ENVIRONMENTAL IMPLICATION OF COMBUSTION: THE MODELING OF COAL COMBUSTION[a]

Abraham A. Asere
Mechanical/Production Engineering and Petroleum Engineering Programmes
Abubakar Tafawa Balewa University, P.M.B. 20248, Bauchi,Nigeria

Introduction

The increasing awareness of environmental effects of the by products of various sources of actions taken in the economic development and its sustenance, in different nations of the world, has prompted the necessity to address the arrest of or mitigate the effect of pollution from source. The growing popularity and public understanding of the dangers posed to man by pollutants has given rise to the formation of political group campaigners such as the Anti-Nuclear Group, CND – Campaign for Nuclear Disarmament – and the Green Peace. These groups have lobbied successfully governments of developed nations of the world to institute various legislation that will see to the banning or reduction of emission of potent pollutants into the atmosphere. This action had led to international agreement in some areas of pollutant emission. In air pollution, the chronic effects are evident primarily in poor visibility, eye irritation, growth reduction yield reduction, widespread population structural changes and permanent physical changes to vegetation.

The short-term effects of some pollutant (Frenkiel [1]) may result in loss of several man-hours at governmental or industrial set up and economic waste in Medicare finances, due to sicknesses and hospitalization of victims as well as accidents on our roads. Long-term effects may be simply quantified as human death, irreversible changes in growth with devastating effects on economy and various deformations to newborn due to genetic defects.

However potent the side effect of some of these pollutants, their sources is such that development cannot totally afford to do without. The energy source for generating electricity and for powering our transport and industrial system, release such pollutants that cause acid rain, nausea, chronic heart diseases, intestinal hemorrhages and death to aquatic lives. The depletion of fossil fuel has led man to investigate the substitution of nuclear fuel, only to find that the side effect of this material's use is very dangerous to life on earth and hence greater precautions and safety factors have to be instituted to mitigate these side effects. The production of various items for economic sustenance from our industries generates pollutants which goes to show vividly that we cannot do without generating pollution if we are to keep pace with development and cutting down on the nauseating by-products seem to be the only option.

[a] AMS Subject classification:80A

The modeling of the combustion of coal is very important for the following reasons:

(a) The combustion of coal is such an environmental issue that provoke violent demonstrations from various political divide activists most especially Green-peace.

(b) The generation of power employing this fuel request for a lot of care in other to meet Environmental Protection Agency's regulation in emission into the environment.

(c) Coal deposit in Nigeria is large and compares favorably with petroleum deposit but for reasons of emissions and inadequate knowledge of combustion procedure this vast amount of energy have been abandon and lies unutilized, with the concomitant of job losses.

(d) Nigeria needs energy for technological progress and current employment of petroleum-derived fuel cannot provide our needs since our foreign earnings depend on crude oil and gas. Nigeria must result therefore to the utilization of her vast deposit of coal if she must get away from nuclear power stations that provoke more problems and political issues than it is the case with coal. United States of America, China (Mass[2]), South Africa, Australia and Britain have large deposits of coal and utilize them for power generation.

(e) The utilization of Nigerian coal will provide the much-needed employment at this time of very high unemployment and stage of our development.

Modeling of the combustion of coal is one sure way of understanding the gravity of the usage of coal. It is the way by which the environmental pollution of its combustion may be solved and helps in the engineering of the combustion chamber to produce efficient combustor system

There are many approaches to the combustion of coal. However the two most efficient methods of coal combustion is pulverized combustion and fluidized bed combustion. Of these two the modeling of the combustion of coal by pulverized method will be discussed here. Save to say here that research into fluidized bed combustion of coal is going on, at ATBU presently, by the author.

Pulverized Coal

Pulverized coal is coal that has been crushed and ground to a fine powder so that it can be carried as a suspension in a stream of air, injected into a combustion chamber[3] and burnt, as if it is a gas fuel, in seconds or less. The typical mean size of the coal particle is in the range of 30 to 70 micron. Pulverized coal could be used for power generation or as a source of heat in the manufacture of cement. Other industrial applications of coal abounds[4,5]. Hence the effective combustion and the understanding of it is very important if we are to utilize this vast resource of fuel in this country (Famuboni[6],Asere[7]) Figure 1 shows the areas of Coal and lignite deposit in Nigeria. The figure is just an indication of part of energy resources that is available for exploitation in this country to resolve the energy needs.

Combustion Camber Burning of Coal

The parameters of the combustion chamber employed in this modelling are horizontal tube of 1.09m in diameter and 6.10m long. Pulverized coal and primary air were fired axially. The input flow rates and velocities required have been determined.

Heat transfer in the combustor was predominantly radioactive, convective transfer was very small. However convection played a significant role in the primary zone of the combustor. An important process in the combustion is that of the char. The coal particle was assumed to be constant-density spheres that burned only at the outside.

Mathematical Model

Mathematical models are constructed on the bases of questions needed to be answered and the degree of precision required. Also of significance in combustion is the magnitude of input required. The purpose of the model is to estimate the fraction of carbon remaining unburnt, U, oxygen partial pressure, radiation to the walls and temperature.

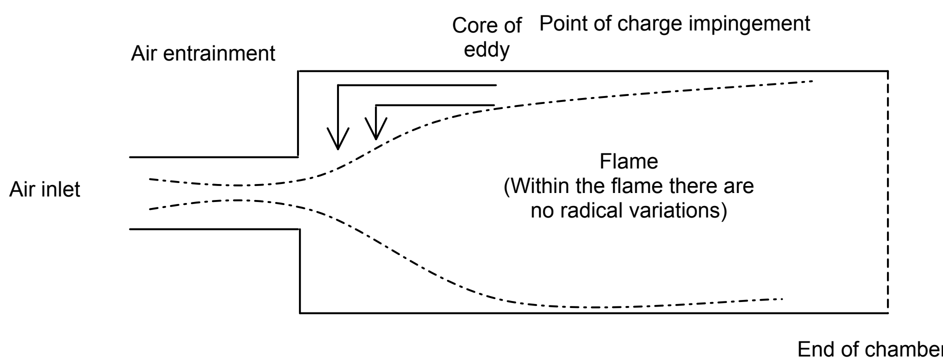

Fig. 2: Combustion Chamber with assumed flow pattern.

These quantities are to be calculated for various numerical values of the factors influencing them.

Some assumption in the model must be made and these are:

(1) Flow pattern is assumed as shown in the above figure. Flame is assumed to mean part of the chamber occupied by coal suspension coming from the primary zone.
(2) The flame expands in Chamber until it reaches the point of impingement and there after fills the combustor.
(3) Area from inlet to impingement zone is occupied by recirculation eddy.
(4) Rate of entrainment of re-circulated fluid and rate of extraction of fluid from flame to eddy are constant.

(5) Combustion in the re-circulated eddy is complete before entering the flame.
(6) No variation of composition, velocity and temperature.
(7) No longitudinal mixing.
(8) Particle moves at the same speed as the gas steam.

Heat transfer assumptions made are:

Isothermal and internally adiabatic heat transfer represents perfect heat and the zero heat transfer longitudinally within the flame. There is radiant heat to the wall. Emissivity of particles, and absorption coefficient of the gas are constant; Radiation from soot, and ash ignored; Gas and particle temperature are equal; dissociation is ignored and specific heat of suspension is assumed to be constant.

Reaction rate assumptions are:

(a) Constant density and size of char particles
(b) Volatile matter burns first
(c) Reaction rate is governed by:

$$q = \frac{p_g}{\left(1/k_{diff} + 1/k_s \right)} \quad (1)$$

$k_{diff} = 24\phi D/xR'T_m$
$P_g =$ Partial pressure of oxygen in the gas.
$K_s =$ Coefficient of surface reaction rate.
ϕ = mechanism factor = 1 for CO_2 and 2 for CO
D = diffusion coefficient of oxygen in the gas
x = particle diameter
R' = gas constant
T_m = mean gas temperature.

(d) Particle burns from particle surface.

Basic Equations for the Model

Combustion Rate of Carbon Particles

Employing the assumption that the char burns from outside the rate of change of coal fraction u_j is

$$\frac{du_j}{dt} = -\frac{u_j^{0.67} w_j^{0.67} s_{jo} p_g(U)}{u_j^{0.33} \frac{w_j^{-0.33}}{k_{diff \cdot jo}} + 1/k_s} \tag{2}$$

where w = weight; and

$$s_{jo} = {6w_j}/{\rho_a x_{jo}}$$

It could be shown that

$$k_{diff \cdot jo} = \overline{k_{diff \cdot jo}} \left(T_m / \overline{T} \right)^{0.75} \tag{3}$$

$$k_s = \overline{k_s} \exp\left(E/R\overline{T} \right) \exp\left(-E/RT_s \right) \tag{4}$$

Here T_s = surface temperature of particle and K_s is the surface reaction rate coefficient at temperature $\overline{T}$.

The unburnt fraction of the whole coal is given as

$$U = \sum u_j \tag{5}$$

Oxygen Concentration

Now the total flow rate of gas within the flame varies with distance from the burner and is given by:

$$m = (1 + B + N)m_p \tag{6}$$

Where m = total mass flow rate of gases within flame
m_p= primary air flow-rate.
B = mass flow of secondary air entrained within flame per unit mass of

primary air.

N = mass flow of entrained recirculated gases per unit mass of primary air.

$$B = B_o \, {}^{s}\!/_{s_2} \quad \text{for } s \le s_2$$

$$B = B_o \quad \text{for } s > s_2$$

where s = axial distance from burner s_2 = distance at which entrainment of secondary air is completed. The mass of entrained recirculated gas also varies as *B* in the form of

$$N = N_{max}\left({}^{s}\!/_{s_c}\right) \quad \text{for } s \le s_c$$

$$N = N_{max}(s_r - s)/(s_r - s_c) \quad \text{for } s_c < s < s_r$$

$$N = 0 \text{ for } s \ge s_r$$

where s_c = distance to core of eddy
s_r = distance to point of impingement
N_{max} = value of N at core of eddy.

For a unit mass of primary air that enters the combustion unit it entrains both secondary and recirculated gas and continues to increase if no combustion takes place in the flame, hence mass of oxygen sample can be stated as:

$$F_{02} = f_0 + Bf_0 + N_m f_0 e/(1+e) \quad (7)$$

where f_o= oxygen mass fraction in air
e = excess air as a fraction of the stoichiometric air
N_m = mass recirculation gases which has been mixed with unit mass of primary air.
N_m = N up to the core of recirculation eddy. Beyond the core the value of N decrease but that of N_m does not hence

N_m = N for $s < s_c$
$N_m = N_{max}$ for $s \ge s_c$

Excess air is defined as

1+ e = Total air supplied to furnace / air required for complete combustion

For complete coal combustion the magnitude of oxygen used per air supplied is

$$\text{Oxygen required for complete combustion} = \frac{(1+B_0)f_0}{(1+e)} \tag{8}$$

Hence after the char, and the fixed carbon had been burnt and the volatile is also burnt oxygen consumed in the sample per unit mass of air input is

$$F0_2\ (\text{Consumed}) = (1-cU)(1+B_0)f_0/(1+e) \tag{9}$$

If the equation of oxygen consumed is combined with equation of oxygen mass fraction then oxygen mass fraction could be determined as

$$\frac{f}{f_o} = \frac{\left[1+B+N_m\, {}^{e}\!/\!{}_{(1+e)}\right] - \left[(1-cU)(1+B_o)/(1+e)\right]}{1+B+N_m} \tag{10}$$

Ignoring changes in molecular weight

$$p_g(u)/p_o = {}^{f}\!/\!{}_{f_o} \tag{11}$$

Time / Distance Relation

The parameters of oxygen concentration such as B and N_m are quantified in distance. However the residence time of combustion is significant both in energy released and total combustion. Hence the relation between distance and time is obtained from velocity in the flame. This varies along the flame but assumed constant across a section.
The relation is:

$$dt = \frac{ds}{v} \tag{13}$$

v = velocity at distance s from the burner. The velocity in a direction parallel to the axis of the combustion chamber is calculated from the volume flow rate at any section divided by the cross-sectional area of the flame:

$$v = 4(1 + B + N)m_p / \rho_g \pi L^2 \qquad (14)$$

where ρ_g = density of the gases at flame temperature
L = flame width assume conical in the combustor

$L = 2[\![r_o + (r_f - r_o) s/s_r]\!]$ for $s < s_r$
$= 2 r_f$ for $s \geq s_r$

r_o = radius of injection nozzle
r_f = radius of the cylindrical combustor.

The gas density is inversely proportional to the temperature and is given as

$$\rho = \overline{\rho_g} \, \overline{T} / T \qquad (15)$$

where ρ = density of air at temperature T. Having determine v at any distant s, the derivative of equation 13 may be integrated to obtain time in relation to distant knowing the temperature.

Temperature in Flame

In computing the flame temperature the plug flow combustion model is considered. Temperature is very important in the combustion of fuel. This is because most pollutant or their ions are formed in relation to temperature fields[8]. At higher combustion temperature nitrogen reacts with oxygen to form nitrogen oxides - NO_x, sulphur becomes sulphur oxides - SO_x. Furthermore at high temperature dissociation and ionization become prevalent. In hydrocarbon combustion at high temperature a lot of radicals are produced whose emission into the atmosphere causes smog and a lot of other problems injurious[9-13] to human and her ecosystem. In this model there are two approaches to the computation of temperature or energy in the flame. These approaches are the isothermal approach in which the temperature is considered uniform and given for each run. The other approach is the internally adiabatic version in which the temperature is considered to vary along the flame.

Considering the internally adiabatic approach. Here the temperature varies along the flame. Heat balance for a thin slice of the flame is employed.

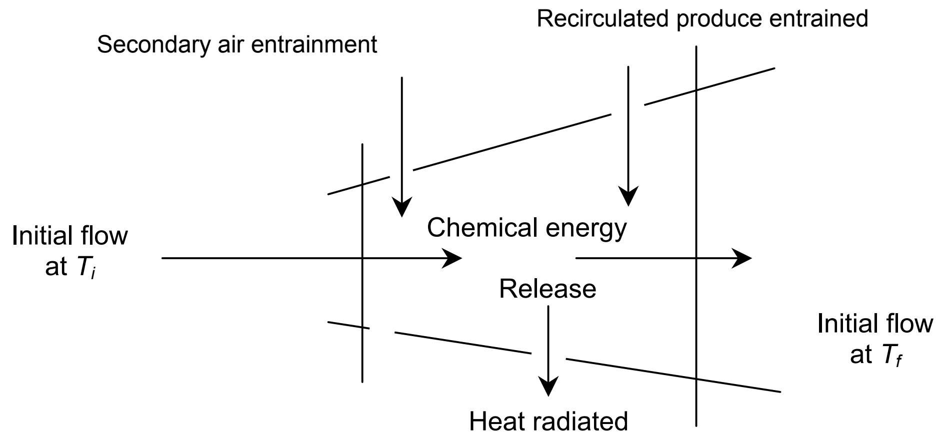

Fig.3 : Heat balance for a thin flame

Heat Balance for a thin slice.

Three zones are identified: (a) Zone up to where volatile combustion is complete
(b) Zone to the recirculation eddy core.
(c) Zone beyond recirculation eddy core.

At the first zone the coal is promised and volatile matter released is burnt warming up the charcoal to its ignition temperature. Here no heat is lost. In the second zone heat balance for a thin slice of flame is obtained as

$$m_e T_e c_p = m_i c_p T_i + \Delta B C_p T_b + \Delta N C_p T_r + \Delta G - \Delta H_{rad} \tag{16}$$

Where C_p = Specific heat of suspension
m_e = mass flow rate of suspension in flame at end of slice
m_i = mass flow rate of suspension in flame at beginning
ΔB = increase of Secondary-air flow rate
ΔN = increase of recirculated gas flow rate
T_b = temperature of secondary air
T_e = temperature at the end.
T_i = temperature at the beginning.
T_r = temperature of recirculated gases entering zone
ΔG = rate of heat generation
ΔH_{rad} = rate of radiation from the zone.

In the 3rd zone the fluid that leaves the flame to recirculation eddy is at the temperature of the flame hence the temperature T_r will be T_i temperature of the flame. Hence

$$m_e T_e c_p = m_i C_p T_i + \Delta B C_p T_b + \Delta N C_p T_i + \Delta G - \Delta H_{rad} \quad \text{for } s > s_c \quad (17)$$

Heat generation in zone 2 is

$$\Delta G = -m_c Q \Delta U \quad \text{for } s \leq s_c 18) \quad (18)$$

where m_c = initial feed rate of residual char
Q = heat released per unit weight of carbon burnt
-ΔU = fraction of initial residual char feed burnt.

In zone 3 the quantity of flow determined to give (1 + B + N)/(1 + B + N_{max}) fraction hence in this zone heat generation is

$$\Delta G = -m_c Q \Delta U (1 + B + N) / (1 + B + N_{max}) \quad \text{for } s \geq s_c \quad (19)$$

Radiative heat to the wall is given as

$$\Delta H_{rad} = A^1 \varepsilon \sigma \left(T^4 - T_w^4\right) \Delta S \quad (20)$$

Where A′ = surface area of flame/unit length of axis = circumference
ε = emissivity of flame
σ = Stefan- Boltzman constant
T_w = Wall temperature.

The emissivity of the flame varies with distance from the burner and is computed as

$$\varepsilon = 1 - \exp(-kL_{eff}) \quad (21)$$

Where k = absorption coefficient of flame
L_{eff} = effective width of flame

$$K = K_p + K_g$$

for grey body particles the absorption coefficient is given as

$$K_p = \frac{1}{4} C_w S_w^1 \varepsilon_p \tag{22}$$

where C_w = concentration of particles
$S_w{}'$ = specific surface area of particles
ϵ_p = particle emissivity.

$$C_w = n_{fc} U \rho_g \,/\, \left(1 + B + N_m\right) \tag{23}$$

n_{fc} = initial mass of residual char per uit mass of primary air.
$S_w{}'$ is the sum of contribution from all size fractions

$$S_w^1 = \sum u_j S_j^1 / U \tag{24}$$

where

$$S_j^1 = \frac{6}{\rho_a x_j}$$

For computation purposes

$$S_w^1 = \frac{\sum u_j S_j^1}{U} = \frac{6}{\rho_a U} \sum \frac{u_j^{0.67} W_j^{0.33}}{x_{jo}} \tag{25}$$

Isothermal Approach

In this approach an initial value of temperature for the flame is assumed. Better temperature at which heat generated is equal heat loss is obtained by preparing an overall heat balance.

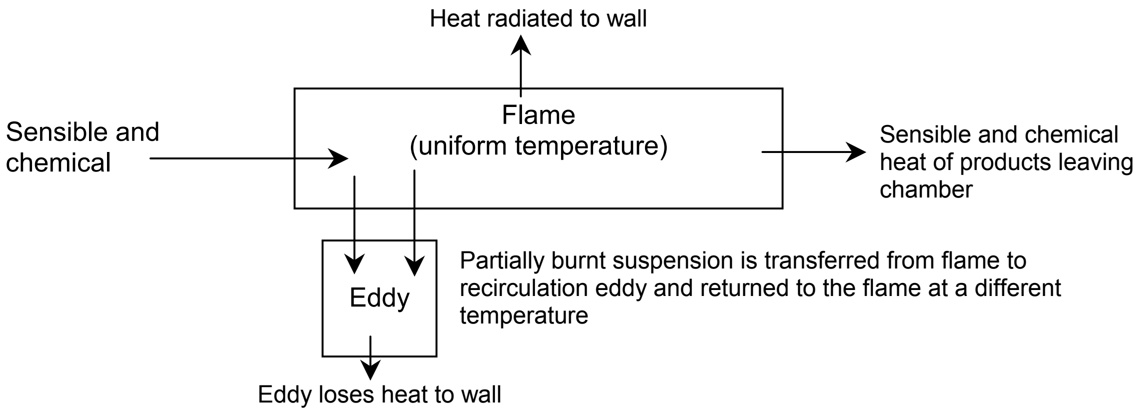

Fig. 4: Combustor sample for isothermal version

The only additional computation needed in the isothermal approach is the net heat loss to the walls via the recirculating partially burnt char returning to the flame at lower temperature T_r but completely burnt.

The loss of Chemical energy is given as

$$\Delta H_{chemical} = -\frac{m_c QU\Delta N}{1 + B_o + N_{\max}} \qquad (26)$$

Total Chemical energy loss to recirculating eddy is computed as a summation from eddy core to the impingement point. Total heat loss as sensible heat and chemical energy is given as

$$H_r = m_p N_{\max}(T - T_r)C_p - \sum_{N=N_{\max}}^{N=0} \frac{m_c QU\Delta N}{1 + B_O + N_{\max}} \qquad (27)$$

Equation 27 gives the rate of heat loss to the wall through recirculation in the system.

The total heat removed is

$$H_{rad} + H_r + m_t C_p \left(T - T_a\right) \tag{28}$$

H_{rad} = total heat radiated from flame
m_t = total mass flux of coal and air
T_a = reference temperature.

Method of Solution

The principle of the method of solution is to calculate the value of a variable at time (t +Δt) from its value at t and the rate of change at time t. The method is typified by

$$y(t + \Delta t) = y(t) + y^1(t)\Delta t \quad .$$

This is known as Euler's method. The method gives satisfactory results at short interval of time; it is also advantageous for flexibility and simplicity. Computer is adopted for the solution of the models. The results show the fraction of unburnt fuel. The computation shows also the influence of various parameters on the combustion efficiency. The surface reaction rate in the sustenance of flame and its stability could be determined. Finally the pollution effect of the combustion by emission of the combustion gas into the atmosphere could be determined.

Concluding Remarks

It is very important that the habit of modeling becomes part of our process in research investigation as through it theoretical prediction can be made and adequate modifications could be made before prototype is built. This way money and energy will be saved. The above shows that with adequate prediction the shortcomings involve in the combustion of coal could be taken care of and claim could be made for it clean use.

References

1. Frenkiel, F.N., 'Atmospheric pollution in growing communities', Proc. Air and Water Pollution, pp 339-369, 1970.

2. Mass, H., 'Chaina's power house', New World, Pub. Siemens Ag, Hamburg No. 3, pp 10-20,
3. Sept. 2001.

4. Field, M. A, Gill, D.W., Morgan, B.B and Hawksley, P.G.W., Combustion of Pulverized Coal; The British, Coal Utilization Research Association, Leatherhead, 1967.

5. Asere, A.A. “Parameters dictating the efficient use of coal with reference to Nigerian coal’, Proc. N.S.E., PP 128-131, 1987.

6. Laditan, G.O.A., ‘Coal carbonization by-products : feedstock for manufacture of industrial products’,

7. Famuboni, A.D. ‘Maximizing exploration of Nigeria’s coal Reserves’, Nigerian Coal: A resource for energy and investments, Ed. Okolo, H.C and Mkpadi, M.C, Pub. RMDC, Abuja, pp 39-62, 1996.

8. Asere, A.A, ‘Thermal Energy Generation’, Energy Crisis in Nigeria-The way forward; NSE- Bauchi Branch, 2001.

9. Suthenthiran, A., Khan, S.A., Ahmed, S.H. and Carabine, M.D., ‘The influence of high temperature and residence time on the formation of SO_3in a premixed laminar flame’, J. Inst. Energy, pp 85-88, 1988.

10. Asere, A.A., “Air Pollution in Developing Economy - A Perspective”, NSE Technical Transactions, Vol. 30, No 4, pp. 11 - 23, 1995.

11. Pegg, M.J. ‘Pilot-scale combustion tests : a comparison of the flames of heavy fuel oil and coal-water mixtures’, J. Inst. of Energy, Vol. LX 11, No. 452, 1989.

12. Kanury, A.M., ‘Introduction to combustion phenomena’, Gordon of Breach Science Publ. New York, 1977.

13. Glassman I., ‘Combustion’, Academic Press, New York, 1977.

14. Mason B.J., ‘Acid Rain : Its causes and its effects on inland waters’, Clarendon Press, Oxford, 1992.

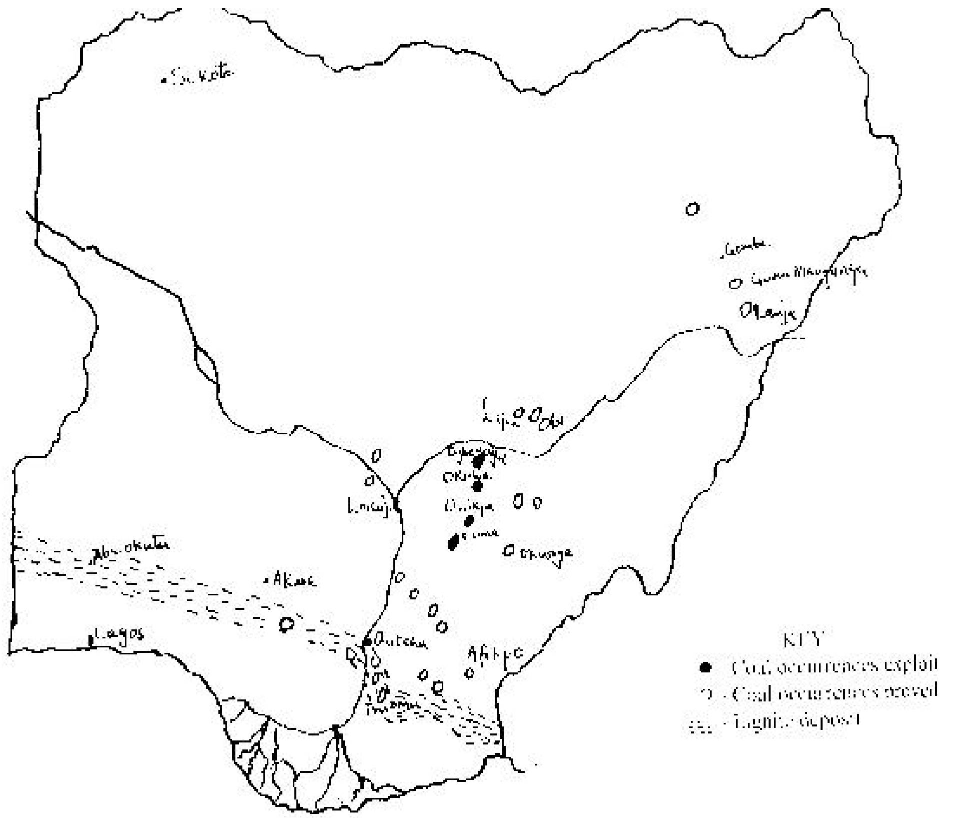

Fig. 1: Coal and lignite deposit in Nigeria