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Chemical process modelling of Underground Coal Gasification (UCG) and evaluation of produced gas quality for end use

Anna Korre, Nondas Andrianopoulos, and Sevket Durucan
Imperial College London (a.korre@imperial.ac.uk)

Underground Coal Gasification (UCG) is an unconventional method for recovering energy from coal resources through in-situ thermo-chemical conversion to gas. In the core of the UCG lays the coal gasification process which involves the engineered injection of a blend of gasification agents into the coal resource and propagating its gasification. Athough UCG technology has been known for some time and considered a promising method for unconventional fossil fuel resources exploitation, there are limited modelling studies which achieve the necessary accuracy and realistic simulation of the processes involved. This paper uses the existing knowledge for surface gasifiers and investigates process designs which could be adapted to model UCG.
Steady state simulations of syngas production were developed using the Advanced System for Process ENgineering (Aspen) Plus software. The Gibbs free energy minimisation method was used to simulate the different chemical reactor blocks which were combined using a FORTRAN code written. This approach facilitated the realistic simulation of the gasification process. A number of model configurations were developed to simulate different subsurface gasifier layouts considered for the exploitation of underground coal seams. The two gasifier layouts considered here are the linked vertical boreholes and the controlled retractable injection point (CRIP) methods. Different stages of the UCG process (i.e. initialisation, intermediate, end-phase) as well as the temperature level of the syngas collection point in each layout were found to be the two most decisive and distinctive parameters during the design of the optimal model configuration for each layout. Sensitivity analyses were conducted to investigate the significance of the operational parameters and the performance indicators used to evaluate the results. The operational parameters considered were the type of reagents injected (i.e. O_2, N2, CO_2, H_2O), the ratio between the injected reagents and the feedstock quantity (i.e. coal), the pressure, the gasification and the combustion temperatures. The performance indicators included the composition and the energy content of the product gas as well as the carbon and energy efficiency achieved under each operational scenario. Different operational scenarios for every model configuration facilitated the cross-comparison among different configurations. The proximate and ultimate analysis data for the coal seams modelled were taken from a number of candidate UCG sites (Durucan et al., 2014) .The model findings were validated using the results of field trials reported in the literature. It was found that, increased gasification temperature leads to higher H2 and CO quantities in the product gas. Moreover, CH4 and CO_2 concentrations increased as reaction pressure increased, while the CH4 quantity reached its highest value at the highest operational pressure, when combined with the lowest gasification temperature. The simulation models developed can be used to design and validate experimental UCG studies and offer significant advantages in terms of time and resource savings. As the UCG process consists of interrelated stages and a number of diverse phenomena, therefore, the gasification designs developed could act as the basis for an integrated UCG model tailored to the needs of a UCG pilot plant.