Chapter-8

Conclusion and Suggestions for Future Work

8.1 Conclusion

The objective of this research work focuses on the chemical characterization of the coal collected from the Gondwana basin of the Permian period in India and its significant beneficiation by using choline chloride and urea-based deep eutectic solvent. The problem was undertaken because of the growing demand for coal for energy production and its contribution to the state's economy and to understand the further consequences of coal burning. The Indian coal characteristics vary in chemical constituents. From the observations made in this research work followings, essential conclusions have been drawn.

i. The Permian coal of the Singrauli basin was stratified in nature. Chemically, they have a medium to high ash yield and high volatile matter content. Proximate analysis suggests that the studied coals were sub bituminous to volatile bituminous rank. Various structural and geological features control the quality of coal in this basin. Moreover, these coals' complex and heterogeneous nature makes them particularly important from an environmental perspective and minimizes their carbon footprint.

ii. Six Permian coal samples, bituminous in rank, have been studied for combustion characteristics, pyrolysis behavior, and kinetics parameters through TGA and DTG analysis. The present study helps to understand the ignition and combustion performance of high-ash and low-ash coal considering the physicochemical constraints. The kinetic parameters were determined using the Arrhenius equation, and activation energies were calculated by using the Coats-Redfern method. Further detailed study of different combustion parameters reveals that the activation energy varies from 63–169 kJ/mol for different coal samples, and, values of activation energies for low-rank coal were found to be high (169.5 kJ/mol). It has been observed that the conversion degree obtained lies in the range of 0.34-0.54, and the mean correlation coefficient (R^2) value lies in the range of 0.965-0.999. This study can be beneficial to understanding the combustion performance of coal and help us use low-rank coal to upgrade environmental and energy constraints efficiently.

iii. The analyzed XRD diffractogram of coal reveals a significant phase of quartz, kaolinite, and gypsum, followed by muscovite, orthoclase, sulfur, hematite, siderite, pyrite, jarosite, and chlorite. These mineralogical elements and their atomic arrangement in the crystal lattice influence coal's physical and chemical properties.

iv. The morphological and mineralogical information about coal and their associations have been revealed by SEM/EDS photo-micrographic study of coal samples. It is very helpful in identifying clay minerals like kaolinite and quartz. Minerals, mainly quartz, are attached to the surface of coal macerals because of drift in origin. Sometimes minerals are present as discrete units, especially quartz. Clay minerals present in coal are seen as lamellar, plate-like, and sandwiched between two coal macerals. Clay is present extensively and non-uniformly in coal, and kaolinite is the most abundant, along with anatase, illite, montmorillonite, and siderite. These adhere to or are incorporated onto the surface of coal particles.

v. FTIR spectra of coal samples reveal that they incorporate oxygen-containing, aliphatic, and aromatic functional groups. There are a considerable number of hydrophobic functional groups such as (CH, CH_2, and CH_3). Oxygen-containing functional groups such as (C=O) carbonyl or carboxide, (C-O,-OH) alcohol, phenol, and (COO-) carboxyl groups are hydrophilic. It is found that Indian Permian coal has fewer hydrophobic groups and more hydrophilic groups, i.e., the inherent hydrophobicity of Indian Permian coal might be high. It also indicates a low degree of ordered microcrystalline units with a low degree of aromatic conformation. The samples have the most significant proportion of oxygenated functional groups, followed by aromatic structures, aliphatic structures, and hydroxyl groups. Results from this study are helpful in the study of molecular structural characteristics of coal and our understanding of properties such as wettability and pore structure.

vi. The XPS survey spectrums confirm the presence of different elements on the surface of the coal. Some of these are C 1s (286.0 eV); O 1s (534.5 eV); N 1s (399.9 eV); S 2p (158.2 eV).The peaks correspond to Si 2p (102.7 eV) and Al 2p (75.6 eV), shows the presence of quartz and clay group minerals in the form of SiO_2 and Al_2O_3. XPS spectra of C 1s confirm a huge amount of aliphatic and aromatic carbon present, which are hydrophobic compared to hydrophilic groups such as alcoholic, carboxylic, and phenolic groups. Hence, it can be said that the natural hydrophobicity of the coal surface is very good and the surface hydrophobicity of coal can also be characterized by using XPS and FTIR characterization.

vii. Raman spectral methods are powerful tools for the non-destructive qualitative and semi-quantitative analysis of coal. Raman spectra in 1000 to 2000 cm^{-1}

range were obtained, revealing two prominent peaks in coal known as the D and G bands, which were located near 1370 cm^{-1} and 1590 cm^{-1}, respectively. G-D1 value for coal 1 was 230, indicating less distorted graphitic structures. The ratio of A_{D1}/A_G represents the degree of growth of aromatic rings in coal, indicating that coal 1 has a less distorted structure. The value of A_{D2}/A_{All} was smaller (0.157) for coal 1 than for the other; hence coal 4 has a more ordered structure and was less amorphous. The A_{D1}/A_G ratio of 0.388 indicates a higher order structure. For Coal 4 A_{D1}/A_G ratio of 0.963 indicates less ordered structure. The samples' G-D1, I_{D1}/I_G ranged from 208 to 230 cm^{-1}, 0.388 to 0.963, respectively. For coal 4, the ratio of I_{D1}/I_G was highest (0.963), which indicates the degree of graphitization was lowest. Coal 1 has a lower ratio value of I_{D1}/I_G (0.388), which signifies a well-graphitized coal structure. The I_D/I_G ratio decrease indicates that graphitization has increased in coal. A decrease in the ratio of A_{D2}/A_{All} indicates a reduction in the amorphous nature of coal and an increase in the order of coal molecular structure. The value of A_{D2}/A_{All} was smaller (0.157) for coal 1 than (0.347) for coal 2. Hence, coal 4 has a more ordered structure and is less amorphous

viii. Besides coal, four different fly ash samples sourced from the thermal power stations were also studied in the present investigation to know the nature of the ultimate product of combustion. The conclusion drawn is that the high-ash Permian coal enriches the mineral oxides in fly ash. It has a significant influence on the properties of fly ash. The amount of mineral fraction (SiO_2+Al_2O_3+Fe_2O_3) in coal contributes to the use of a pozzolanic material. The material has good potential to be used in cement-based pozzolanic materials. It can also be utilized as a cement-based building material for the manufacturing of fly ash bricks.

ix. The wet beneficiation study was conducted to learn about coal samples' interaction and dissolution properties with deep eutectic solvents (DES), choline chloride, and urea. DES was synthesized using choline chloride as a hydrogen bond donor (HBD) and urea as a hydrogen bond acceptor (HBA) in an equimolar amount. The swelling of DES-treated coal is obtained over the raw coal samples in the 1.12 to 1.43 range. An FTIR study of raw and treated coal samples has been carried out, confirming the reduction of oxygen-containing and phenolic functional groups. The ultimate and proximate analysis of raw and DES-treated coal samples was estimated, showing a decrease in ash yield. Calorific value in the form of fixed carbon content was also increased. The DES is a green solvent that is easy to synthesize, low cost, and useful for the increasing efficiency of coal.

8.2 Suggestions for Future Work

The limitations can be improved, and there is still room for more research. The following suggestion is put forward for further development of coal quality and its beneficiation, thereby improving the environment and value of coal.

1. Other subsidiaries of Coal India Ltd. should be included to investigate the chemical characteristics of coal for more comprehensive results.

2. In this work, the prime focus was on Indian Permian coal, so there is a lot to highlight and compare with other coal types like lignite for the betterment of marketability and strategies of the Indian coal industry.

3. There is ample scope, and we still need to work with XPS, FTIR, Raman spectroscopy, and TGA to obtain a more comprehensive picture of the coal components involved in oxidation at low temperatures(30-150°C).

4. There is a vast scope for research because the new opencast coal mines are drastically affecting the citizen's life in all aspects, i.e., coal mines dust polluting society and surroundings.

5. There is a huge opportunity for study and research as coal is the country's prime energy source for various industries. Also, it is a vital source of revenue for the country, and it also creates enormous employment for the citizens directly or indirectly.

6. Some toxic elements like arsenic and mercury are present in coal. More study is required for the source apportionment. Further investigation is needed to know the toxicological relationship between morphological features and physical-chemical characteristics of fly ash.

7. Coal beneficiation studies with other suitable chemical and green solvents must be studied.