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Kinetics of pyrolysis and combustion of a South African coal using the distributed activation energy model

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Abstract

Most of the energy requirements in South Africa are met by conversion of coal. Kinetics of these coal conversion reactions are necessary for these processes to be run efficiently. In this work, the kinetics of pyrolysis and combustion of a South African coal have been studied. Thermo-gravimetric experiments were carried out on coal and char samples under nitrogen and oxygen atmospheres, at different heating rates. The results were used with appropriate models in order to determine the reaction kinetics.

The Distributed Activation Energy Model (DAEM) is commonly used to describe the coal pyrolysis process. The model states that coal devolatilizes according to a number of first order reactions, each with unique activation energy (E). An algorithm has been developed to invert this model in order to calculate the fraction reacting, E and pre-exponential factor (A) of each reaction using thermo-gravimetric data. The algorithm was tested on pyrolysis data from real and simulated TGA experiments. The parameters obtained were used to model the reaction at different heating rates. It was found that the DAEM is suitable to model the pyrolysis reaction

Further scrutiny of the inversion algorithm has shown that the calculation of the activation energy is a model-free method. The algorithm was therefore applied to real and simulated thermo-gravimetric data for coal combustion. Results show that the DAEM can be used as a model-free method to calculate the E of coal combustion. However, the calculation of the A requires the use of an appropriate structural sub-model. For this particular coal, the shrinking core model was not suitable to describe the combustion reaction. Finding the correct model did not form part of this work.

In addition, the assumption of a constant heating rate used in the algorithm was investigated. Examination of TGA data showed that there was a lag between the program temperature and the actual sample temperature. This temperature lag, however small, impacted the heating rate of the sample. Instantaneous values for the heating rate were used in the algorithm. Again, the algorithm proved able to calculate kinetic parameters.

Finally, data obtained from coal and char combustion reactions was compared. Both the E and temperature at the maximum devolatilization rate indicate that raw coal is more suitable for use in industrial boilers than char.