CHE 3804 NUCLEAR ENGINEERING

SECTION 1

NUCLEAR PHYSICS

ATOMIC STRUCTURE

Atoms are made up of a nucleus of *protons* and *neutrons* which is surrounded by a cloud of *electrons*. Different *elements* have different numbers of protons in the nucleus while different *isotopes* of the same element have different numbers of neutrons in the nucleus. All isotopes of all elements are commonly known as *nuclides*. Hence there is a Chart of Nuclides showing all isotopes of all elements. The number of negatively charged electrons is always equal to the number of positively charged protons. For the lighter elements the number of neutrons in the nucleus is approximately equal to the number of protons.

The masses of a proton and a neutron are exceeding low being only about 1.67×10^{-27} kg $(1.67 \times 10^{-24} \text{ g})$. The mass of an electron is very much less being about 0.00091×10^{-27} kg $(0.00091 \times 10^{-24} \text{ g})$. The electron mass is practically negligible in comparison with a proton and a neutron. The neutron has a slightly greater mass than the proton since a neutron is made up of a proton plus an electron.

ATOMIC NOTATION

The atomic number is designated Z. This is the number of protons in the nucleus. It also designates a particular element. The *neutron number* is designated N. This is the number of neutrons in the nucleus. Together neutrons and protons are termed *nucleons* and the *atomic mass number*, designated A, is the total number of nucleons in the nucleus. The atomic mass number is related to the *isotopic mass* (or atomic weight) of the element but is an integer whereas the isotopic mass (or atomic weight) is the actual mass of the particular isotope (or element). The usual way of designating a particular isotope X is as follows:

Isotope ${}^{A}X_{Z}$ Element = X Mass Number = A Protons = Z Neutrons = A - Z

ATOMIC MASS SCALE

Since atomic masses are so minute, it is convenient to introduce a very small unit, known as the *atomic mass unit* (u), to simplify the arithmetic. This unit is defined by taking the mass of the neutral atom of the isotope carbon-12 to be precisely 12 u. From this, it follows that the equivalence between the atomic mass unit and the kilogram is:

 $1 u = 1.660566 \times 10^{-27} kg$

The masses of the atomic constituents in atomic mass units are:

Proton	1.0072765 u
Neutron	1.0086650 u
Electron	0.0005486 u

The isotopic masses of all other elements are given relative to Carbon-12. Isotopic masses for all isotopes are given in the Chart of Nuclides. The atomic weight M of an element is calculated by adding the products of the isotopic masses and the relative abundances of the individual isotopes.

$$M = \gamma_A M_A + \gamma_B M_B + \gamma_C M_C + \dots$$

Note that the isotopic masses are the total masses including electrons. If the mass of the nucleus only is required then the masses of electrons must be subtracted. For nuclear reaction equations where the same number of electrons appear on each side of the equation the masses of electrons may be neglected since they cancel one another.

MASS-ENERGY EQUIVALENCE

It is well known that energy E is related to mass m according to the following equation where c is the velocity of light.

 $E = mc^2$

From the above the mass of one atomic mass unit is:

$$1 u = 1.660566 \times 10^{-27} kg$$

The velocity of light is:

$$c = 2.998 \times 10^8 \text{ m/s}$$

The energy equivalent of one atomic mass unit may therefore be calculated as follows:

$$1 u = 1.4925 \times 10^{-12} J$$

In nuclear physics it is common to use *electron volts* (eV) or *mega-electron volts* (MeV) as a measure of energy where:

$$1 \text{ eV} = 1.6022 \text{ x } 10^{-19} \text{ J}$$

Making this substitution gives the energy equivalent of one atomic mass unit as

$$1 u = 931.5 MeV$$

AVOGADRO'S NUMBER

It is often required in nuclear engineering that the number of atoms or nuclei in a given sample be calculated. This number can be obtained from Avogadro's Number given as:

$$N_A = 6.022 \times 10^{23}$$

Note that to facilitate calculations it is better to write it immediately as:

$$N_A = 0.6022 \times 10^{24}$$

This relationalises the exponent and allows it to be easily cancelled by other exponents also written using the engineering notation for exponents.

The number of atoms N in a given sample of mass m is given by the following equation where m is the mass in grams and M is the atomic weight

$$N = (Na / M) m$$

In many cases since the atomic mass number A is very nearly equal to the atomic weight M of an element the following approximate relationship may be used

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$$N \approx (N_A / A) m$$

If the sample consists of a mixture of isotopes with one predominating then the atomic mass number of the predominant isotope may be used. This approximation gives results within an acceptable range of accuracy in engineering calculations where other simplifying assumptions are made.

As an example of the use of this relationship consider the potential power output of the total consumption of 1 kg of pure Uranium-235 per day. The number of Uranium-235 atoms in 1 kg of pure fuel is:

 $N = (0.6022 \times 10^{24} / 235) \times 1000$

 $N = 2.562 \times 10^{24}$ atoms

If this number of atoms is totally consumed (fissioned) in one day and if each fission produces 200 MeV of energy then energy is released at the following rate:

$$P = 0.005932 \times 10^{24} \text{ MeV} / \text{s}$$

If this is converted to watts and megawatts the rate of heat energy production is:

$$P = 950 \text{ MW}$$

If used in a nuclear power plant with a thermal cycle efficiency of about 30% this would be equal to approximately 300 MW of electrical power.

If in the above equation the atomic weight of Uranium-235 (235.043924) had been used instead of the atomic mass number (235) the difference in the answer would have been negligible.

ATOMIC DIMENSIONS

The dimensions of atoms are exceedingly small and impossible to visualise. It is therefore necessary to draw comparison and to compare the size of a complete atom with that of its nucleus.

The diameters of atoms range from about 75 picometres to about 500 picometers with the

larger atoms generally being towards the bottom left hand side of the Periodic Table of Elements.

The radii and diameters of nuclei are given by the following formulae where A is the atomic mass number:

$$r = 1.25 \times 10^{-15} A^{1/3} m$$

 $d = 2.5 \times 10^{-15} A^{1/3} m$

Considering Helium as an example the following dimensions are obtained;

Atom diameter = $100 \times 10^{-12} \text{ m}$ = $100 000 \times 10^{-15} \text{ m}$ Nucleus diameter = $0.004 \times 10^{-12} \text{ m}$ = $4 \times 10^{-15} \text{ m}$

The atom diameter is thus some 25 000 times that of the nucleus. It is evident that the atom consists mainly of empty space. This is an important concept when considering the passage of neutrons and other atomic particles through a material. Uncharged particles such as neutrons pass freely through millions of atoms before eventually striking or interacting with a nucleus.

ENERGY LEVELS

The electrons surrounding a nucleus may be excited to discrete energy levels up to the energy level at which the electron is separated from the nucleus and ionisation occurs. When an electron drops down from a certain energy level to another lower level or to the ground state, energy corresponding to the drop is emitted in the form of *x*-*rays*. The wavelength of these x-rays depends upon the associated energy drop. The energy levels are measured in electron volts and excitation may be induced by electromagnetic influences. The nucleons within the nucleus behave in a similar manner. There are also discrete energy levels to which the nucleons can be excited. In dropping back to lower energy levels or to the ground state, the excess energy is emitted in the form of γ -*rays*. These energy levels are measured in mega-electron volts. Since the energy levels are roughly a million times greater than those for electrons, the excitation generally arises from particle interactions with the nucleus.

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During the decay of radio-active isotopes, particles such as β -particles may be emitted. Since each such particle carries away a discrete amount of energy, it may leave the nucleus in an energy state higher than the ground state of the newly formed isotope. This excited isotope will then drop down to the new ground state by the emission of a γ -ray of appropriate energy. Invariably any nuclear reaction involving the absorption or emission of a particle by a nucleus results in the emission of a γ -ray.

NUCLEAR STRUCTURE

If the structure of various atoms is studied it is found that, for the light elements, the number of neutrons and protons in the nucleus is about equal but, for the heavy elements, the number of neutrons exceeds the number of protons. If the number of neutrons in the nucleus is plotted against the number of protons for all stable isotopes of various elements a graph, that shows progressive departure from the line where the neutron number N equals the proton number Z, is obtained.

Within the nucleus there are *short range strong nuclear forces* and *long range weak electrostatic forces*. All nucleons attract one another due to the short range nuclear forces irrespective of type or charge but these forces only act on adjacent nucleons. The long range electrostatic forces however act over the entire nucleus causing a repulsion between the similarly charged protons. As the nucleus becomes larger with increasing atomic mass number the influence of the long range electrostatic forces becomes greater since more positively charged protons are present. Under this influence the nucleus becomes unstable and, in order to hold it together, more neutrons are required. These additional neutrons help to bind the nucleus together with their short range nuclear forces and so dilute the effect of the long range electrostatic forces. At very high atomic mass numbers even these additional neutrons are not able to maintain a stable nucleus and all elements with an atomic number Z above 83 (Bismuth) are unstable.

Nuclei with too many neutrons or too few neutrons are also unstable. If there are too few neutrons the excessive electrostatic forces of the protons create instability. If there are too many neutrons the natural instability of the neutrons creates instability. In both cases there is a change in the nucleus to bring the isotope in question closer to the zone of stability. This zone is a curved band just above the N = Z line on a plot of number of neutrons versus number of protons.

RADIO-ACTIVITY

Radio-activity is the emission of particles or waves from the nucleus of an atom. There are four types of *radiation* common in nuclear engineering:

 α -particles β -particle γ -rays neutrons

Radiation is a stream of these particles or waves. Radiation arises from the spontaneous or induced decay of atoms.

Alpha Decay, in which α -particles (Helium nuclei) are emitted, results in the nucleus of the original isotope X losing two protons and two neutrons to form a new isotope Y

$$^{A}X_{Z} \rightarrow ^{A-4}Y_{Z\cdot 2} + {}^{4}\alpha_{2}$$

 $^{234}U_{92} \rightarrow {}^{230}Th_{90} + {}^{4}\alpha_{2}$

Heavy nuclei decay in this way to reduce the charge on the nucleus.

Negative Beta Decay, in which β -particles (electrons) are emitted, results in the nucleus of the original isotope X losing an electron to form a new isotope Y. This electron arises from the disintegration of a neutron into a proton and an electron. The result is the creation of an additional proton in the nucleus and the loss of a neutron. The atomic mass number remains the same.

$${}^{A}X_{Z} \rightarrow {}^{A}Y_{Z+1} + {}^{0}\beta_{-1}$$
$${}^{1}n_{0} \rightarrow {}^{1}p_{1} + {}^{0}\beta_{-1}$$
$${}^{32}P_{15} \rightarrow {}^{32}S_{16} + {}^{\circ}\beta_{-1}$$

Positive Beta Decay in which β^+ -particles (positrons) are emitted results in the original isotope X losing a positron to form a new isotope Y. The positron arises from the conversion of a proton into a neutron. An alternative reaction producing the same result is electron capture

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$${}^{A}X_{Z} \rightarrow {}^{A}Y_{Z-1} + {}^{0}\beta_{1}$$
$${}^{1}p_{1} \rightarrow {}^{1}n_{0} + {}^{0}\beta_{1}$$
$${}^{13}N_{7} \rightarrow {}^{13}C_{6} + {}^{0}\beta_{-1}$$

Electron Capture results in the nucleus of the original isotope X gaining an electron to form a new isotope Y. This electron is integrated with a proton to form a new neutron.

$${}^{A}X_{Z} + {}^{0}e_{-1} \rightarrow {}^{A}Y_{Z-1}$$

 ${}^{1}p_{1} + {}^{0}e_{-1} \rightarrow {}^{1}n_{0}$
 ${}^{59}Ni_{28} \rightarrow {}^{0}e_{-1} + {}^{59}Co_{27}$

Proton Decay was discovered only in 1970 and is rare. A proton is emitted from the nucleus immediately after creation of the unstable nucleus

$${}^{A}X_{Z} \rightarrow {}^{A-1}Y_{Z-1} + {}^{1}p_{1}$$

 ${}^{53}Co_{27} \rightarrow {}^{52}Fe_{26} + {}^{1}p_{1}$

Neutron Radiation is the result of nuclear fission reactions where a surplus of neutrons is produced. A few radioactive isotopes emit neutrons directly but this is rare in the absence of prior nuclear fission. Free neutrons that are not absorbed by other nuclei eventually disintegrate into a proton and an electron (β -particle).

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$${}^{1}n_{o} \rightarrow {}^{1}p_{1} + {}^{0}\beta_{-1}$$

$${}^{A}X_{Z} \rightarrow {}^{A}Y_{Z+1} + {}^{0}\beta_{1} \rightarrow {}^{A-1}Z_{Z+1} + {}^{1}n_{0} + {}^{0}\beta_{-1}$$

$${}^{87}Br_{35} \rightarrow {}^{87}Kr_{36} + {}^{0}\beta_{-1} \rightarrow {}^{86}Kr_{36} + {}^{1}n_{0} + {}^{0}\beta_{-1}$$

$${}^{137}I_{53} \rightarrow {}^{137}Xe_{54} + {}^{0}\beta_{1} \rightarrow {}^{136}Xe_{54} + {}^{1}n_{0} + {}^{0}\beta_{-1}$$

The half life of this reaction is 12 minutes.

RADIO-ACTIVE DECAY

A fundamental law of nature is that the number of random events occurring is proportional to the total number of active elements in the sample. For example the death rate in a certain population is proportional to the number of people making up that population. This can be expressed mathematically as

Number of events / unit time \propto Number in sample

$$dN / dt = -\lambda N$$

The proportionality constant λ is negative if the number of events reduces the number in the sample. This is the case for the decay of radioactive isotopes which, once decayed, cease to exist since they are transformed into different isotopes.

The solution to this differential equation is given as follows where N_0 is the initial number in the sample and N_t is the number in the sample after time t:

$$N_t = N_0 e^{-\lambda t}$$

The *half-life* $t_{1/2}$ of a decay process or radio-active isotope is the time taken for the total number in the sample to be reduced to one half of its initial value:

$$N_{t1/2} = (\frac{1}{2}) N_0$$

At the point of one half-life the previous equation becomes:

$$N_{t1/2} = N_0 e^{-\lambda t 1/2}$$

Combining these two latter equations gives:

$$(\frac{1}{2}) N_0 = N_0 e^{-\lambda t 1/2}$$

The solution of this equation is:

$$t_{1/2} = 0.693 / \lambda$$

This is the very important relationship between the half-life $t_{1/2}$ and the decay constant λ .

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This is important since it is always the half-life that is given in tables or charts but it is the decay constant that is required in calculations.

The *mean life* t_{ave} is the average life of a radioactive isotope. It may be found by integrating the area under the decay curve (total lives of all nuclei) and dividing by the initial number in the sample.

$$t_{ave} = \int_{0}^{\infty} Ndi/N_{o}$$

After substitution for N this gives the following result

$$t_{ave} = 1 / \lambda$$

RADIO-ACTIVE CHAIN

Often a radio-active isotope A decays into an isotope B which itself is radio-active. This second isotope B decays in turn into a third isotope C.

 $A \rightarrow B \rightarrow C$

The rate of decay of A is proportional to the number of nuclei of isotope A.

$$dN_A / dt = -\lambda_A N_A$$

The rate of build-up of B is equal to the rate of decay of A.

 $dN_B / dt = + \lambda_A N_A$

Since isotope B in turn decays the rate of decay of B is given by:

$$dN_B / dt = -\lambda_B N_B$$

The net rate of change of B is then:

$$dN_B / dt = \lambda_A N_A - \lambda_B N_B$$

The solution to this equation is given by the following where N_A is the number of nuclei of isotope B present after time t

 $N_{B} = [\lambda_{A} / (\lambda_{A} - \lambda_{B})] N_{A0} [e^{-\lambda At} - e^{-\lambda Bt}]$

RADIO-ACTIVE BUILD-UP (NEUTRON ACTIVATION)

If radio-active materials are created by the reactions within the nuclei of certain isotopes the rate of build-up of that isotope will be equal to the reaction rate R.

$$dN / dt = R$$

If this isotope decays the rate of decay will be equal to the number of nuclei created at time t.

$$dN / dt = -\lambda N_t$$

The net rate of change of the number of nuclei is then:

$$dN / dt = R - \lambda N_t$$

Eventually an equilibrium condition will be reached where the number decaying is so great that the decay rate is equal to the creation rate. The creation rate usually depends upon external factors and remains essentially constant with time.

$$dN / dt = 0$$
$$R = \lambda N_{m}$$

The equilibrium number prevailing under these conditions is N_{eq} . By substituting this into the previous equation the following differential equation is obtained:

$$dN / dt = \lambda N_{eq} - \lambda N_t$$

The solution to this equation is given by the following:

$$N_t = (R / \lambda) [1 - e^{-\lambda t}]$$

 $N_t = N_{eq} \left[1 - e^{-\lambda t} \right]$

BUILD-UP AND DECAY

If a radio-active isotope is created by a nuclear reaction and subsequently isolated from the creating influence it will subsequently decay according to the formulae given above.

Most radioactive isotopes are created by nuclear irradiation and the artificial nuclides so produced may then be used subsequently in irradiation facilities or radio-active systems while they decay. The radioactivity or simply activity of the radioactive nuclide is at a peak at the time of removal from its initial irradiation. This *activity* α is equal to the rate of decay of the radioactive nuclei.

$$\alpha = dN / dt$$

BINDING ENERGY

Binding energy is the force of attraction between nucleons in the nucleus. Nucleons attract one another and, as they approach one another and bind together, a certain amount of energy is accumulated and released. A force is required to separate the nucleus and the work required in separating them against this force is equal to the binding energy. Thus energy must be supplied to separate nucleons from the nucleus.

There is an analogy between this binding energy and potential energy. Free balls on a flat plane will accumulate kinetic energy on rolling into a shallow well. When they collide this kinetic energy will be dissipated as heat energy. The potential energy has thus been released. In order to lift them back onto the flat plane energy, equal to the potential energy required to lift them out, will have to be supplied. The difference between the two potential energy levels of the balls is analogous to the binding energy of the nucleons.

An analysis of the masses of individual nucleons and various nuclei will reveal that the mass of a nucleus is always less than the sum of the masses of the nucleons. In assembling a nucleus some mass has disappeared. This mass is equal to the binding energy. In order to separate the nucleus into its individual nucleons energy equivalent to the mass deficiency must be supplied. This mass deficiency is known as the *mass defect* and is defined as follows:

Mass Defect = Mass of Nucleons - Mass of Nucleus

The binding energy is equal to the mass defect:

Binding energy may be measured in joules and can be calculated from:

$$E = m c^2$$

Binding energy is more commonly given in mega-electron volts in which case:

$$BE_{nucleus} = (Z m_P + N m_N - {}^{A}M_Z) \times 931.5$$

To obtain the binding energy per nucleon the above value is divided by the atomic mass number:

$$BE_{nucleon} = BE_{nucleus} / A$$

If the binding energy per nucleon is plotted against the atomic mass number a curve is obtained. This curve starts at zero, rises rapidly to a maximum of nearly 9 MeV and then falls slowly to about 7 MeV. The maximum occurs at an atomic mass number of about 80. This indicates that mid-range elements have higher levels of binding energy than light or heavy elements.

If the analogy with potential energy is used again one can consider balls on a flat plane rolling into wells of differing depths. The depth of the well is related to the magnitude of the binding energy. Deeper wells require more potential energy to lift the balls out so deeper wells signify a greater binding energy (energy to separate the nucleons). As the balls drop into deeper wells more energy is released as they come together. The same applies to the mid-range elements which have the higher binding energies per nucleon. If a heavy element fissions into two mid-range elements the excess binding energy is released just as balls falling into deeper wells will release additional energy. This happens when Uranium fissions into two lighter fission fragments. If two light elements fuse into a heavier element the excess binding energy is also released. This happens when Hydrogen fuses into Helium.

If the plot of binding energy per nucleon is inverted it becomes analogous to the flat plane with shallow well to visualise the potential energy. As the balls roll down into deeper wells more potential energy is released. The shape of this curve of binding energy versus atomic mass number is the reason for being able to obtain energy from both nuclear fission and nuclear fusion.



Atomic Notation



Atomic Mass Scale

- * Atomic mass is based on Carbon-12 Atom
- * Atomic mass of Carbon-12 Atom is exactly 12
- Atomic masses of other elements are given relative to Carbon-12
- Atomic Mass (^AX_z) = 12 [Mass (^AX_z)/Mass (¹²C)]
- Atomic Masses are given in the chart of nuclides. Note that the atomic mass includes the mass of the electrons
- When determining the mass of the nucleus only, the mass of the electrons must be subtracted (or cancelled)



OH 1.7



OH 2.24

OH 1.2

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DECAY CONSTANT

NUMBER OF EVENTS SECOND & NUMBER IN SAMPLE

$$\frac{dN}{dt} = -\lambda N$$

WHERE A IS PROPORTIONALITY CONSTANT





HALF LIFE IS TIME FOR NUMBER TO DECAY TO HALF OF THE INITIAL VALUE

$$N_{t} = N_{e} e^{-\lambda t}$$

$$N_{t_{1}} = N_{e} e^{-\lambda t}$$

$$M_{t_{1}} = \frac{1}{2}N_{e}$$

$$\frac{1}{2}N_{e} = N_{e} e^{-\lambda t}$$

$$E = e^{\lambda t}$$

$$k_{e}e^{2} = \lambda t_{1} k_{e}e^{2}$$

$$0.693 = \lambda t_{2}$$

$$t_{1} = \frac{a_{695}}{\lambda}$$

MEAN LIFE



MEAN LIFE IS AVERAGE LIFE OF ATOM OF RADIOACTIVE MATERIAL

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 $\begin{array}{rcl}
\text{OF} & \text{RADIOACTIVE} & \text{MATERIAL} \\
&= & \int_{0}^{\infty} N \, dt \, \big/ \, N_{0} \\
&= & \int_{0}^{\infty} N_{0} \, e^{-\lambda t} \, dt \, \big/ \, N_{0} \\
&= & \int_{0}^{\infty} e^{-\lambda t} \, dt \\
&= & \left[-\frac{1}{\lambda} e^{-\lambda t} \right]_{0}^{\infty} \\
&= & -\frac{1}{\lambda} e^{-\alpha} + \frac{1}{\lambda} e^{-\alpha} \\
&= & 0 + \frac{1}{\lambda} \\
&= & \frac{1}{\lambda}
\end{array}$



HALF LIFE

DECAY OF A

$$\frac{dNA}{dT} = -\lambda_A N_A$$
AMOUNT OF A AFTER TIME t

$$N_{At} = N_{A*} e^{-\lambda_A t}$$
Build-up of & (DECAY OF A)

$$\frac{dNs}{dt} = \lambda_A N_A$$
DECAY OF B

$$\frac{dNs}{dt} = -\lambda_B N_B$$
NET RATE OF CHANGE OF B

$$\frac{dNs}{dt} = \lambda_A N_A - \lambda_B N_B$$

$$= \lambda_A N_{A*} e^{-\lambda_A t} - \lambda_B N_B$$

$$\frac{dNs}{dt} + \lambda_B N_B = \lambda_A N_{A*} e^{-\lambda_B t}$$
THE SOLUTION TO THIS EQUATION IS:

$$N_{Bt} = \frac{\lambda_A}{\lambda_3 - \lambda_6} N_{A*} (e^{-\lambda_A t} - e^{-\lambda_B t})$$

RADIO-ACTIVE BUILD-UP

THIS IS A FIRST ORDER DIFFERENTIAL EQUATION THE SOLUTION TO THIS EQUATION IS :

. Nt • Nog $\left[1 - e^{-\lambda t}\right]$ Nt = $R/\lambda \left[1 - e^{-\lambda t}\right]$

