



Full Length Article

Innovative thermodynamic underground coal gasification model for coupled synthesis gas quality and tar production analyses



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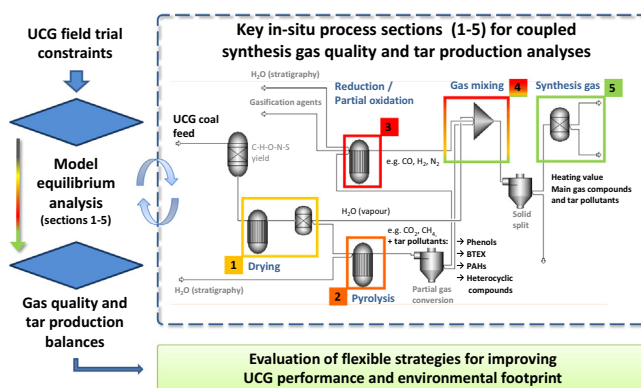
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HIGHLIGHTS

- A first-time UCG modeling approach for coupled synthesis gas quality and tar production analyses is introduced.
- Main UCG chemical sub-processes, operating parameters and tars down to single pollutant level are considered.
- The model is successfully validated against available literature data.
- Mixing of different sub-process related gas fractions and affiliated cracking leads to reduced tar yields in synthesis gas.
- Best-fit future prognoses in plan regarding reachable UCG gas qualities at simultaneously reduced tar production.

GRAPHICAL ABSTRACT



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ABSTRACT

Underground Coal Gasification (UCG) technology is steadily improving due to high scientific and industrial efforts in currently over 14 countries worldwide. A fundamental UCG objective refers to syngas production for multiple end-uses, accompanied by environmental impact mitigation focusing contaminant reduction. In terms of this topic, the control of groundwater quality endangering tars has been a key problem rarely addressed in UCG publications so far. Considering UCG main sub-processes, operating parameters and tar spectrum knowledge grounded upon established thermodynamic equilibrium principles, an innovative and flexible model approach for coupled gas quality–tar production balances is presented here. The model is validated against literature data of the Hanna-I and Centralia-Partial Seam CRIP (PSC) field trials. For both trials good matching results were found. Main gas compounds and Lower Heating Values (LHVs) results are close to reported data partly reaching less than 10% deviation (relative error range for main compounds 4.32–18.6%, LHV 6.60–21.7%). Tar literature trend-modeling comparisons down to the single pollutant scale are addressed for the first time considering published data. Results here

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successfully reflect main qualitative tar tendencies, while current quantitative prognoses are on a satisfactory level, and expected to be further improved with the availability of more comprehensive in-situ data.

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1. Introduction

Underground Coal Gasification provides a promising technical and economic potential to solve current long-term power supply conflicts worldwide by controlled in-situ conversion of otherwise non-mineable coal reserves [1–7]. While the technique itself is a rather simple concept in theory, experience from major international field trials over the last decades shows its control in practice is much more complicated. Various factors during the in-situ UCG reactor operation often hamper a continuously stable process performance (e.g. water ingress, heat losses), in consequence partially leading to lower synthesis gas qualities and undesired hazardous by-products [1,3,8–14]. Pollutant charged gas leakage from the UCG reactor due to roof rock failure as a thermo-mechanical response of in-situ pressure and temperature conditions recently marks one of the most severe potential environmental impacts [1,6,15–19]. With focus on the growing public debate on gas leakage affiliated with organic groundwater pollution risks as well as general tar plugging problems, a key future UCG by-product challenge thus lies in better tar production control and aligned organic pollutant minimization in UCG gases [20–23]. Principle UCG tar related organic pollutant groups, primarily consisting of BTEX, Phenols, PAHs and heterocyclic compounds have been well documented in diverse preceding publications [10,11,21,24–26]. Besides environmental motives, the tar control topic may also be deeper analyzed from an economic valuable tar perspective, regarding tar yield and spectrum optimization for marketable products [27]. Whether addressing environmental or economic targets, in terms of subsurface tar control factors and quantitative tar effects to date, overall few hard fact knowledge exists and rare literature data are available covering these issues. UCG chemical in-situ processes are of major relevance in terms of tar build up and transformation. In this context, previous studies indicate that UCG mixed synthesis gas tars can be interpreted as a reduction/partial oxidation induced lighter- and lower molecular weight/boiling point-fraction of heavier primary pyrolysis tars, whereby pyrolysis is consistently reported as main source process for tar build up. Tar spectrum and related quantities can depend on several factors, including gasification stage, inner-system variables such as coal type chemistry, in-situ gas temperature, as well as outer ones, e.g., choice of oxidant [10,26,28–30].

Due to complex reaction routes involved in tar chemistry and the numerous factors that contribute to the final UCG tar product, so far tars have seldom been explicitly focused in UCG modeling. Whenever considered in former compositional gas models, they were commonly treated as pseudo species [31–34]. In awareness of the recent debate on potential gas leakage and compound related water cycle restrictions, however a deeper tar modeling scale down to the specific single pollutant level becomes mandatory to deduce corresponding quantitative data on single compounds and optimization potentials regaining trust in UCG's environmental performance.

2. Materials and methods

Using the established commercial simulator Aspen Plus[®], we introduce a new UCG synthesis gas quality related tar model, which considers main chemical in-situ sub-processes of drying,

pyrolysis, reduction/partial oxidation, related mixing of gas fractions, water influx, optional gas losses and respectively a selected model tar set including typical single pollutants [1,3,8,10,24,25]. The model is based on chemical and phase equilibrium balances under minimization of Gibbs energy referring to the Peng Robinson Equation of state [35,36]. Equilibrium modeling has successfully been conducted within diverse previous UCG studies among other focusing basic test operating alternatives as well as economic analyses [37–39]. Considering these former modeling equilibrium approaches, we provide an innovative coupled main gas- and detailed tar compound accounting model. In this context we respectively chose the equilibrium balancing option faced to the fact that it marks an established approximation strategy, which is independent of reaction pathways [3,40], helping to overcome uncertainties and reduce complexity in terms of more than 500 potentially participating tar reaction routes [41]. While UCG may be performed with different technical setups [1,42] the focus here is on a general coal model establishment, considering the previously named main chemical in-situ processes as key elements of all UCG schemes. The model can be applied for environmental risk assessments and critical in-situ data estimation down to the sub-process level as important support for future laboratory and field setups. It may also be used as valuable support tool for tar yield optimization and composition analyses regarding surface gas processing plant design. In more general terms, it allows deeper insight into in-situ out-of-sight processes and respectively preferred operating modes to achieve coupled clean as well as high quality synthesis gas production solutions.

Corresponding to the process model development, standard Aspen Plus[®] software modules were governed as depicted in Fig. 1. An overview of selected model components, including the principal tar pollutant set balanced within the model is outlined in Table 1. Relevant information on parameterization for specific modules is provided in Table 2 [43–58]. In view of essential model validation test data only few precise background data on former UCG field trials are available to the public. As a starting point, here we used data related to the early North American trials Hanna I and Centralia PSC [43–47,53–57].

In deeper view of the basic flowsheet build-up procedure, the integration of main sections (1–5) was oriented at the in-situ reactor zone distribution known from principal previous UCG field experiments and related excavation experiences that have been well documented in several preceding UCG publications [1,3,8,59,60]. The basic reactor distribution is thus characterized by development of an oxidant impacted high-temperature reduction/partial zone near the injection well (cf. Fig. 1, section 3), in direction of the production well gradually followed by a mid-temperature pyrolysis section (cf. Fig. 1, section 2) and a low temperature drying section (cf. Fig. 1, section 1). In consequence of gas mixing between the previously named zones (cf. Fig. 1, section 4), finally a mixed synthesis gas stream forms (cf. Fig. 1, section 5).

Referring to the detailed process modules individual coal type chemistry is first defined using a basic material stream (cf. Fig. 1, STC). The coal chemistry information is subsequently transferred to an elementary C–H–O–N–S yield distribution in a RYield reactor (module RY) with a calculator block added for dry to wet basis transformation. The C–H–O–N–S yield distribution is a general essential data form for RGibbs balance calculations that we tested

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