

Abstract

A particular field of interest in the development and understanding of current coal-based fuel and energy production is the determination of reaction kinetics of various materials. A more efficient and accurate method would improve the design and operation of current technology used in fuel and energy production.

An established DAEM-based algorithm was further developed to determine the reaction behaviour of materials reacting in CO₂ by means of incorporating the Random Pore Model (RPM). A method for modifying the algorithm to accurately use any other reaction model (for both isothermal and non-isothermal cases) was developed. It was found that the multiple reaction approach characteristic to the DAEM resulted in far more accurate reaction behaviour predictions than conventional methods that presuppose a single overall reaction.

The novelty in this research was the determination of multiple reactions occurring in RPM systems. Despite specifying multiple reactions, a single RPM structural parameter ($\phi=12.2$) was still suitable, and produced accurate data fits. Charred Coal-CO₂ reactivity data was processed with the algorithm and activation energy values of $E_1=261.7\text{kJ/mol}$, $E_2=246.4\text{kJ/mol}$ and $E_3=227.6\text{kJ/mol}$ were found. Grouped pre-exponential factor values were found to be $A_1^*=1.60\text{E}+07\text{s}^{-1}\cdot\text{m}^{-1}$, $A_2^*=2.08\text{E}+06\text{s}^{-1}\cdot\text{m}^{-1}$ and $A_3^*=2.75\text{E}+06\text{s}^{-1}\cdot\text{m}^{-1}$. The corresponding mass fractions were $f_{0,1}=0.31$, $f_{0,2}=0.32$, $f_{0,3}=0.37$. These proved to predict the reaction behaviour better than the conventional single reaction approach which found activation energy and grouped pre-exponential factor of $E=254.5\text{kJ/mol}$ and $A^*=1.0\text{E}+07\text{s}^{-1}\cdot\text{m}^{-1}$ respectively.

The algorithm was then used to compare reactivities of plain South African coal char and of the South African coal-pinewood blend char in CO₂. This particular combination was found to exhibit improved reactivity as compared to the plain coal. The coal-pine blend was found to have a lower structural parameter value ($\phi=11.7$) compared to plain coal char. The change in the structural parameter value suggests structural changes as a result of the biomass addition, which improved reactivity.

The findings show that the algorithm can be successfully adapted to process RPM (and other reaction model) data and produce accurate and reliable results. The biomass-blend results indicate the potential benefits of co-feeding the two feedstocks commercially; this must however be investigated further.