? Why do some chemicals boil over a range of temperatures and some have a unique boiling temperature? Why do reference sources sometimes disagree?

### Different Chemical Names

In the previous example we looked up information for methanol. The information was displayed under methyl alcohol. Methanol is a synonym for methyl alcohol. It is a fact of life that the same chemical can go by different names. Some chemicals can go by as many as 30 or 40 different synonyms, not to mention different names for chemicals in different languages.

Why so many names? One reason is chemists have a code for naming complex chemicals. These names may be very long in the case of complex organic chemicals, so short names of only a few letters are invented because they are easy to remember. There are also different codes or methods of naming chemicals resulting in different names. The International Union of Pure and Applied Chemistry (IUPAC) has established rules for naming complex chemicals by chemists [visit the website for rules on naming organic chemicals]. A chemist using a proper code name for the particular chemical can give it to another chemist, and that chemist will know the chemical structure. The PEAC tool contains both chemical code names and common names for the chemical. For example, a certain pesticide has a chemical name "1-[2-Chlorophenylsulfonyl]-3-[methoxy-6-methyl-1,3,5-triazin-2-yl]urea", but the pesticide is more commonly known by the names "chlorsulfuron" or "chlorosulfuron" [chlorsulfuron is the name registered with the EPA]. If one selects the long-handled chemical name, "1-[2-chlorophenyl…" into the PEAC tool, it is linked up to the more common name for the chemical. The 'long-handled name" has meaning to chemists, but first responders may choose to use the shorter, common name. This same chemical is known by another long chemical name, 1-chloro-N-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide. There may be situations where the "long chemist name" is used but not the common name. If this is not bad enough, there may be variations in how the chemical is spelled or how the number and component parts are ordered, for example, chlorosulfuron or chlorsulfuron is also known by 2-chloro-N-[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)aminocarbonyl)benzenesulfonamide. Sometimes the chemical is known by brand names (short names used by the manufactuer). Examples of brand names are "Glear", "Telar", and "Trilixon". Teilixon is a powder containing chlorsulfuron and methabenzthiazuron as active ingredients.

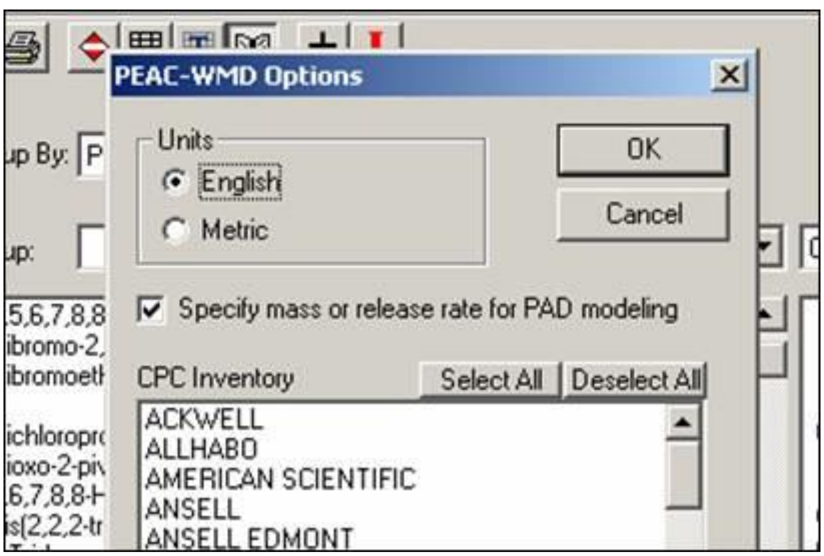



Why not use only common names which are more easily remembered? A particular chemical may have many common names, and the names are also different in different languages. Generally, the long chemical name is the same in any language but there are some exceptions to this.

The American Chemical Society has assigned a unique number for each chemical called the “Chemical Abstract Service” or CAS number. The original intent of the number was to aid scientists and other researchers to locate information about the chemical in the literature, a sort of catalog system for chemicals. The CAS number for Chlorsulfon is 64902-72-3. This number can be typed in many computerized data bases including the PEAC tool to pull up information about the chemical. It also appears on many labels listing product ingredients supplied with chemicals. The CAS number is internationally recognized. When in doubt whether the name matches a data base, get a match for the CAS number.

<u>Different Units of Measurement</u>

The PEAC tool user has the option of selecting English or metric (international) units for display. To select this option, the user clicks on “edit” at the top of the screen, then “options”. A screen pops up like the one below over other screens. The user can select “English” or “metric”.




When getting information from different data sources, the data may be expressed in different units. A good conversion table and pocket calculator are necessary.

Table 1. Conversion Table

| Measurement Type | To Convert From: | To Convert To: | Do This |
|---|---|---|---|
| Temperature | $^{o}$ F | $^{o}$ C | Subtract 32 from $^{o}$F and multiply result by 5/9 |
| Temperature | $^{o}$ C | $^{o}$ F | Multiply by 9/5 and add 32 |
| Concentration | ppm | $mg/m^3$ | Multiply ppm by the molecular weight and divide the result by 24.45 |
| Concentration | $mg/m^3$ | ppm | Multiply $mg/m^3$ by 24.45 and devide the result by the molecular weight |
| Concentration | Volume % | ppm | Multiply by 10000 |
| Pressure | mm Hg | atm | Divide by 760 |
| Pressure | atm | mm Hg | Multiply by 760 |
| Pressure | psi | atm | Multiply by 0.06805 |
| Pressure | atm | Inches Hg | Multiply by 29.921 |
| Pressure | atm | KPa (kilopascals) | Multiply by 101.325 |
| Pressure | atm | psi | Multiply by 14.696 |
| Pressure | Torr | mm Hg | Multiply by 1 |
| Pressure | Torr | KPa | Multiply by 0.13332 |
| vap. pressure | atm | Vap by volume | Multiply by 100 |
| Weight/mass | Pounds | grains | Multiply by 7000 |
| Weight/mass | Pounds | kilograms | Multiply by 0.45359 |
| Weight/mass | kilograms | Pounds | Multiply by 2.2046 |
| Volume | Gallons | Cubic Feet | Multiply by 0.13368 |
| Volume | Gallons | Liters | Multiply by 3.785 |
| Volume | Gallons | Cubic meters | Multiply by 0.003785 |
| Volume | Barrels (oil) | gallons | Multiply by 42 |
| Power | Horsepower (British) | Horespower (metric) | Multiply by 1.0139 |
| Power | Watts | B.T.U./hr | Multiply by 3.413 |
| Power | Watts | Joules/second | Multiply by 1 |
| Work | Joules | B.T.U. | Multiply by 0.000948 |
| Work | Joules | Calories | Multiply by 0.2389 |
| Work | Joules | Kilowatt-hours | Multiply by 0.00000027778 |
| Work | Kilocalories | Joules | Multiply by 4186.8 |
| Length | Feet | Meters | Multiply by 0.3048 |
| Length | Miles | Meters | Multiply by 1609.3 |
| Length | Miles | km | Multiply by 1.6093 |
| Radiation Activity | Becquerel (Bq) | Disintegrations/second | Multiply by 1 |
| Radiation Activity | Becquerel (Bq) | Curies | Multiply by $2.703 \times 10^{-11}$ |

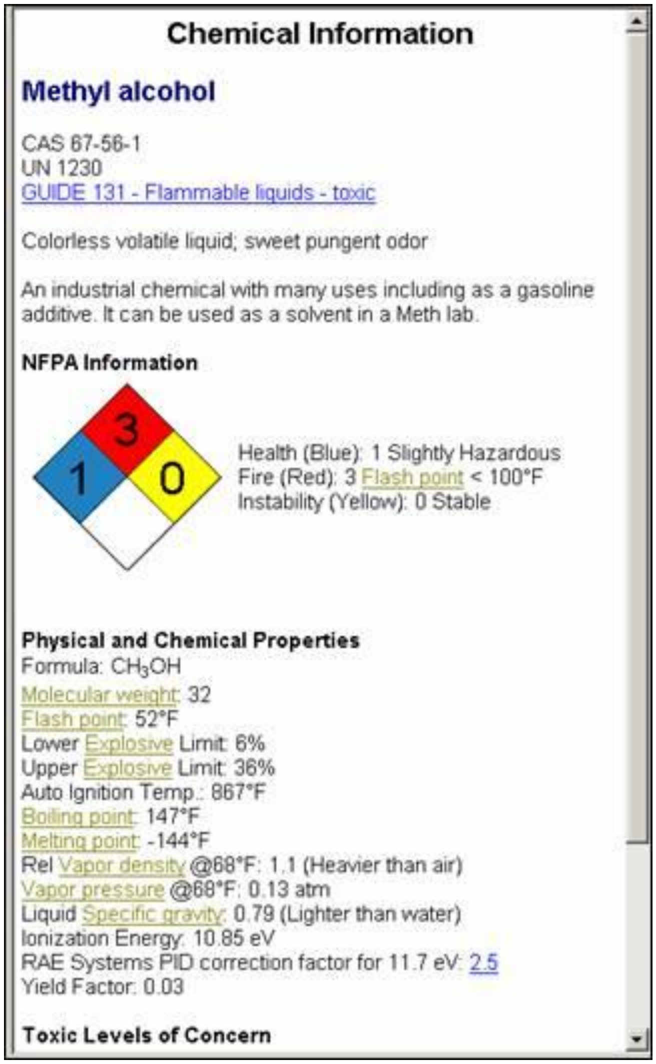
| | | | |
|---|---|---|---|
| Radiation dose | Roentgen | rem | Dose absorbed is equivalent for gamma and x radiation, different factors apply for neutron and other radiation |
| Radiation dose | rem | Sievert | Multiply by 0.01 |

**Example:** The concentration of sulfur dioxide is 5 ppm. What is the concentration in $mg/m^3$?
Answer: The molecular weight of sulfur dioxide is 64.1. The concentration in $mg/m^3$ (milligrams per cubic meter) is 5 x 64.1/24.45 = 13.11 $mg/m^3$ (call it 13 $mg/m^3$ , the numbers are usually rounded).

Someone might ask: Wouldn't the answer be different if the temperature is hot or cold, as the cubic meter will expand if the temperature is hot or become more dense if it is cold?. Also, wouldn't the cubic meter be less dense at Leadville CO where the elevation is 10000 feet as opposed to sea level. The answer is no. By convention, a standard cubic meter when expressing concentrations. The standard cubic meter is at 1 atmosphere pressure and $20^oC$ ($68^oF$).

Someone might again ask, why don't data bases express concentrations entirely in "ppm" or "$mg/m^3$" rather than using a mixed set of units? Answer: A lot of people favor using ppm (parts per million) when expressing concentrations of gases and organic vapors in the air. But this does not work with dusts and particulates because the weight of particulates in the air per unit volume is what is important; also, many dusts and particulates do not have a defined molecular weight. It is possible to express concentrations of gasses, vapors, metal fumes, and particulates in terms of $mg/m^3$. But only gases and organic vapors can be correctly expressed in ppm.

**Another Example**: Will methanol catch fire at $60^o$ F ($20^o$ C) if exposed to an ignition source (e.g. a match or a spark)?




When we type in "methanol" in the PEAC tool, the above display is seen (bottom is cropped in this illustration). Methyl alcohol is a synonym for methanol. The flash point is 52$^o$F meaning that methanol will ignite if the temperature is 52$^o$F or higher.

Another way of approaching the problem is to note that the liquid vapor pressure is 0.13 atm at 68$^o$F. This means that the vapor concentration just above the methanol liquid is 13%. We see that the lower explosive limit for this chemical is 6%. The chemical will ignite since actual interface concentration of 13% is greater than the lower explosive limit of 6%. In fact, if enough vapor has built up above the liquid and has not dispersed, there could be an explosion when exposed to an ignition source.

**A More Complex Example:** An explosive device has been detonated in a public building. Structural damage to the building appears to be minimal, at least this is an initial assessment. There is some fine dust in the air inside the building. A preliminary sample of the air inside the building showed the particulate level to be up to 50 $mg/m^3$. Of greater concern was that the air sample displayed an elevated radioactivity compared with background. The gamma radiation count for various air samples taken inside the building was upwards of 5000 counts per second per milliliter of sample. The energy level of the gamma radiation was 0.662 MeV, which is characteristic of a Cesium 137 fingerprint. Can a CBRN negative pressure respirator, with a particulate filter rated at 99.97% particulate removal, provide adequate protection against inhalation of Cesium 137 particulates by inhalation? How much more radiation exposure would a responder receive using a particulate filter rated at 99.97% particulate removal compared with using SCBA?

Answer: This is a much more complex situation than the previous examples, as several things must be considered. The radiation dose is a combination of gamma and beta radiation external to the body plus from any inhaled radioactive isotope. We will assume that an assessment has been made on radiation dose for emergency response personal in Level A protection using SCBA, and answer the question as to what additional radiation dose might a person receive if he/she used a particulate filter rated at 99.97% particulate removal rather than SCBA. We will assume a moderate to heavy work load resulting in a breathing rate of 65 liters/minute. The suit is assumed to adequately shield against the harmful effects of beta particles, at least for the duration of use.

What additional radiation exposure would be acceptable? For the purpose of this calculation, we will go with 5 rem (0.05 sievert) radiation dose, which is the annual inhalation limit recommended exposure by adult workers exposed to radioactive isotopes [see 10 CRF Part 20 Appendix B], over and above background [typical background is 0.3 to 0.5 rem per year]. The regulations do allow up to 100 rem exposure limit for emergency, life-saving operations, but studies have shown that there is an increased cancer risk at these higher exposure levels. The damage from radiation exposure is accumulative, meaning if someone receives a dose of 5 rem one day and another dose of 5 rem on a later date, his/her total dose is 10 rem.

OSHA regulations recommend that the particulate filter be replaced after a loading of 200 mg. Based on a breathing rate of 65 liters/minute, an ambient particulate concentration of 50 $mg/m^3$, we can calculate the useful service life of the respirator cartridge:

Service Life (minutes) = 200 x 1000 /(65 x 50) = 62 minutes [comment:  200 mg x 1000 liters/$m^3$ x (1/65) minutes/liter x (1/50) $m^3$/mg = 62 minutes]

To calculate how much additional radiation exposure the person would receive using a particulate filter rated at 99.97% removal as opposed to using SCBA (assuming the same breathing rate), we need to calculate the amount of radiation inhaled.   The ambient radiation count per milliliter is 5000 per second.   The intensity (% of disintegrations) of gamma radiation at 0.662 MeV is 100% (see PEAC tool display below) meaning that the number of gamma radiation counts can be equated to the number of disintegrations per second.  Each count represents 1 disintegration per second, or one Becquerel.    The person's breathing rate is 65 liters/minute.   There are 1000 milliliters per liter.   Cesium 137 is in particulate form, and we will base our calculation on 99.97% removal of Cesium 137.  [1 – 0.9997 = 0.0003] The amount or radiation inhaled per minute is calculated to be,

5000 x 0.0003 x 65 x 1000 = 98000 Becquerels/minute.

The next step is to relate 98000 Becquerels/minute to the radiation exposure, in rems or sieverts.   Using the PEAC tool,  the annual worker dose for inhalation of Cesium 137 equivalent to 0.05 sieverts is 7.4e+006 Becquerels.    Although the regulations (10 CFR Part 20 Appendix B) list 5 rem annual dose limit for workers, the 7.4e+006 in the regulations is linked to a 5 rem dose and not to time.    The number 7.4e+006 is the same as 7,400,000.     A person will receive a 0.05 sievert (5 rem) dose after 7400000/98000 = 66 minutes.

This number might be acceptable for an emergency situation for less than one hour, but SCBA is the better choice.

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Theses examples have in common taking information out of data bases and performing some calculations or unit conversion to help in the decision process regarding action for a particular situation

Radioactive Isotope Information

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## Cesium 137

Man-made-has been detected at nuclear power plants. Uses include food irradiation, soil density testing, industrial radiography.

Symbol: Cs 137

Half Life: 30.2 years
Atomic Weight: 136.9071
Atomic Number: 55

**Radiation**
Activity: 86.6912 Ci/g
Alpha Radiation: None
Beta Radiation: 1.176 MeV (100%)
Isomeric Transition Radiation: None
Orbital Electron Capture: None
Spontaneous Fission: None

**Gamma Radiation**, energy level (MeV) and intensity (% of disintegrations):
0.6616 MeV (100.0%)

**Beta Particle Travel**
Beta particle travel distance in air (sea level, ambient temp.): 164.8 in
Beta particle travel distance in air (6560 ft elevation, ambient temp.): 219.67 in
Beta particle travel distance into human flesh if radioactive isotope is on the skin: 0.2 in

**Daughter Isotopes**
Barium 137m (half life 2.55 minutes), then Barium 137 (stable)
Daughter Isotope Radiation: Ba k x-ray

**Inhalation and Ingestion Exposure Limits**
Annual Limit by Inhalation for 5 rem annual exposure:
2.0e+002 microcuries

Occupational Derived Air Concentration for 5 rem annual exposure:
6.0e-008 microcuries/ml (breathing rate 20 liters/minute, exposed 2000 hours/year)