Diffusion Modeling in TGA in Context of CO2 Gasification of Char

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Abstract

The Thermo- Gravimetric Apparatus (TGA) is often used for kinetics determination. A typical TGA experiment is performed by filling cylindrical crucible with a few milligrams of char. The gasifying agent flows across the top of the crucible at a constant concentration and temperature. With this kind of setup, gasification reaction may be limited by the reach (diffusion) of the gasification agent to the internal surfaces of the char particles. In addition to this, after some time, ash is formed between the bulk of the gas and the upper surface of char as well as the char bed consists of small particles surrounded by empty spaces, through which the gasification agent has to diffuse to reach the external surfaces of the porous char particles. Furthermore, if the endo/exothermicity of the reaction is higher, and if the external heat transfer process is not fast enough, the temperature of the external layer of the char bed may be significantly different than that of the bulk of the gas. The present modeling exercise is aimed at examining the diffusion effects on TGA gasification experiments using CO2 as a gasification agent. The diffusion processes may seriously affect the observed gasification rate and must be considered when interpreting results of laboratory studies and determining the kinetic parameters. CO2 gasification data (weight of char vrs time and temp) and kinetics parameters determined by single layer TGA experiments are available. (Ramesh Mandapati, 2012). Initially the simulations were run with a constant temperature of char, that was taken to be equal to temperature of bottom wall of TGA crucible (available in TGA data). This assumptions was considered to be valid as the heat of reaction as well as rate of reaction of gasification are not very high and the TGA crucible is very small. To check the validity of constant temperature assumption, heat transfer enabled simulation is carried out. It was observed from the results that variation in temperature is very less. Minimum temperature attained in crucible is 0.6 K less than the initial temperature. So our assumption of constant temperature stands valid in case of CO2 gasification, as it has very less effect on conversion. But the same will not be true with any highly endo/exotheric fast reaction e.g. char oxidation.