

## COMPARING THE REACTIVITY IN TWO MEDIUM RANK NIGERIAN COALS: RAW AND DEMINERALIZED FORMS

*A.O. Odeh and E A. Oyedoh*

Department of Chemical Engineering, Faculty of Engineering, University of Benin, Benin-City, Nigeria.

### *Abstract*

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*Nigeria as a nation is greatly endowed with natural resources. Among these natural resources, coal is considered to be vastly available second to crude oil. However, a lack of comprehensive data on physico-chemical and thermal properties of Nigerian coals has greatly limited their utilization. Hence, in this study, two Nigerian medium rank coals of different grades, one low volatile bituminous (MBT) and a high volatile bituminous (AFZ) were demineralized and characterized. The thermal analysis under different process condition were also examined to determine the impact of demineralization on the coal's reactivity.*

*The results indicate that the coals contain high proportions of percent carbon and a sufficiently high heating value (HHV) for energy conversion: 77% carbon content and 20.4 MJ/kg gross calorific value MBT coal and 82% and 26.8 MJ/kg for the AFZ coal. The thermal analysis of both the raw and demineralized coal on reactivity were found to confirm to well-established trends. The effect of temperature in the high temperature range was, however, strongly affected by pore and film diffusion during combustion. The coal classification revealed the thermochemical and pyrolytic fuel properties of the coal and indicates that the coal can potentially be utilized for future clean energy applications in Nigeria.*

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**Keywords:** Nigerian coal; char, coal transformation; energy efficiency; energy recovery; technical performance

### **1. Introduction**

Pyrolysis will remain an important process for thermo-chemical coal conversion either as an individual process for char and tar/oil production or as a step in other coal conversion processes such as combustion, gasification, and liquefaction. During fixed bed gasification, coal passes through four distinct stages: drying, pyrolysis, reduction, and combustion [1]. In the pyrolysis stage, volatiles devolatilization occurs and the properties transformation from coal to char can be dramatic for some coals. The behavior of coal under pyrolysis can be linked to coal properties and process conditions such as coal rank, particle size, porosity, surface area, mineral content, petrographic composition, process temperature, process pressure, catalyst, and heating rate [2 - 8]. Thus, among other aspects the time-temperature histories will have an influence on the char reactivity and behavior. While the inorganic component are sometime responsible for poor and unstable performance of coal conversion processes [9 - 12]. However, in other conversions, such as direct liquefaction the pyrite mineral is beneficial to the yield of the process [13 - 14].

Tracing char structure evolution during coal conversion process allows an improved evaluation of the conversion mechanism [15]. Of the many rank indicators and char properties the fuel ratio (a commonly used factor in the design of unit operations for coal conversion processes and also a useful parameter in the selection of coals used in coal blending plant) has not commonly evaluated but may prove to be useful indicator in the coal to char conversion process [16]. Most power plants utilized coals with fuel ratio in the range of 1.0 - 2.5 due to their combustion characteristics of calorific values, ignitability, and combustibility [6]. Fuel ratio is considered to give an indication of coal reactivity as coals with fuel < 1.5 are thought to combust more smoothly whereas coal with fuel ratio > 1.5 combust with difficulty [17]. The pulverized coal combustion characteristics of high-fuel-ratio coals with fuel ratio in the range of 1.46 to 7.10 were examined and the

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Corresponding Author: Odeh A.O., Email: Andrew.odeh@uniben.edu, Tel: +2348033188797

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researchers concluded that as the fuel ratio increases, nitrogen oxides ( $\text{NO}_x$ ) emission reduces significantly and that the char's external surface area decreases with increase in the fuel ratio of the coal [15]. Fuel ratio of demineralized coal and slow-heating coals are not readily available in the open literature. Thus the fuel ratio is a somewhat forgotten rank parameter that may have utility in coal to char transitions. However, detailed evaluation of typical Nigerian coals has been least investigated and as such there is limited information available at present in the open literature on Nigerian coals. The lack of data on the thermo-chemical fuel properties of the coals is an impediment to more accurate assessment of their technological applications and efficient industrial utilization. With the knowledge of coal deposits in nations like Nigeria, its importance as an industrial and commercial commodity will unquestionably increase in the future. However, the studies on the fuel properties and potential applications of coals in Nigeria are limited.

Therefore, the main objective of this paper is to characterize and examine the physico-chemical and thermal properties of two medium rank Nigerian coals. The paper also presents novel data on the reactivity of the two coals and comparison in reactivity between the raw and demineralized coals form under the same process conditions which serves as a fundamental requirement for assessing its future potential utilization in the clean coal technology age. This is vital for the engineering design, modelling and optimization of thermochemical processes, conversion equipment, and environmental impact assessment of coals in Nigeria.

## 2. Experimentals

### 2.1 Sample preparation

Two medium rank coals, a low volatile bituminous coal from the middle belt trough coal field in Kogi state denoted as MBT and a high volatile bituminous coal from the Afuze coal field in Edo state denoted as AFZ, Nigeria, were used for this study. The coal samples were pulverized to coal particle size of  $\leq 75 \mu\text{m}$  by employing a mechanical size reduction jaw crusher (Samuel Osborne (SA) LTD, model: 66YROLL) and a Fritsch P-14 rotary mill containing ceramic balls (Model number: 46 – 126). The required particle size of  $\leq 75 \mu\text{m}$  was finally obtained from screening the particles from the rotary mill using a  $75 \mu\text{m}$  screen. The prepared samples were stored under argon prior to analysis in sealed bags. The prepared coal samples were acid washed by sequential leaching with hydrofluoric acid (HF) and hydrochloric acid (HCl) as detailed in Strydom et al. [17]. The HF (48%) and HCl (32%) were obtained from Turraco Industrials Ltd, Nigeria.

### 2.2 Apparatus and procedure

The coal samples (20g) were placed in a ceramic boat in a horizontal tube furnace at atmospheric conditions initially. The samples were flushed with nitrogen (AFROX, ultra high purity grade) at atmospheric conditions, to remove oxygen from the oven for 15 min. at a flow rate of 1 litre/min. The furnace was then heated at  $20 \text{ }^\circ\text{C}/\text{min}$  to the target temperature, and held isothermally for 60 minutes. The target temperature ranged from 450 to  $700 \text{ }^\circ\text{C}$ , while keeping the samples under a nitrogen atmosphere. The char samples were stored in sealed bags.

The calorific value and conventional chemical analyses (proximate and ultimate analyses) of the raw coal, acid treated and heat treated samples were performed according to the ISO 1928, ASTM 3172 and ASTM 3176 standards respectively at Eunandy laboratories, Warri, Nigeria. The surface areas of the various samples were determined using the carbon dioxide adsorption BET method on a Micromeritics ASAP2020 surface area analyser as detailed in [19]. Prior to  $\text{CO}_2$  adsorption, the samples (about 0.20 g) were degassed under vacuum ( $10.0 \mu\text{mHg}$ ), for 48 hours at 25 and  $380 \text{ }^\circ\text{C}$  for the coals and chars respectively. The evacuated sample was analysed at  $0 \text{ }^\circ\text{C}$  in an ice bath. The results were processed using the Accelerated Surface Area and Porosimetry System (ASAP) 2020 software linked to the Surface Area Analyzer. The coal morphology and that of the resultant char obtained in the transition of coal to char was observed using scanning electron microscope (SEM) model FEI Quanta 250 with FEG emitter, equipped with an EDS detector that does the elemental composition analysis. The spectra used in obtaining the structural properties of both the coal and char were obtained from the Fourier-transform infrared spectrometer equipped with an attenuated total reflectance (FTIR-ATR), model Perkin-Elmer Spectrum 400. The procedure of FTIR-ATR as detailed by Odeh, 2015, was used [20]. Aromaticity ( $f_a$ ) was obtained from the ratio of aromatic bands in the  $900 - 700 \text{ cm}^{-1}$  region to the aliphatic and aromatic bands in the  $3000 - 2815 \text{ cm}^{-1}$  region [18]. The vitrinite reflectance of the parent coals were obtained following the procedure and equipment at the advanced coal technology, Coal and coal products laboratory, South Africa as detailed in and reported in Odeh, 2015b [19].

Thermogravimetric analyses of the chars were carried in a Leco TGA701 thermogravimetric analyzer with pneumatic carousel assembly with capacity of being loaded with 19 samples per run. The analyses were performed at Coal and Carbon laboratory, University of Pretoria, South Africa. The char combustion experiments were carried out isothermally at four different temperature ranging from 365 to  $410 \text{ }^\circ\text{C}$ . The samples were heated under nitrogen from ambient temperature to the target temperature for an hour, after weight stabilization the nitrogen was replaced by oxygen atmosphere (10 volume %) [18], and held isothermal for six hours at a heating rate of  $10 \text{ }^\circ\text{C}/\text{min}$ . Sample masses of approximately 2g, with a particle size distribution of  $\leq 75 \mu\text{m}$ , were used to reduce mass transfer effects [15]. The selection of these experimental conditions were based on recommendations from researchers on the need for the samples to be distributed uniformly on the bed of the analyzer and not having a bed thickness  $> 1 \text{ mm}$  [5]. The specific reactivity of the char was calculated by:

$$R = \frac{1}{W} \frac{dW}{dt} \quad (1)$$

Where  $W$  is the weight of the char (daf basis) at any given time  $t$ . The intrinsic reactivity was obtained by normalizing the specific reactivity of the char by the DR micro-pore surface area obtained from the ASAP 2020 surface area analyzer [12].

### 3. Results and discussion

The coal samples used for the investigation are of the same rank but of different grades and as such it is expected that the chemical composition and physical properties will demonstrate considerable differences as a result of demineralization and heat treatment. Samples are referred to as "MBT450, AFZ700" to clearly indicate the sample identity and the temperature to which it was heat treated. From Table 1, the carbon content of the coals on dry ash free basis (daf) varies from 77.4 to 80.7% for the bituminous coal (MBT) between the parent coal (untreated coal) and the demineralized version. For the AFZ, the variation is from 81.6 to 83.6 for both the parent coal and the demineralized coal. The low total sulphur content of 0.5 and 1.2% (daf basis) for the MBT and AFZ coals, which together with the other properties would make this parent coal desirable for combustion in conventional pulverised boilers, thus, making both coals, choice coal for combustion processes. The effect of charring temperature is as given in Table 2 and it can be seen that there is a significant reduction of the volatiles at 700°C to 3.7% as compared to 14.7% at 450°C from a parent coal with a value of 21.3% (air dried basis) for the MBT coal. Similar significant reduction in the volatiles was also observed for the AFZ coal with values of 3.8% at 700°C, 13.8% at 450°C and 26.8% (air dried basis) respectively. Observation of the atomic H/C ratio in this study is generally consistent with previous reports on coal systems in that the low volatile bituminous coal (MBT) has the higher value of H/C (0.70) compared to the high volatile bituminous (AFZ) that has a H/C value of 0.68. The same trend was obtained for the demineralized coal and the heat treated coal samples. The trend of decrease of H/C ratio with increasing charring formation temperature for the acid treated (demineralized) coals was the same which converged to almost the same value of 0.13 at the charring temperature of 700°C. Similar trend of decrease with increasing charring formation temperature were observed for the atomic O/C (Table 2). There was, however, unlike the low rank coals as reported by Odeh, 2015b, there was no convergence to the same value at a temperature of 650 °C. This implies that the maximum temperature to get the heat effects of the bituminous coals is not necessary 650 °C. The calorific value determined for the MBT coal was 20.4 and 31.0 MJ/kg for the parent coal and the demineralized version respectively. While for the AFZ coal, the determined calorific values of 26.8 and 32.0 MJ/kg for the parent and demineralized coals respectively. The impact of demineralization is visible as the calorific value increased in value. From the proximate analysis, the fuel ratio, which is the ratio of the fixed carbon to volatile matter content, was calculated (Table 1 and 2). It can be seen that the fuel ratio increases with increase in coal rank, AFZ coal has a higher fuel ratio compared to the MBT coal and with increase in charring formation temperature. Though slight differences can be observed in the values obtained both the parent coal and the demineralized coals, the impact is more noticed in the heat treated coals and there is a convergence to a value of 24 MJ/kg around 700 °C (Table 2). The spectra obtained from the FTIR were used to determine the aromaticity, which is a technical performance index for measuring the maturity and usefulness of coal in coal conversion processes was calculated (Table 1 and 2). The aromaticity was determined to be in the range of 0.84 - 1.00 for the MBT coal and 0.83 - 1.00 for the AFZ coal. The aromaticity shows similar trend that converged to the same value at the charring temperature of 700 °C (Table 2). The internal structure and morphology of both coal and coal chars demonstrated similar behaviour (Figure 1, 2 and Table 2). The BET surface area determined is consistent with the rank of the coal [17]. The surface area for the heat treated coals were determined to be in the range of 139 – 222 m<sup>2</sup>/g and 132 – 227 m<sup>2</sup>/g for the MBT and AFZ coals respectively. Since the pathway for the formation of char is affected by the heating rate, the results of the surface area obtained from the slow heating rate used in this study corroborates results reported by Odeh [18]. This gives an indication that the MBT is likely to be more porous than the AFZ coal. It can be depicted from both Figures 1 and 2 that the pores in the coals opens up at elevated temperature most especially at 550 °C. Figures 1 and 2 also illustrates the impact of heat on coal during utilization processes when viewed under petrographic microscope. It can be seen that there is a colour change from grey to white when the lowest charring temperature of 450 °C is compared to the highest charring temperature of 700 °C. This colour change can be attributed to the spontaneous reaction of the reactive components (vitinite + liptinite) of the macerals in the coals when subjected to elevated temperatures.

In this communication, the data obtained from the thermogravimetric analyser were fitted experimental. The best fit for the data obtained was a fourth order polynomial (Figures 3 and 4). Both the parent and the demineralized version of the two coals subjected to heat treatment were fitted to the fourth order from where the kinetic parameters were calculated to define the coals reactivity. (It should be noted that the coals were demineralized to reduce the amount of mineral matter present in them as well as to minimise their influence during quantitative analysis and the reactivity of the coals). This initiative of demineralization is a drive towards clean coal technology for efficient and effective uses of coal and coal products resources. From the specific and intrinsic reactivity data generated from the thermogravimetric analysis in Table 3, It can be seen that both the specific and intrinsic reactivity decreases with increasing charring for the four combustion programme employed for this investigation. The decrease of reactivity with increasing charring temperature has been reported to be due to the reduction of the hydrogen content in chars which is related to the reduction of active sites giving room for more desorption reaction with oxygen [18]. Previous research reports has demonstrated some level of inconsistencies with the data obtained for combustion reactivity for the medium rank coals. However, in this report, the inconsistencies were limited as reflected in Table 3. The inconsistency can be attributed to the irregular and random distribution of the specific reactivity with increasing char formation temperature. To correct the irregular phenomenon of the specific reactivity, the specific reaction rate data were normalized to the measured CO<sub>2</sub> adsorption surface area to get the intrinsic reactivity, which gives better representation and interpretation of the reactivity of a coal sample. On comparing the reactivity between the parent and the demineralized coal, the parent coal seems to be more reactive than the demineralized coals (Table 3). Odeh [19], reported that inherent minerals in the medium rank coals do have favourable catalytic effects during coal processing. These inherent minerals would have been removed or reduced in content in the course of the demineralization in this study. These minerals are mostly found in clay minerals (calcite and dolomite) consisting of aluminium oxides

and oxides of calcium and potassium which plays active role in the de-alkylation and dehydrogenation reaction at high charring temperatures and in the cracking (decarboxylation/decarbonylation reactions) of oxygen functional groups at charring temperatures [6]. For a better and greater insights of this investigation, the activation energy for the demineralized coals, which is a temperature predominant parameter of the intrinsic reaction rate was determined. The activation energy was determined to be in the range of 174 to 87 KJ/mol for MBT from 450 to 700 °C. While for AFZ, the activation energy was determined in the range of 397 to 118 KJ/mol. The activation energy is found to vary dramatically over the course of the combustion analysis, exhibiting a sharp maximum in the early stages of char combustion. This dramatic behaviour can be attributed to the fact that when coal is heated, two processes occur competitively: one is the depolymerization process through which gas, water vapour and tar are formed and the other is the condensation or repolymerization which leads to char formation [20]. The determined average activation energy of 104 KJ/mol for the MBT and 142 KJ/mol for the AFZ coal obtained in this work falls within the range of values previously reported in the open literatures. From the detailed characterization and energy content evaluation, the two medium rank Nigerian coals can be considered to possess great energy potentials.

#### 4. Conclusion

Nigeria as a country is a great nation endowed with so much natural resources. The fall and rise of oil wells and price, the GDP of countries such as Nigeria, which is monopolistic in nature would be affected. Hence the dire need to investigate the properties of Nigerian coal for effective and efficient utilization cannot be over-emphasized in this context. Coal when subjected to chemical and heat treatment undergoes changes as observed in this study. This changes affects the chemical, physical, mechanical, heat and electrical properties of the coal.

It can be concluded that the two medium rank Nigerian coals show a similar behaviour in char properties, when subjected to elevated temperatures; the (O/C) and (H/C) ratio, decrease with temperature, while the aromaticity, fuel ratio and BET surface area increase with charring temperature. The order of the determined characteristics is consistent with the rank of the parent coal when compared to what obtains in open literatures. This demonstrates the great potentials embedded in the Nigerian coals waiting to be explored and exploited for energy recovery. Since pyrolysis has been identified potentially as a promising, sustainable conversion process for the utilization of carbonaceous fuels such as coal into clean fuels and power generation. The data and knowledge obtained from this study would be vital for the future implementation of clean coal technologies and applications in Nigeria.

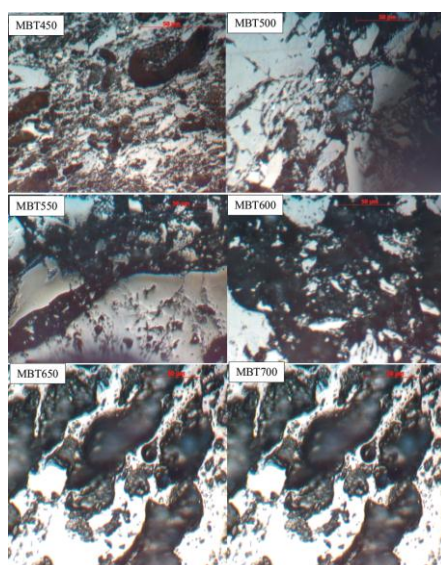


Figure 1: Photomicrographs of the transition of coal to char (450 – 700 °C) for MBT samples

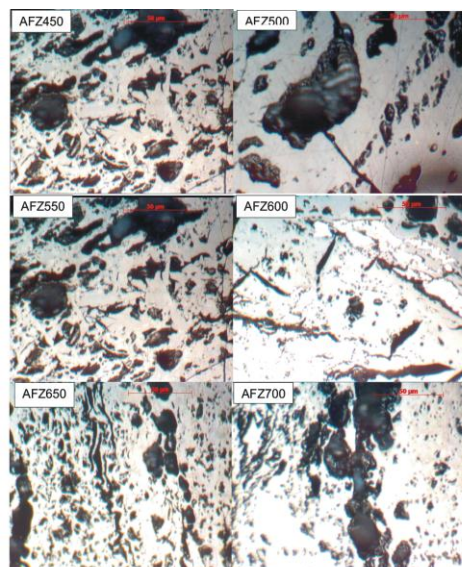


Figure 2: Photomicrographs of the transition of coal to char (450 – 700 °C.) for AFZ samples

Table 1: Properties of both coal

Coal	MBT	MBT-D	AFZ	AFZ-D
Inherent moisture(air dried) wt.%	4.2	1.4	2.2	2.7
Ash (air-dried) wt.%	29.1	3.5	16.1	1.2
Volatile matter (air-dried) wt.%	21.3	24.9	26.8	27.2
Fixed carbon (air-dried) wt.%	45.4	70.6	54.9	68.9
Carbon (daf) wt.%	77.4	80.7	81.6	83.6
Hydrogen (daf) wt.%	4.5	4.3	4.6	4.5
Nitrogen (daf) wt.%	2.1	2.3	2.0	2.1
Oxygen (daf) wt.%	15.5	12.4	10.7	9.1
Sulphur (daf) wt.%	0.5	0.3	1.2	0.8
Gross calorific value (MJ/kg) (air-dried)	20.4	31.0	26.8	32.0
H/C (daf).	0.70	0.63	0.68	0.66
O/C (daf)	0.15	0.09	0.10	0.11
f <sub>a</sub>	0.70	0.73	0.71	0.74
Fuel ratio	2.1	2.6	2.1	2.8
CO <sub>2</sub> BET surface area (m <sup>2</sup> /g)	93	109	86	97
Rank (mean random vitrinite reflectance %)	0.76	0.77	0.73	0.78

MBT-D demineralized coal      AFZ-D demineralized coal

Table 2: Derived properties of heat treated coals (chars)

CHAR	Wt % (air dried)				Wt % (daf)						daf				m <sup>2</sup> /g
	Mois.	Ash	V.M	F.C	C	H	N	O	S	O/C	H/C	f <sub>a</sub>	FR	BET	
450	1.6	3.5	14.7	80.2	88.2	3.0	2.2	6.3	0.4	0.06	0.42	0.84	5.8	139	
500	1.4	3.6	12.4	82.6	89.6	2.8	2.2	5.2	0.3	0.05	0.38	0.88	6.7	153	
550	1.1	3.5	9.6	85.8	89.7	2.4	2.1	5.4	0.3	0.05	0.33	0.90	9.1	197	
600	0.9	3.7	7.6	88.0	89.6	2.1	2.1	5.4	0.3	0.05	0.27	0.93	11.3	201	
650	0.9	4.1	5.6	89.6	91.8	1.5	2.1	4.2	0.3	0.04	0.23	0.97	16.2	217	
700	1.1	4.2	3.7	91.0	92.5	0.8	2.3	4.1	0.3	0.03	0.13	1.00	24.1	222	
AFZ															
450	1.2	1.3	13.8	84.1	88.1	3.3	2.1	5.7	0.8	0.05	0.45	0.83	6.3	132	
500	1.1	1.3	11.3	86.3	89.0	2.9	2.1	5.4	0.7	0.04	0.38	0.86	7.8	157	
550	1.0	0.8	8.9	89.4	91.3	2.6	2.2	3.4	0.5	0.03	0.34	0.88	10.4	182	
600	0.9	1.1	7.4	90.6	92.1	2.2	2.1	3.1	0.5	0.03	0.28	0.93	12.2	208	
650	0.9	1.1	5.1	92.9	93.1	1.7	2.1	2.5	0.6	0.02	0.22	0.96	18.5	216	
700	0.9	1.1	3.8	94.2	95.6	1.2	2.0	0.9	0.6	0.01	0.13	1.00	24.2	227	

FR Fuel ratio fa Aromaticity

Table 3: Specific and Intrinsic reactivity of chars

CHAR	R <sub>s</sub> (g/g.s) x 10 <sup>-5</sup>	R <sub>i</sub> (g/m <sup>2</sup> .s) x 10 <sup>-7</sup>	R <sub>s</sub> (g/g.s) x 10 <sup>-5</sup>	R <sub>i</sub> (g/m <sup>2</sup> .s) x 10 <sup>-7</sup>	R <sub>s</sub> (g/g.s) x 10 <sup>-5</sup>	R <sub>i</sub> (g/m <sup>2</sup> .s) x 10 <sup>-7</sup>	R <sub>s</sub> (g/g.s) x 10 <sup>-5</sup>	R <sub>i</sub> (g/m <sup>2</sup> .s) x 10 <sup>-7</sup>	E <sub>a</sub>	E <sub>a</sub>
C/TEMP	415 °C		400 °C		385 °C		370 °C		KJ/mol	KJ/mol
MBT450	8.04	3.33	7.63	3.13	7.43	3.05	8.41	3.46	174	104
MBT500	7.00	2.75	7.11	2.83	6.92	2.72	8.37	3.29	165	
MBT550	6.93	2.10	6.92	2.09	6.81	2.07	7.14	2.16	56	
MBT600	6.77	2.02	6.26	1.86	6.63	1.96	7.47	2.21	97	
MBT650	6.43	1.70	5.61	1.76	6.05	1.64	6.21	1.69	46	
MBT700	5.72	1.41	5.90	1.46	6.16	1.51	5.86	1.47	87	
AFZ450	6.72	3.26	6.03	2.91	5.56	2.73	8.17	3.97	397	
AFZ500	6.51	2.5t	5.47	2.15	5.81	2.31	6.31	2.48	143	
AFZ550	6.46	2.23	5.32	1.84	5.66	1.92	6.26	2.12	71	
AFZ600	5.73	1.71	5.33	1.91	5.51	1.68	5.51	1.68	52	
AFZ650	5.13	1.45	4.76	1.35	4.76	1.36	5.16	1.51	69	
AFZ700	5.25	1.48	4.02	1.11	3.37	0.91	2.27	0.66	118	

R<sub>s</sub> Specific reactivity R<sub>i</sub> Intrinsic reactivity E<sub>a</sub> Activation energy

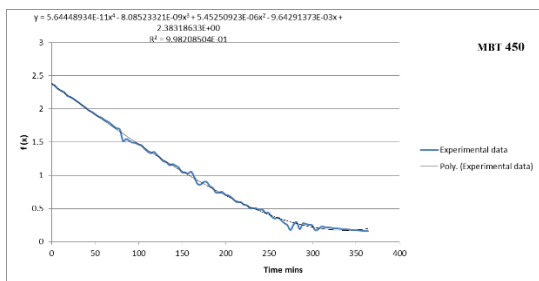


Figure 3a: Curve fitting of experimental data for the demineralized MBT coal

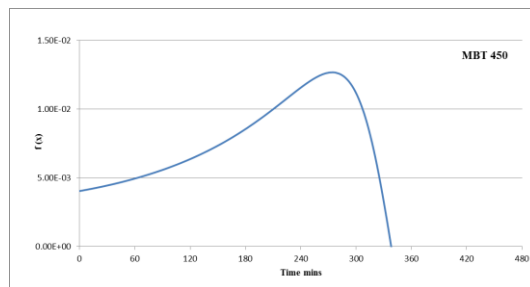


Figure 3b: Curve fitting of experimental data for the demineralized MBT coal

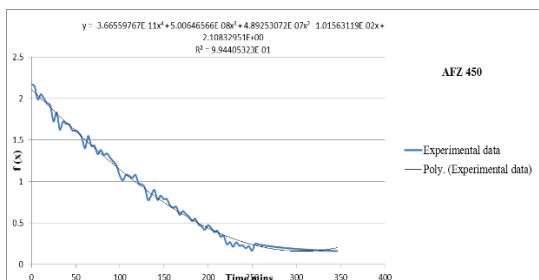


Figure 4a: Curve fitting of experimental data for the demineralized AFZ coal

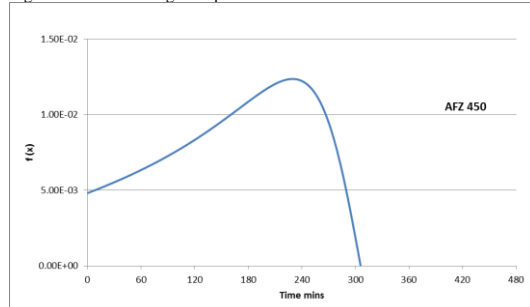


Figure 4b: Curve fitting of experimental data for the demineralized AFZ coal

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