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Applications of basic chemical composition on heat expansion of solids in an internal combustion engine

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Abstract Almost all materials experience slight deformation in response to changes in temperature. The purpose of this study was to investigate the application of basic chemical composition of heat expansion of solid in an internal combustion engine. It was found that solids are compose of atoms, ions and molecules held by bonds, metallic solids are held by metallic bounding arranged in an orderly repeating pattern, called crystals. Within solid, molecules are typically located in close proximity to one another, contributing to the defined shape of the structure. As the temperature rises, molecules begin to vibrate at a more rapid speed and push away from one another. This increased separation between the individual atoms causes the solid to expand, thus increasing the volume of the structure.

Keywords chemical composition, expansion, internal combustion, chamber engines.

Introduction

According to Ganesan (2012) internal combustion engine is a system in which the combustion of the fuel occurs in a chamber within the system. When the fuel burns inside the combustion chamber, high pressure and high temperature gases are produced. These gases exert a direct force on the walls of the combustion chamber. This linear force is converted into useful reciprocating rotational motion by the connecting rod and the crankshaft mechanism. This favors the internal combustion engine efficiency [1].

Furthermore, combustion also known as burning is the basic chemical process of releasing energy from a fuel and air mixture. In an internal combustion engine (ICE), the ignition and combustion of the fuel occurs within the engine itself. The engine then partially converts the energy from burning to useful working principles. The engine consists of a fixed cylinder connecting rod, crankshaft and a moving piston. The expanding combustion gases push the piston. This in turn rotates the crankshaft and ultimately through a system of gears in the power train drives the vehicles wheels.

There are two kinds of internal combustion engines currently in use, the spark ignition gasoline engine and the compression ignition diesel engine. Most of these are four-stroke cycle engines, meaning that four piston strokes are needed to complete a cycle. The cycles include four distinct processes: intake or induction, compression, combustion or power stroke, and exhaust.

The Spark ignition gasoline and compression ignition diesel engines differ in how they supply and ignite the fuel. In a spark ignition engine, the fuel is mixed with air and then inducted into the cylinder during the intake process. The piston compresses the fuel-air mixture; the spark ignites it, causing combustion. The expansion of the combustion gases pushes the piston during the power stroke. In the diesel engine, only air is inducted into the engine and then corn pressed. Diesel engines then carry out combustion by spraying the fuel into the hot air compressed air at a suitable, measured rate.

Types of internal combustion engine and application of four stroke cycle

There are two types of internal combustion engines. They are:

- Four Stroke Internal Combustion Engine
- Two Stroke Internal Combustion Engine

Fundamental of Internal Combustion Engine

According to Heywood (1988) a lot of research works was carried out in the 20th century to get the maximum utilization of heat and to convert it into useful work, as a result we have IC engines. The second law of thermodynamics also states that energy cannot be completely converted into useful work but the idealized device of Carnot heat engine is designed to help us overcome this problem to a large extent. Carnot engine basically uses the heat to convert it into useful work in a cyclical or repetitive manner [3].

The four strokes of the cycle are intake, compression, power, and exhaust.

1. **Intake:** During the intake stroke, the piston moves downward, drawing a fresh charge of vaporized fuel/air mixture. In the illustrated engine features above, a poppet intake valve is drawn open by the vacuum produced by the intake stroke. Some early engines worked on this principle; however, most modem engines incorporate an extra cam/lifter arrangement as seen on the exhaust valve. The exhaust valve is held shut by a spring.

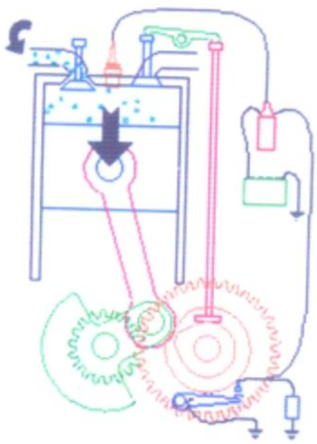

Figure 1: A diagram showing the intake stroke.

2. **Compression:** As the piston rises, the poppet valve is forced shut by the increased cylinder pressure. Flywheel momentum drives the piston upward, compressing the fuel air mixture.

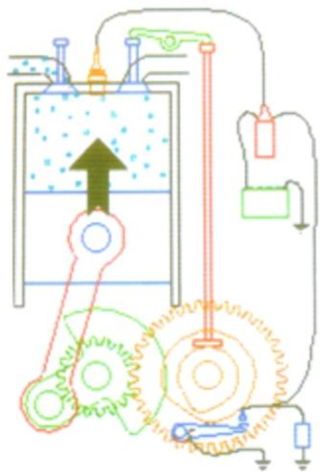

Figure 2: a diagram showing the compression stroke

3. **Power:** At the top of the compression stroke, the spark plug fires, igniting the compressed fuel. As the fuel bums it expands, driving the piston downward.

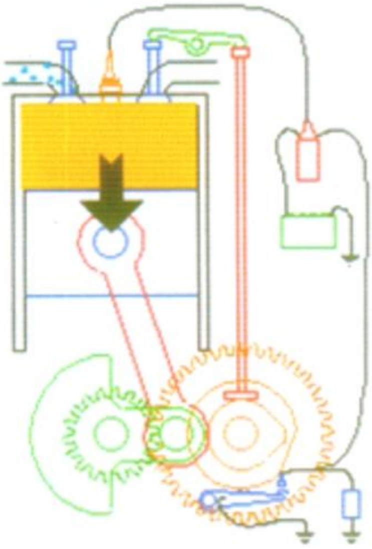

Figure 3: a diagram showing the power stroke

4. **Exhaust:** At the bottom of the power stroke, the exhaust valve is opened by the cam/lifter mechanism. The upward stroke of the piston drives the exhausted fuel out of the cylinder.

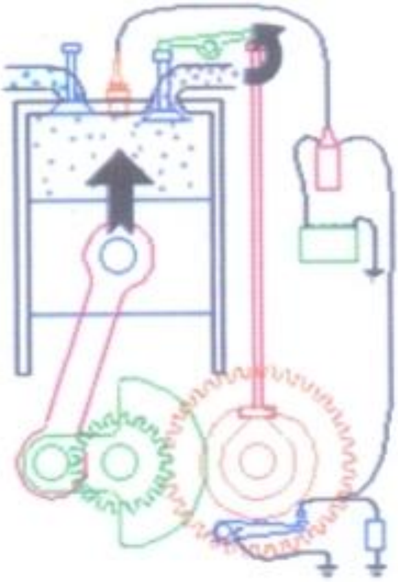

Figure 4: a diagram showing the exhaust stroke

Applications: Two-stroke engines are generally less expensive to build compared to four-stroke engines, and they are lighter and can produce a higher power-to-weight ratio. For these reasons, two-stroke engines are ideal in applications such as chainsaws, weed trimmers, outboard motors, off-road motorcycles and racing applications. Two-stroke engines are also easier to start in cold temperatures, making them ideal for use in snowmobiles

Four-stroke engines, on the other hand, produce more torque at lower resolution per minute rpm, generally providing greater equipment durability than high-revving two-stroke engines, while also providing greater fuel efficiency and lower emissions. For these reasons, four-stroke engines are ideal in applications such as motorcycles, ATVs and personal watercraft [4].

Basic Chemical Composition in the Expansion of Solid

Chemistry: Is the branch of science concerned with the substances of which matter is composed, the investigation of their properties and reactions, and the use of such reactions to form new substances. The chemical composi1ion and properties of a substance or body are essential in heat expansion of solids.

Solid is one of the four fundamental states of matter (the other being liquid, gas and plasma). It is characterized by structural rigidity and resistance to changes of shape or volume. Unlike a liquid, a solid object does not flow to take on the shape of its container, nor does it expand to fill the entire volume available to it like a as does. The atoms in a solid are tightly bound to each other, either in a regular geometric lattice (crystalline solid which include metals and ordinary ice) or irregularly (an amorphous solid such as common window glass). Metals typically are strong, dense, and good conductors of both electricity and heat. Mixtures of two or more elements in which the major component is a metal are known as alloys. Metallic solids are held together by a high density of shared, delocalized electrons, known as "metallic bonding" In a metal, atoms readily lose their outermost ("valence") electrons, forming positive ions. The free electrons are spread over the entire solid, which is held together firmly by electrostatic interactions between the ions and the electron cloud [5]. The large number of free electrons gives metals their high values of electrical and thermal conductivity. The free electrons also prevent transmission of visible light, making metals opaque, shiny and lustrous

Figure 5a: *Square Array Layering*

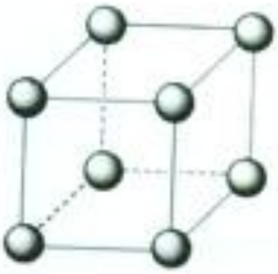

Figure 5b: *Simple Cubic lattice*

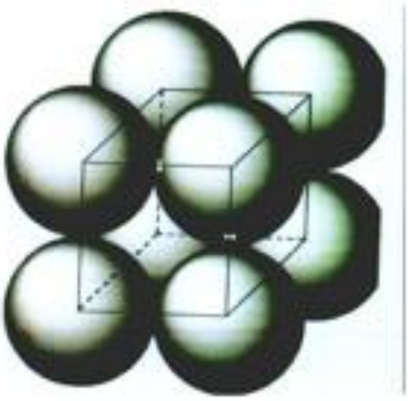

Figure5c: *Space Filling Simple Cubic lattice*

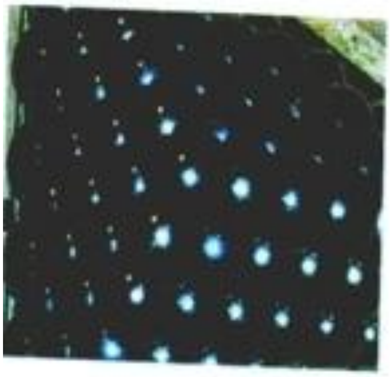

Figure 5d:

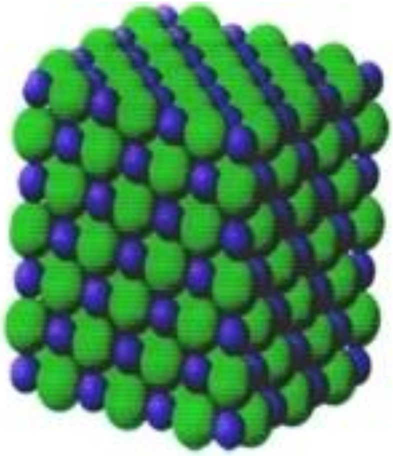

Figure 5e:

Pictorial presentation of atoms arrangement in solids (source: Wikipedia, 2015)

Expansion in Solids

Materials in general will usually change their size when they are been heated to a certain temperature, if held in that temperature for a while. Solid materials, are usually not appreciably affected by temperature in their size and so, for solids, it's usually not necessary to specific that the pressure be held constant.

Common engineering solids usually have coefficients of thermal expansion that do not vary significantly over the range of temperatures where they are designed to be used, so where extremely high accuracy is not required, practical calculations can be based on a constant, average, value of the coefficient of expansion [6].

Thermal expansion is the tendency of matter to change in volume in response to a change in temperature, through heat transfer. Temperature is a monotonic function of the average molecular kinetic energy of a substance. When a substance is heated the kinetic energy of its molecules increases; thus, the molecules begin moving more and usually maintain a greater average separation. Materials which contract with increasing temperature are unusual; this effect is limited in size, and only occurs within limited temperature ranges. The degree of expansion divided by the change in temperature is called the material's coefficient of thermal expansion and generally varies with temperature.

Linear expansion

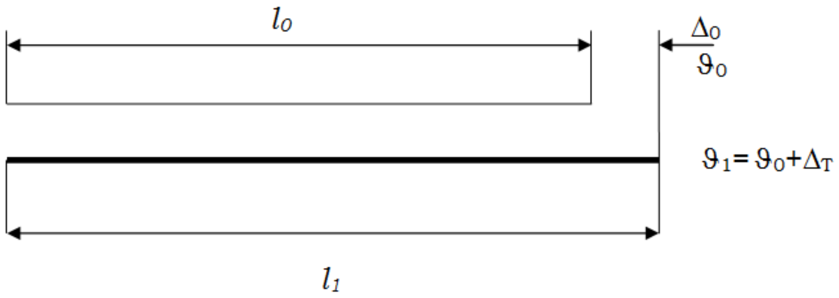

Figure 6: Change in length of a rod due to thermal expansion.

To a first approximation, the change in length measurements of an object ("linear dimension" as opposed to, e.g., volumetric dimension) due to thermal expansion is related to temperature change by a "linear expansion coefficient". It is the fractional change in length per degree of temperature change. Assuming negligible effect of pressure, we may write: $\alpha_L = \frac{1}{L}\frac{dL}{dT}$ (1)

Where L is a particular length measurement and dL/dT is the rate of change of that linear dimension per unit change in temperature.

The change in the linear dimension can be estimated as: $\frac{\Delta L}{L} = \alpha_L \Delta T$ (2)

This equation works well as long as the linear-expansion coefficient does not change much over the change in temperature ΔT. If it does, the equation must be integrated.

Effects expansion on strain

For solid materials with a significant length, like rods or cables, an estimate of the amount of thermal expansion can be described by the material strain, given by $E_{thermal}$ and defined as:

$$E_{thermal} = \frac{L_{final} - L_{initial}}{L_{initial}} \quad (3)$$

Where $L_{initial}$ is the length before the change of temperature and "final is the length after the change of temperature.

For most solids, thermal expansion is proportional to the change in temperature:

$$E_{thermal} \alpha \Delta T \quad (4)$$

Thus, the change in either the strain or temperature can be estimated by:

$$E_{thermal} \alpha_L \Delta T \quad (5)$$

Where $\Delta T = \left(T_{final} - T_{initial}\right)$ (6)

is the difference of the temperature between the two recorded strains, measured in degrees Celsius or Kelvin, and is the linear coefficient of thermal expansion in "per degree Celsius" or "per Kelvin", denoted by $^{O}D^{01}$ or K^{01}', respectively. In the field of continuum mechanics, the thermal expansion and its effects are treated as eigenstrain and eigenstress.

Area expansion

The area of thermal expansion coefficient relates to the change in a material's area dimensions to a change in temperature. It is the fractional change in area per degree of temperature change. Ignoring pressure, we may write:

$$\alpha_A = \frac{1}{A}\frac{dA}{dT} \quad (7)$$

Where *A* is some area of interest on the object, and dA/dT is the rate of change of that area per unit change in temperature.

The change in the area can be estimated as:

$$\frac{\Delta A}{A} = \alpha_A \Delta T \quad (8)$$

This equation works well as long as the area expansion coefficient does not change much over the change in temperature δT . If it does, the equation must be integrated.

Volume expansion

1. For a solid, we can ignore the effects of pressure on the material, and the volumetric thermal expansion coefficient car' be written where *V* is the volume of the material, and dV/dT is the rate of change of that volume with temperature [7].

$$\alpha_V = \frac{1}{V}\frac{dV}{dT} \quad (9)$$

This means that the volume of a material changes by some fixed fractional amount, for example, a steel block with a volume of 1 cubic meter might expand to 1.002 cubic meters when the temperature is raised by 50 K. This is an expansion of 0.2%. If we had a block of steel with a volume of 2 cubic meters, under the same conditions, it would expand to 2.004 cubic meters, again an expansion of 0.2%. The volumetric expansion coefficient would be 0.2% for 50K, or 0.004% K^{1}.

Since already know the expansion coefficient, then we can calculate the change in volume

$$\frac{\Delta V}{V} = \alpha_V \Delta T \quad (10)$$

Where $\Delta V/V$ is the fractional change in volume (e.g., 0.002) and ΔT is the change in temperature (50°C).

The above example assumes that the expansion coefficient did not change as the temperature changed. This is not always true, but for small changes in temperature, it is a good approximation. If the volumetric expansion coefficient does change appreciably with temperature, then the above equation will have to be integrated:

$$\frac{\Delta V}{V} = \int_{Ti}^{T} \alpha_V(T)\, dT \quad (11)$$

Where $\alpha_V(T)$ the volumetric expansion coefficient as a function of temperature *T*, and Ti, T_f are the initial and final temperatures respectively [7].

Fuel

A fuel is a substance that releases energy. Some fuels, for example coal, wood, candle, papers, kerosene, petrol, diesel, uranium, etc. Uranium release energy from nuclear reactions. Most fuels release their energy by reacting with oxygen in the air (burning). A fuel burns more rapidly and releases energy at a faster rate if it is supplied with pure oxygen instead of air. High temperature torches for metal welding a mixture of pure oxygen with a fuel called acetylene (ethyne). The question is what substance makes a good fuel?

A substance is a good fuel if it is easily available, releases a large amount of energy, produces a small amount of pollutant products and is easy to store and transport. The amount of energy released by a fuel can be measured using a simple calorimeter.

Heat is simply the transfer of energy from a hot object to a colder object. Heat is a form of energy.

According to Berger (2005) the flames caused as a result of a fuel undergoing combustion (burning) [8]. Combustion or burning is a high-temperature exothermic redox chemical reaction between a fuel and an oxidant, usually atmospheric oxygen, which produces oxidized, often gaseous products, in a mixture termed as smoke. Combustion in a fire produces a flame, and the heat produced can make combustion self-sustaining. Combustion is often a complicated sequence of elementary radical reactions. Solid fuels, such as wood, first undergo endothermic pyrolysis to produce gaseous fuels whose combustion then supplies the heat required to produce more of them.

Combustion reactions according to De Leon (2013) always involve molecular oxygen O_2. Any time anything burns (in the usual sense), it is a combustion reaction. Combustion reactions are almost always exothermic (i.e., they give off heat) [9].

Wood as well as many common items that combust are organic (i.e., they are made up of carbon, hydrogen and oxygen). When organic molecules combust the reaction products are carbon dioxide and water (as well as heat).

$$\begin{array}{l}\text{Organic} \\ \text{Molecules} \\ \text{with } (\text{C}, \text{H and O})\end{array} + 02 \rightarrow co_2 + H_2 0 + \text{Heat}$$

For example consider the combustion of methanol (rubbing alcohol):

$$CH_3OH + 0_2 \rightarrow CO_2 + 2H_2 0 + \text{Heat} \quad (12)$$

Of course, not all combustion reactions release CO_2 and water, e.g., the combustion of magnesium metal:

$$2Mg + 0_2 \rightarrow 2MgO + \text{Heat} \quad (13)$$

Combustion is often hot enough that light in the form of either glowing or a flame is produced. A simple example can be seen in the combustion of hydrogen and oxygen into water vapor, a reaction commonly used to fuel rocket engines. This reaction releases 242 kJ/mol of enthalpy (heat):

$$2H_2(g) + O_2(g)' \ 2H_2O(g) \quad (14)$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \quad (15)$$

Complete combustion equation of methane and a hydrocarbon

The combustion of methane, a hydrocarbon

In complete combustion, the reactant bi4rns in oxygen, producing a limited number of products. When a hydrocarbon burns in oxygen, the reaction will primarily yield carbon dioxide and water. When elements are burned, the products are primarily the most common oxides. Carbon will yield carbon dioxide, sulfur will yield sulfur dioxide, and iron will yield iron (III) oxide. Nitrogen is not considered to be a combustible substance when oxygen is the oxidant, but small amounts of various nitrogen oxides (commonly designated NO*x* species) form when air is the oxidant.

Combustion is not necessarily favorable to the maximum degree of oxidation, and it can be temperature-dependent. For example, sulfur trioxide is not produced quantitatively by the combustion of sulfur. NO' species appear in significant amounts above about 2,800 °F (1,540°C), and more is produced at higher temperatures. The amount of NO*x* is also a function of oxygen excess [10]

In most industrial applications and in fires, air is the source of oxygen (O_2). In air, each mole of oxygen is mixed with approximately 3.71 mol of nitrogen. Nitrogen does not take part in combustion, but at high temperatures some nitrogen will be converted to NO*x* (mostly NO, with much smaller amounts of NO_2). On the other hand, when there is insufficient oxygen to completely combust the fuel, some fuel carbon is converted to carbon monoxide and some of the hydrogen remains un reacted. A more complete set of equations for the combustion of a hydrocarbon in air therefore requires an additional calculation for the distribution of oxygen between the carbon and hydrogen in the fuel.

The amount of air required for complete combustion to take place is known as theoretical air. However, in practice the air used is 2-3x that of theoretical air [10].

Incomplete Combustion

Incomplete combustion will occur when there is not enough oxygen to allow the fuel to react completely to produce carbon dioxide and water. It also happens when the combustion is quenched by a heat sink, such as a solid surface or flame trap.

For most fuels, such as diesel oil, coal or wood, pyrolysis occurs before combustion. In incomplete combustion, products of pyrolysis remain unburnt and contaminate the smoke with noxious particulate matter and gases. Partially oxidized compounds are also a concern; partial oxidation of ethanol can produce harmful acetaldehyde, and carbon can produce toxic carbon monoxide.

Various other substances begin to appear in significant amounts in combustion products when the flame temperature is above about 1,600 K. When excess air is used, nitrogen may oxidize to NO and, to a much lesser extent, to NO_2. CO forms by disproportionate of CO_2, and H_2 and OH form by disproportionate of H_2O.

Metallic Bonding and the Properties of Metals

A metal is a lattice of positive metal 'ions' in a 'sea' of delocalized electrons.

Metallic bonding refers to the interaction between the delocalized electrons and the metal nuclei.

The physical properties of metals are the result of the delocalization of the electrons involved in metallic bonding.

According to ATJS-e-TUTE (2014) the physical properties of solid metals could be explained under the following, as:

1) Conduct electricity and heat: Solid and liquid metals conduct heat and electricity. The delocalized electrons are free to move in the solid lattice. These mobile electrons can act as charge carriers in the conduction of electricity or as energy conductors in the conduction of heat.
2) Generally high melting and boiling points: In general, metals have high melting and boiling points because of the strength of the metallic bond.
   The strength of the metallic bond depends on the number of electrons in the delocalized 'sea' of electrons. (More delocalized electrons results in a stronger bond and a higher melting point.)
3) Packing arrangement of the metal atoms. (The more closely packed the atoms are the stronger the bond is and the higher the melting point). Strong
4) Malleable: Metals are malleable and ductile. The delocalized electrons in the 'sea' of electrons in the metallic bond, enable the metal atoms to roll over each other when a stress is applied (can be hammered or pressed out of shape without breaking) ductile (able to be drawn into a wire) metallic lustre
5) Opaque (reflect light): Metals typically have a shiny, metallic luster. Photons of light do not penetrate very far into the surface of a metal and are typically reflected, or bounced off, the metallic surface [11].

Summary

Metals expand when heated and contract when cooled. This is an important factor to consider for machine parts or structural components that exist in environments with fluctuating temperatures. If a part expands, it can create stresses on other structural part s and possibly cause failure. The exact deformation of any object depends on its geometry and it's constant of thermal expansion. The internal combustion engine works on the principle of combustion (burning), excessive heat generated as a result of pre-ignition, detonation, spark knock, combustion instability pinging, etc. Create intense high frequency pressure waves and vibration that buckle or damage engine components resulting to engine knock or break down. Adequate knowledge of composition and expansion of solid is required to overcome this phenomenon.

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