Mineral Matter Transformation During Sasol-Lurgi Fixed Bed Dry Bottom Gasification – Utilization of HT-XRD and FactSage Modelling

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Abstract

Coal is generally accepted to be a heterogeneous resource where coal properties can vary extensively between geographical sites or within a mine. However, detailed coal characteristics are essential to predict gasification performance. Mineral matter transformation and slag formation are specific properties of a coal source that provide more information on the suitability for combustion or gasification purposes. Therefore, the chemistry and mineral interaction have to be understood in order to determine the suitability for fixed bed gasification purposes with regards to mineral matter transformations and slagging properties. Agglomeration of ash particles provides the desired porosity of the ash bed for adequate agent (steam and oxygen) flow and distribution, whereas excessive slagging inside the gasifier can cause channel burning, pressure drop problems or unstable operation, resulting in cut backs on gasifier load, which implies a direct loss in gas production.

The principle aim of this paper is to understand the chemistry and interpret mineral matter transformation during Sasol-Lurgi Fixed Bed Dry Bottom (S-L FBDB) Gasification by means of high temperature X-ray diffraction (HT-XRD), in combination with FactSage modelling.

Conventional ash fusion temperature (AFT) analyses are currently used to predict slagging properties of coal sources. Normal AFT analyses give an average flow property and do not indicate exactly at what temperature the first melt/slag is occurring. Operating experience indicates that even when the gasifiers are operated at temperatures above the flow temperature as given by AFT analysis, a low percentage of slag is formed. HT-XRD results indicated (up to a temperature of 500°C) that the starting assemblage mainly consisted of kaolinite ($Al2SiO5(OH)4$), calcite ($CaCO3$) and dolomite

($CaMg(CO_3)_2$). From 500°C, kaolonite decomposes first, followed by calcite and dolomite. Around 1000°C, anorthite ($CaAl_2Si_2O_8$) becomes stable probably due to partial melting of the phase assemblage. Mullite decomposes at 1200°C, while quartz and anorthite were observed up to 1350°C. Above 1350°C the whole phase assemblage of the coal was molten. The HT-XRD findings were further supported with FactSage thermochemical modelling of the gasifier, and indicated that feldspar formation (including anorthite) correlated with slag formation at temperatures around 1000°C.

It can be concluded that HT-XRD and FactSage modelling supply insight into specific mineral reactions and slag formation. Although the amount of melt was fairly low at 1000°C, a percentage of melt is definitely present, which at this temperature is not reflected by AFT analyses. The specific value for Sasol in using FactSage, in combination with HT-XRD is that it can be used to analyse equilibrium conditions for reactions occurring between inorganic and organic materials together, as well as provide insight into mineral transformation and slag formation. This can improve the interpretation of flow properties of the reacted mineral matter in coal and assist in identifying and quantifying slag formation in gasifier operation at temperatures not reflected by normal AFT analyses.