



Full Length Article

Optimization of synthesis gas heating values and tar by-product yield in underground coal gasification



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ABSTRACT

Increasing global energy demand is a central challenge of the 21st century. Apart from renewable energy concepts, sustainable bridging and buffering technologies are needed which simultaneously offer long-term energy supply guarantees. Underground coal gasification (UCG) shows a promising potential to meet these requirements of future energy markets by in situ conversion of coal to a valuable synthesis gas that can be used in various industrial applications. Currently conducted in more than 14 countries worldwide, a main focus of international UCG efforts lies in improved technical control to reach the desired high gas qualities and simultaneously reduce the tar by-product yield as a potential source of groundwater contamination. Referring to an innovative thermodynamic UCG model parameterized with exemplary base-case data from the UCG field trials Hanna-I, Centralia-Partial Seam CRIP (PSC) and Pricetown, we investigated pyrolysis temperature, operating pressure, water influx and gasification agent injection, optimizing synthesis gas heating values and reduced tar production. General best-fit scenarios were performed assuming an idealized UCG reactor. Besides these best-fit simulations, selected worst-case scenarios considering gas losses were tested. Overall, the model results indicate that operational process improvement potentials vary over wide ranges in the order of few percent to more than 50% compared to the examined base cases. In view of selected available literature data, near-zero tar production rates and simultaneous Lower Heating Value (LHV) improvements in the range of ~2–40% are feasible.

1. Introduction

Underground coal gasification shows a profound potential to provide competitive alternative energy solutions for several decades up to a few hundred years. Main technical advantages include economic utilization of deep global coal deposits as well as flexible product design options [1–5]. Due to vast international research efforts, the understanding of in situ processes and technical operation of UCG constantly increased and introduced improved reactor concepts such as the Controlled Retraction Injection Point (CRIP) system, optimized post-phase reactor clean-up procedures (Clean Cavern Concept), as well as reduced greenhouse gas emission strategies in terms of Carbon Capture and Storage (UCG-CCS) [1,4,6–23]. Regardless of these positive perspectives,

to date UCG still remains a challenging technology, both from economic as well as environmental performance perspectives [4,19,24–26]. Besides coal feedstock [27–30], main operating challenges in the past UCG trials were especially maintaining effective reactor pressures and temperatures, controlling the water influx, and choosing suitable gasification agent mixtures in view of potential gas losses. These may induce the release of BTEX (Benzene, Toluene, Ethylbenzene, Xylenes), Polycyclic Aromatic Hydrocarbons (PAHs), Phenol and heterocyclic compounds to nearby groundwater resources [1,4,8,11,26,30–34]. In view of the latter, gas loss-related water pollution risks, the past debates in Australia and Scotland point out that future industrial-scale UCG acceptance will substantially depend on environmental long-term sustainability issues [35,36]. Referring to this

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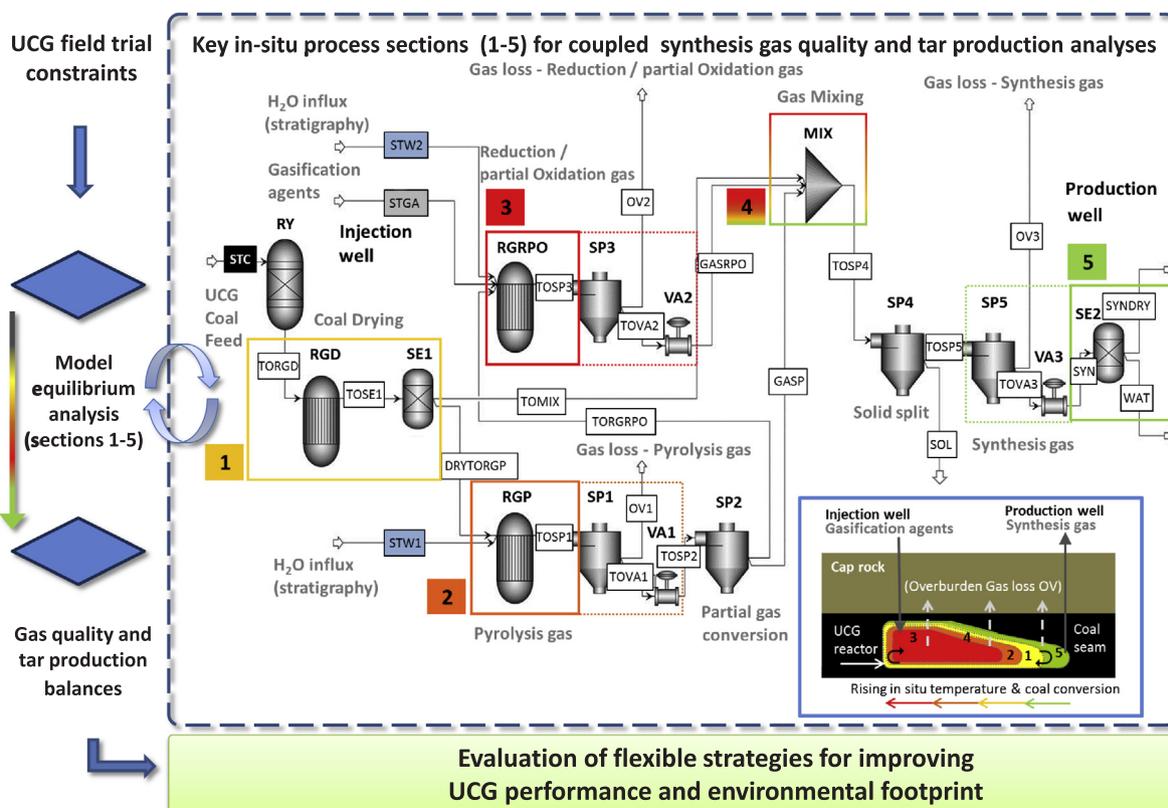


Fig. 1. UCG flow sheet [51,52] considering gas losses from main gas sections (dashed lines). Note: OV1 = gas loss stream pyrolysis gas, OV2 = gas loss stream reduction/partial oxidation gas, OV3 = gas loss stream synthesis gas, RY = RYield reactor, coal chemistry yield transformation to elemental C-H-O-N-S distribution essential for Gibbs reactor balancing, RGD = Gibbs equilibrium reactor for drying section (1), product balancing by minimization of Gibbs energy, RGP = Gibbs equilibrium reactor for pyrolysis section (2) RGRPO = Gibbs equilibrium reactor for reduction/partial oxidation section (3), (balancing cf. RGD), MIX = mixer module, mixing of section 1–3 related gas types (4), SE1 = coal moisture separator unit, SE2 separator unit for dry synthesis gas balancing (5). SP1 = pyrolysis gas loss splitter, SP2 = pyrolysis gas splitter unit for partial pyrolysis gas conversion, SP3 = reduction/partial oxidation gas loss splitter, SP4 = splitter unit for solid separation from gas phase via material stream SOL, SP5 = mixed synthesis gas loss splitter, GASP = material stream residual pyrolysis gas to mixing section, GASRPO = reduction/partial oxidation gas stream to mixing section, STC = material stream coal/coal chemistry definition, STGA = material stream for gasification agent definition, STW1/STW2 material streams for water influx definition to pyrolysis- and reduction/partial oxidation sections, SYN = material stream mixed wet synthesis gas, SYNDRY = material stream dry synthesis gas, TOMIX = material stream coal moisture re-added to mixing section, (balancing cf. RGD), TORGRPO = material stream partial pyrolysis gas consumed in reduction/partial oxidation gas section, TOSP1 = material stream pyrolysis gas, TOSP2 = material stream reduction/partial oxidation gas, TOSP5 = material stream mixed wet synthesis gas, TOVA1 = material stream to VA1, TOVA2 = material stream to VA2, TOVA3 = material stream to VA3, VA1 = volume control valve gas loss pyrolysis section, VA2 = volume control valve gas loss reduction/partial oxidation, VA3 = volume control valve synthesis gas loss section, WAT = material stream residual water.

problem, many preceding studies showed the benefit of modeling analyses which can offer an effective and safe path to gain a better understanding of UCG optimization potentials. In terms of gas composition, previous UCG modeling studies successfully investigated gas shift effects for product optimization considering, e.g., CO, H₂, CH₄, CO₂ and N₂ [12,23,37–42]. However, tars were rarely considered in a modeling context so far, with few authors considering bulk tar as a pseudo compound [12,43–45]. Besides these studies, only limited deeper analyses have been conducted with regard to tar formation and related compound conversion. In this context, lighter and lower molecular weight synthesis gas tars were found due to reduction/partial oxidation-induced cracking of heavier pyrolysis tars, partly accompanied by plugging problems [33,46–50]. Overall, profound knowledge of tar production control under varying in situ conditions is still missing. Using a new thermodynamic model for coupled synthesis gas

quality and tar production analysis of underground coal gasification [51], the present modeling study provides a predictive UCG analysis taking into account tar production control and economic gas quality constraints to achieve optimum operating options in view of synthesis gas quality and reduced tar production.

2. Materials and methods

A detailed overview of the established Aspen Plus thermodynamic model methods and its adaptation to the UCG process has been previously addressed [51]. Fig. 1 illustrates the basic flowsheet including the UCG process chain integration from injection to production well and related descriptions of the utilized Aspen standard units. A comprehensive model documentation is given in [52]. Corresponding to the available knowledge on the UCG chemical reaction zone and the

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