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A new HYSYS model for underground gasification of hydrocarbons under hydrothermal conditions

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ABSTRACT

A new subsurface process model was developed using the ASPEN HYSYS simulation environment to analyse the process energy and gasification efficiency at steady-state equilibrium conditions. Injection and production wells were simulated using the HYSYS pipe flow utilities which makes use of the Beggs and Brill flow correlation applicable for vertical pipes. The downhole reservoir hydrothermal reactions were assumed to be in equilibrium, and hence, the Gibbs reactor was used. It was found that high W/C ratios and low O/C ratios are required to maximise gasification efficiency at a constant hydrocarbon feed flowrate, while the opposite is true for the energy efficiency. This occurs due to the dependence of process energy efficiency on the gas pressure and temperature at surface, while the gasification efficiency depends on the gas composition which is determined by the reservoir reaction conditions which affects production distribution. Another effect of paramount importance is the increase in reservoir production rate which was found to directly enhance both energy and gasification efficiency showing conditions where the both efficiencies are theoretically maximised. Results open new routes for techno-economic assessment of commercial implementation of underground gasification of hydrocarbons.

Introduction

Underground gasification of fossil fuels is a promising technology for economic and environmentally benign production of hydrogen and syngas for power generation or chemical applications [1]. Many studies have been reported on the modelling of underground gasification of fossil fuels, particularly coal, showing that it is technically and economically feasible, and it is capable of producing syngas with high heating values [1–8]. Other studies have demonstrated the thermodynamic thermal efficiency of steam reforming and partial oxidation of hydrocarbons and biomass models [2,9–11] showing the upper theoretical limit for the thermal efficiency which may be useful in process optimisation. For instance, Lutz et al. [10,11] reported that, the thermal efficiency decreases as the O/C increases due to the increased combustion of carbon feedstock compared with steam reforming. They defined the thermal efficiency as the ratio of energy output to energy input for a given system with defined boundaries. They showed that the thermal efficiency of steam reforming of heptane increases with increasing steam to

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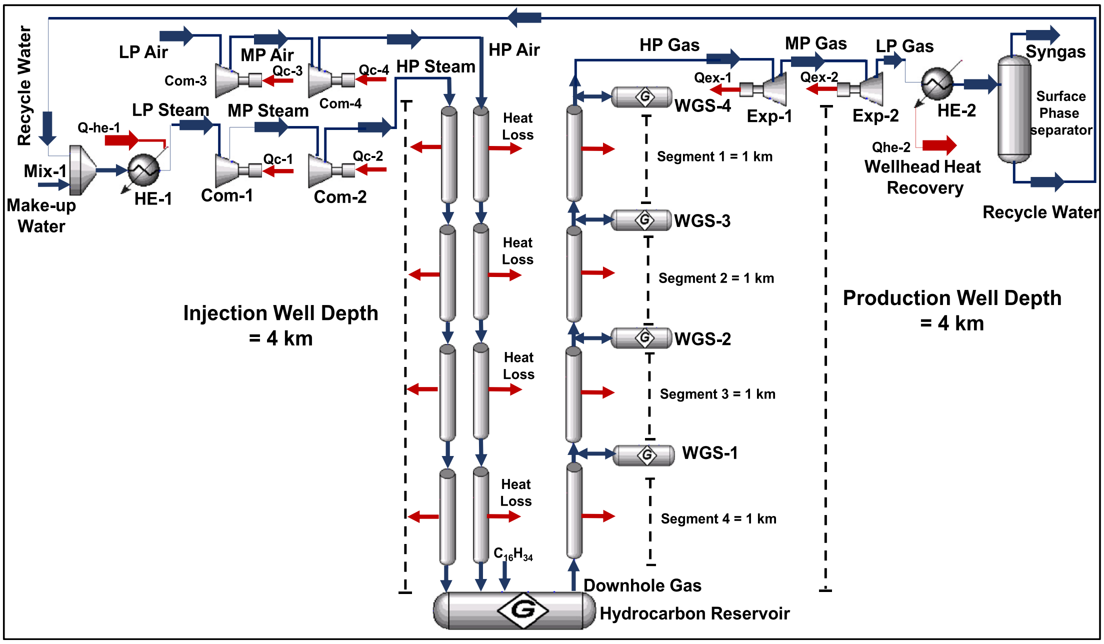

Fig. 1 – HYSYS model for an underground gasification of hydrocarbons.

carbon ratio with a slight decrease as the ratio exceeds 3.5. The increase on the oxygen to carbon ratio showed the opposite effect, during partial oxidation, causing the thermal efficiency to decrease due to the increase of fuel consumption and decrease of hydrogen yield [10]. Prins et al. [2] investigated on the effects of fuel composition comparing between coal and biomass gasification efficiency in terms of exergy losses which were found to increase when gasifying wood, at O/C of around 0.6, compared with gasifying coal at O/C of around 0.2. Withag et al. [9] presented an ASPEN model for supercritical water gasification of biomass emphasising the importance of heat exchangers effectiveness for maximising thermal efficiency at a given biomass concentration. More Recently, Bhutto et al. [12] reviewed the technical fundamentals and recent advances in underground coal gasification highlighting the importance of thermodynamic simulations as well as kinetic models to optimise downhole gasifiers. Furthermore, Afgan and Vezirlogu [13] also highlighted the key role of oil, with a low heating value of 7000 kJ/kg, as contributor to supplying efficient production of hydrogen with a reforming of efficiency of 34 UScent/kgH_2, which may be favourably compared to the oil market energy cost of 4 UScent/kJ.

In our previous work [14], we reported the analysis of equilibrium gas yield of hydrothermal gasification of n-hexadecane under oxidative and non-oxidative conditions showing optimal conditions for maximising the theoretical yield of hydrogen and syngas. In this work, we extend our previous theoretical equilibrium analysis into an integrated subsurface well system analysing the energy and gasification efficiency during the injection of steam and air, and production of syngas at surface under hydrothermal conditions. Although this model is based on equilibrium steady-state conditions, it provides useful insight into how underground gasification may behave under kinetically controlled regimes, in order to establish conditions where energy and gasification efficiencies are maximised.

Subsurface system modelling

Based upon the thermodynamic analysis reported in our previous work [7], a subsurface flow system, comprising the injection and production wells, was developed in order to predict to the change in temperature, pressure, and gas composition over a well depth of 4 km, which accounts for the distance between the reservoir and wellhead. At different segments of vertical elevations, the Beggs and Brill [8] pipe flow correlation was used to estimate the change in temperature and pressure, while the change in gas composition was estimated using the Gibbs reactor embedded between different pipe segments in the production well. The equation of state used in this analysis is PRSV which may predict the thermodynamic properties of fluid components, as carried out in our previous work [7]. This analysis was useful in estimating the temperature and pressure and gas composition of at the wellhead enabling immediate recovery of clean energy, through the gas heat and momentum, in addition to producing hydrogen, syngas, and methane. The HTFS correlation was used to predict the heat transferred between the pipe and surrounding insulation (Concrete) which is assumed to be contained in ground sandstone medium. This enabled prediction of pressure drops, and heat losses across the pipe enabling direct estimation of temperature and pressure gradients of injection and production fluids. The downhole pressure of injection fluids (steam, and air) was maintained at a range between 222 and 230 bar which is slightly above than the reservoir pressure (220 bar). The effects of varying the oxygen to carbon ratio (O/C), water to carbon ratio (W/C), well