DrNuc Instructions

DrNuc® is a registered trademark of Oilfield Nuclear Software LLC.

There are 6 calculators in this app:

1. **Lithology Calculator** - good for clean limestone sandstone or dolomite formations with water oil gas and/or CO2.
2. **Clay Calculator** - good for sandstone formations with the clays illite kaolinite and/or smectite.
3. **SuperNuc Calculator** - a very powerful calculator for modeling complex formations and pore fluids. The SuperNuc can do everything that the other calculators can do and more. Use it for complex oil and gas compositions and/or complex formation matrix compositions.
4. **Mineralogy Calculator** - good for examining the petrophysical properties of pure minerals (approx. 100 in the app's database).
5. **Saline Water Calculator** - petrophysical properties of saline water.
6. **Weight Percents Calculator** - designed for chemical or elemental assays of rock or fluid samples.

A segmented control will allow you to:

1) run the calculator
2) clear all fields
3) set default values
4) show a basic help message
5) save the results
6) email the saved results

You must explicitly click on 'save' to save the current calculator information for emailing. The app is only collecting data identified by the user.

Units used in all of the calculators:

- Porosity in porosity units (100 pu = 100% = 1). Valid range is 0 to 100 pu.
- The fluid saturations Sw, So, Sg, and Sco_2 are in saturations units (100 su = 100% = 1).
- Densities are in g/cc.
- Water salinity is in kppm (1 kppm = 0.1% by weight). From 0 to 250 kppm (0 to 25% NaCl).
- Temperature can be in °C or °F.

- Pressure in psi absolute (1 atm = 14.7 psia).
- Formation matrix defined with weight percents. Sum has to be 100%.
- Neutron capture cross-sections (sigma) in capture units (cu) [1 cu = 0.001 cm^{-1}].
- PEF and HI are unitless.
- DPHI in pu using the base mineral density.

Rules:

- Saturations Sw + So + Sg + Sco_2 must equal 100.
- Weight percents must sum to 100%.
- The oil composition is assumed to be CH_2 in the Lithology and Clay calculators but the density can be set.
- The gas composition is assumed to be methane CH_4 in the Lithology and Clay calculators but the density can be set.
- Use the SuperNuc calculator for all other oil or gas compositions.

Clay compositions used in the Clay Calculator are:

- Illite = K0.7 Al0.66 Mg0.66 Fe0.66 Al0.67 Si3.33 O10 (OH)2
- Kaolinite = Al2 Si2 O5 (OH)4
- Smectite = Na0.33 Al1.67 Mg0.33 Si4 O10 (OH)2

Use the SuperNuc calculator if your clays have a different composition.

When entering data, if you click on an input value it will automatically clear and you will have to re-enter the data if you don't want it to be zero.

If an input field is empty, a value of 0 is assumed and used in the calculations.

Most input boxes can only handle 4 to 5 characters. The code is not accurate to more than 3 or 4 decimal places.

Additional SuperNuc Instructions:

Mineral or hydrocarbon compositions must be in the form of Element # Element #. The 'element' is the one or two letter symbol for the element (such as H O Si Ca...).

If a # isn't listed after an element symbol, a value of 1 is used. For example, valid hydrocarbon compositions in the SuperNuc calculator are

CH2 CH1.9 C4H9 ...

Valid matrix compositions are

SiO2, CaCO3, Na0.33 Al1.67 etc.

The 5 minerals in the SuperNuc calculator can be defined using chemical formulas or by selecting a standard composition from the mineral library. For example, anhydrite could be defined in 3 ways:

i. using the mineral table (click the ▸ symbol and select **anhydrite**)

ii. by typing **anhydrite** in the mineral input field.
iii. by entering **CaSO4** in the mineral input field.

Note that you must enter the mineral matrix density separately. The matrix density is an input because the matrix may be composed of multiple minerals and may have a unique density.

The matrix is a mix of up to 5 minerals plus either $CaCO_3$ $CaMg(CO3)_2$ or SiO_2. DrNuc will calculate the weight percent of the base mineral to achieve 100%.

If you want to model limestone dolomite or sandstone, you must enter the corresponding matrix density (2.71 2.85 and 2.65 respectively).

The matrix density is the theoretical density (i.e. assuming no porosity).

Element symbols are obviously case sensitive. SI is Sulfur Iodine and is not Silicon. Co is cobalt and is not Carbon Oxygen.

Chemical formulas cannot contain parentheses. You must write out any chemical formulas. For example, dolomite is often written as $CaMg(CO_3)_2$ but that is illegal in DrNuc. Valid formulas for dolomite are: CaMgCO3CO3, CaCO3MgCO3 and CaMgC2O6.[1]

The relative atomic number is important. Ca0.5 Mg0.5 C O3 will give the same answer as CaMgC2O6.

When you select a mineral, you may also use the slider to set the weight percent for that mineral.

After selecting a mineral or typing it in the mineral text field, you can add more elements to the description. But the info will be lost if you use the mineral library again.

For example, it's possible to create gypsum by typing '**anhydrite H4O2**' in a mineral field which is interpreted as CaSO4 H4O2.

It's possible to type multiple mineral names on a line or to have a mineral and a chemical formula. For example, you could enter **calcite quartz** or **calcite SiO2** but it is using the atom numbers not weight fractions. So **calcite SiO2** is being replaced with **CaCO3SiO2**. That is not equal to 50% calcite + 50% SiO2 (by weight). It is 50% by atom number. If you want 50%/50% by weight, you have to enter each on separate lines.

The SuperNuc 'saved' results include the elemental number densities which can be used to calculate element ratios such as C/O.

The SuperNuc calculator is using more sophisticated software than the Lithology or Clay calculators. There may be some differences in the 3rd or 4th decimal places.

[1] The only exception is that $(OH)_N$ is allowed.

Saved Output

The output of the DrNuc calculators can be saved and then emailed to yourself or others. The **Save** action will update the values and then save the results. The **email** action will allow you to review the data, send the data and to clear the saved results. The results are not saved in the app or on your device.

The 'saved' results are useful for reviewing your input parameters because they only list the values used in the calculation. Unused values will not appear in the 'saved' results.

Detailed elemental number densities are only calculated with the SuperNuc calculator.

Bug reports and other requests can be sent to DrNuc from the 'Feedback & Bug Reports' page.

If you have internet access you can access the DrNuc website from the 'Access the DrNuc Website' page.

Mineralogy Calculator:

Click on the ▸ symbol to open up the mineral library.

Many 'minerals' are a class of similar minerals. In those cases, a common formula is being used in DrNuc. Field or formation specific mineral compositions can be defined in the SuperNuc calculator.

Nuclear parameters are listed for the nominal mineral density.

The list of minerals is shown at the end of this document.

Saline Water Calculator:

The calculator computes the density hydrogen index and capture cross section (sigma) of saline water at pressure and temperature. Fresh water vapor pressures are determined from a table of values.

Weight Percents Calculator Instructions:

This calculator is designed for chemical and elemental assays of rock samples. The matrix is a mix of up to 8 minerals/elements/chemical/materials. DrNuc will calculate the weight percent of the 1st mineral to achieve 100%. The 8 minerals can be defined using chemical formulas or by selecting a composition from the mineral library. Same rules as the SuperNuc calculator.

DrNuc Accuracy

Accuracy is typically better than 0.1% compared to SNUPAR the world-wide standard for nuclear petrophysical properties. Typical accuracies are shown on the 'Benchmark Tests' page. The “test runs” may take several seconds to complete.

Capture cross sections are set to match the SNUPAR values. See

McKeon D.C. & Scott H.D. (1988). SNUPAR - A Nuclear Parameter Code for Nuclear Geophysics Applications. Nuclear Geophysics 2(4) 215-230.

Examples are shown in a companion document.

Petrophysics / Nuclear Logging 101

There are multiple nuclear measurements that are used to evaluate rock formations to determine if they are a viable oil or gas well. Nuclear instruments (logging tools) are lowered into oil and gas wells to measure different petrophysical properties. Other measurements are often used too (such as resistivity). Oil reservoirs are usually very complex geological features with a complex history spanning hundreds of millions of years. The goal of nuclear logging is to identify if the rock formation has oil/gas how much it has and how easy or hard it is to produce the oil from the rock. Developing an oil well is a business proposition and nuclear and other measurements are used to evaluate the economics of developing a well. Three nuclear tools used in exploration are the natural gamma-ray litho-density and neutron porosity. Once a well has been developed at some point enhanced recovery techniques are usually employed to produce more of the oil left in place. The nuclear thermal-decay time measurement is often used to evaluate the reservoir and any enhanced recovery programs.

The Litho-Density tool has a gamma-ray source and measures the counts in a pair of nuclear detectors. The detector counts are a function of the density of the rock and to a lesser extent the elemental composition of the rock. With this information, it is often possible to estimate the amount of pore volume in the rock. The 2 petrophysical parameters of interest are the electron density ('rhoe' very close to the bulk density) and the photoelectric factor (PEF). This app calculates both of those petrophysical parameters. Assuming a rock type and water in the pore volume the parameter DPHI (density porosity) puts the information into a more useful parameter (porosity).

The neutron porosity log uses a neutron source and neutron detectors to measure the amount of hydrogen in the rock. While the measurement responds to mineralogy it is a strong function of the hydrogen index (HI) which is calculated with this app. The Clay Calculator and the SuperNuc Calculator can be used to understand the nuclear response of formations with complex lithologies clays and other minerals.

After a well has been producing oil for some time oil production will decrease and enhanced oil recovery techniques are used to increase oil production. A neutron tool with a neutron accelerator is used to measure the overall neutron capture cross section of the formation. This is a function of the rock the porosity the amount of oil and the amount and salinity of water. Oil has a much different capture cross section than saline water. So as oil is produced and replaced with saline water the amount of remaining oil can be determined. During water or CO_2 floods the measured capture cross section (sigma) helps understand the effectiveness of the enhanced recovery program. However, when the water is low in salinity it is difficult to distinguish oil from water. This

app calculates the hydrogen index (HI) and the neutron capture cross section (sigma) of complex formations.

Nuclear measurements are combined with other logs core data fluid samples and other information to understand and evaluate rock formations as potential oil/gas wells and to evaluate enhanced recovery programs in existing wells. Some of the key nuclear parameters are shown below for pure rocks and fluids. The DrNuc app calculates those petrophysical parameters in complex environments based on lithology mineralogy porosity water salinity oil and gas compositions. Below are parameters for some materials.

Material	Density	PEF	HI	Sigma
Sandstone	2.65	1.81	0	4.55
Limestone	2.71	5.08	0	7.08
Dolomite	2.85	3.14	0	4.67
Fresh water	1.0	0.36	1.0	22.2
250 kppm	1.19	1.32	0.89	122
Oil	0.85	0.12	1.09	24.4
Gas	~0.1	0.09	0.22	5.00
CO_2	~0.5	0.37	0	0.03

Density is in g/cc. PEF and HI are unitless. Sigma is in capture units.

List of Minerals in the Mineral Library

Albite
Almandine
Aluminum Oxide
Alunite
Analcite
Anhydrite
Ankerite
Ankerite2
Anorthite
Anthracite
Antigorite
Aragonite
Augite1
Augite2
Augite3
Barite
Beidellite
Biotite
Bituminous-Coal
Boehmite
Brucite
Calcite
Carnallite
Celestite
Chalcopyrite
Clinozoisite
Corundum
Cristobalite
Diesel
Diopside
Dolomite
Dravite
Enstatite
Epidote
Fayalite
Fe-Chlorite
Ferroactinolite
Fluorapatite
Fluorite
Forsterite
FreshWater
Gadolinium Oxide
Galena
Gibbsite
Glauconite
Goethite
Gypsum
Halite
Halloysite
Hedenbergite
Hematite
Heulandite1
Heulandite2
Hydroxyapatite
Hyperstene
Illite
Ilmenite
Kaolinite
Langbeinite
Laumontite
Lignite
Limestone
Limonite
Magnetite
Methane (32F 1 atm)
Mg-Chlorite
Molybdenum Oxide
Monazite
Montmorillonite
Mordenite
Muscovite
Natron
Nickel Oxide
Nontronite
Oil
Opal
Orthoclase
Peat
Perovskite
Phlogopite
Polyhalite
Pyrite
Pyrope
Pyrrhotite
Quartz
Rutile
Saline Water 250 kppm
Sandstone
Saponite
Sea Water (35 kppm)
Siderite
Smectite
Sphalerite
Sphene
Spinel
Strontianite
Sylvite
Thermonatrite
Tridmyite
Trona
Vermiculite
Water
Zinc Oxide
Zircon