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### Full Length Article

# Influence of coal quality on combustion behaviour and mineral phases transformations



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#### HIGHLIGHTS

• Evaluation of chemical and mineralogical compositions of Prajapara coal samples of Ib coal basin.

- Petrographical analysis of Prajapara coal of Ib valley coal basin, Odisha, India.
- Correlation of chemical and mineral composition to ash fusion temperatures.
- FactSage prediction of equilibrium phase transformations and ash fusion behaviour.
- Detailed characterisation of coal quality and combustion behaviour.

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#### ABSTRACT

Coal is still an important resource for power generation. The combustion behaviour of various types of coal is dependent on its ash properties. These are the most important fuel characteristics in the design and operation of commercial boilers. The present study aims to evaluate the whole coal seam quality, coal ash behaviour, fundamental mechanisms, which more closely simulate the conditions of a pulverised coal-fired boiler. The authors formed seven representative samples from overall 126 band-by-band samples of Prajapara coal block (PCB) borehole of Ib valley coal basin, Odisha, India. Authors have carried technological, elemental and petrographical analysis of coal samples. The major oxides and minerals present in coal ash samples were characterised by inductively coupled plasma optical emission spectrometer (ICP-OES) and X-ray diffraction (XRD). The volatile matter (VM<sup>daf</sup>) and ash (A<sup>d</sup>) yields vary from 42.05-44.49 and 30.82-32.12 wt% respectively. The mean vitrinite reflectance ranges from 0.46 to 0.64%. Moreover, FactSage thermodynamics Model (FactSage 6.3) was used for understanding of the coal ash fusion behaviour in boiler operation and to predict the phase transformations that occur during the process of coal combustion which is a chemical thermodynamic models of oxide systems. FactSage provides mineralogical characteristics of coal which are in agreement with XRD analysis of coal. SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, K<sub>2</sub>O appears to influence positively fusion characteristics where as Fe<sub>2</sub>O<sub>3</sub> and MgO have negative effect on it.

The datasets provide information about the contribution of major oxides towards the ash fusion temperatures (AFT). The linear regression analysis of high temperature ash (HTA) composition and AFT indicate trend, which may be used to determine the predictive indices for slagging, fouling, and abrasion propensities during combustion practices.

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#### 1. Introduction

Coal-fired power plants are still the major producer of electricity in India, which utilizes large amount of non-coking coal reserve [1,2]. A long standing problem for users of coal-based power generation technologies is the prediction of the behaviour of the

\* Corresponding author. *E-mail address:* vmishrageology@gmail.com (V. Mishra). organic and inorganic constituents of coal during combustion [3–8]. Combustion profiles depend on different coal properties and characteristics such as particle size, rank, maceral composition and mineral matter content [9–12] whose separate effects are difficult to determine.

During combustion, ash composition, which is derived from inorganic impurities in coal, can be a major operational problem [13]. The problems have been discussed in detail in the coal combustion and ash chemistry literatures [3,4,7,14–18]. The



association and abundance of inorganic components in coals is extremely diverse. Minerals in coal generally occurred as elements required for the growth of the original plant life from which the coal was formed and as inorganic material, typically sand, silt, or clay, deposited in the accumulating plant debris as discrete particles of foreign material. This also may have been deposited later by mineral-laden water percolating through the coal seam. Hence, there are two types of "ash" available, one is "inherent" and another is "extraneous" or "adventitious". Iron, calcium, magnesium, phosphorus, potassium and sulphur are commonly present in inherent ash but iron, calcium, magnesium and sulphur invariably are present in much larger quantities in the adventitious ash [17]. Coal ash deposition on furnace wall is called slagging. The characterisation of coal ash for its tendency to slag and foul has been traditionally related to the bulk chemistry of the ash and ash fusion temperatures (AFT) which includes deformational (DT), softening (ST), hemispherical (HT) and fusion (FT) temperatures [13]. Ash-fusion characteristics are used to predict the behaviour of coal ash under high-temperature conditions at which the various stages of ash softening and melting takes place and is still the most widely accepted means of assessing the deposition characteristics of coal in pulverised fired combustion system. AFTs have been strongly related to coal-ash composition [19–24] as molten ash has the varying viscosity [25,26]. Iron-bearing minerals and calcium bearing minerals in coal are easy to form ash deposits during combustion [27-33]. The effects of major oxides, the ratio of silica to alumina (SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>) as well as acid and basic fluxes on the AFTs of coal ashes have been studied by various methods [34–36]. It is possible to make a reliable prediction of ash fusion characteristics based on the major oxides in coal ash and their AFTs, having significant implications in coal utilization and furnace design. Li et al. [37] recognised the effects of Fe, Ca, Na and K also. Besides, many publications indicated that increased P<sub>2</sub>O<sub>5</sub> content enhances the development of low-melting-point phases in the ash [38–40]. Shao et al. [41] reported phosphates together with the eutectics of Fe<sub>2</sub>O<sub>3</sub>and SiO<sub>2</sub> might play the most important role in bed agglomeration during sludge combustion, by forming low melting point compounds with alkalis. Dvk and Kevser [42] suggest, correlation between AFT and ash composition indicate that, although the regression approaches are more complicated, in many cases they are no more accurate than the approaches based on the acid-base formula.

Recently, studies on the prediction of AFT were undertaken with the aid of computer thermodynamic model of FactSage [43–46]. FactSage was introduced in 2001 and was developed jointly by both the FACT-Win/F\*A\*C\*T and ChemSage/SOLGASMIX thermo-chemical packages [47]. It is a powerful predictive tool, which can be applied to a wide range of coal utilization technologies [48]. FactSage allows calculating and predicting multiphase equilibria, liquidus temperatures, and proportions of the liquid and solid phases in a specified atmosphere for the multi-component system.

Despite the common application of this test within the coal industry, little has been published in India on variability in ashfusion temperature (AFT) within a single mine or within a seam, or on the geologic controls on this property.

The prime objective of this study is to quantify the quality of the coals of Prajapara coal block (PCB) of Ib-valley coal basin, using technological, elemental and petrographical analyses. The other aim is to predict the influence of coal ash material on slag-liquid formation and ash flow temperature such as, coal ash composition and their correlation with thermodynamic model, FactSage, on combustion behaviour in thermal power plants. The ash fusion temperatures of various PCB coal samples were determined and these values were compared to the FactSage modelling results. PCB coals have typically high iron content. Iron bearing minerals

are effective fluxing agent that have a significant role on combustion behaviour of coal.

#### 2. Geological settings

Mahanadi basin is one of the five major coal bearing basins of India [49]. Ib-river Gondwana basin derives its name from the river Ib, a tributary of Mahanadi and comprises a part of the upper Mahanadi valley basin located in Odisha which is bounded by 2 1°30′–22°60′N and 83°37′–84°10′E [49,50]. The coal basin extends over an area of 1460 sq km and covers parts of Sambalpur, Jharsuguda and Sundargarh districts of Odisha. It is characterised by a north-westerly plunging synclinal flexure [51,52]. The boundary of the basin in the southwestern part is marked by a fault, which juxtaposes the Barren Measures and Raniganj Formations against the underlying Precambrian metamorphic rocks.

The Ib Valley coal basin was first mapped by Ball [53]. Subsequently it was resurveyed by Mehta and Anandalwar; Raja Rao [54,55], Central Mine Planning and Design Institute Limited [56,57] and Pal et al. [58]. The Geological map and the stratigraphy succession of the Ib-valley coal basin area is presented in Fig. 1a and Table 1 [59,60].

#### 3. Materials and methods

#### 3.1. Sampling and preparation

To assess the PCB seam quality, overall sample preparation method [61] was followed. In this method definite percent of band by band samples were taken and mixed well to generate one overall sample. 126 band by band coal core samples from one borehole (Fig. 1b) were selected on the basis of coal quality. The bands having the total ash and moisture content  $\leq$ 40 wt% was considered as coal and the bands having the same ranging between 40 wt% and 55 wt% was considered as shaly coal. These samples were assorted to seven representative samples with reference to depth by taking a definite proportion of samples from each band and mixing them well.

#### 3.2. Proximate, ultimate and ash analyses

The proximate analyses viz. moisture content, volatile matter and ash yields were carried using TGA-1000 automated proximate analyser (Navas Instruments, USA). The ultimate analysis (elemental composition) was done using Vario EL III CHNS analyser (Elementar GmbH, Germany). Chemical analysis of major inorganic elements present in coal ash samples were carried out by using VARIAN Vista MPX Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES) after microwave digestion as per ASTM [62].

#### 3.3. Petrographical and mineral matter characterisation

Maceral identification was based on the ICCP classification [63–65] of coal following BIS procedures [66] on polished mounts under the polarised light microscope (Leica DM4500).

Mineral matter composition of the coal ash samples were determined using D8 Discover XRD instrument (Bruker, Germany). Ni-filtered Cu K $\alpha$  was the radiation source and the scan was performed at 2 $\theta$  range of 6–120° at a scan rate of 2°/min. High Score Plus software package was used to analyse the XRD curves.

#### 3.4. Ash fusion temperatures and thermodynamic calculations

Ash fusion temperature (AFT) was measured under oxidising atmosphere (air) using LECO AF-700 electric furnace. In this pro-

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