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Research article

Modelling, simulation and design of an integrated radiant syngas cooler and steam methane reformer for use with coal gasification

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ABSTRACT

In this work, a novel process intensification design is proposed to integrate the Radiant Syngas Cooler (RSC) utilised to cool the coal-derived synthesis gas in entrained-bed gasifiers and a steam methane reformer (SMR). The feasibility of the proposed integrated system is analyzed by developing a rigorous, dynamic, multi-dimensional model and establishing design heuristics for the integrated system. Two different flow configurations are explored; co-current and counter-current. The simulation results show that the proposed concept is feasible that allows for methane conversions as high as 80% in co-current mode and 88% in counter-current mode. The results also demonstrate that the counter-current design, though with higher conversion and cooling duty provided when compared to co-current designs, is limited by the tube wall material limitations. Our analysis shows that the total avoided CO_2 emissions is 13.3 tonnes/h by using the proposed integrated configuration in place of an external reformer for the natural gas feed rates considered in this study. In addition, a sensitivity analysis is performed on key model assumptions and the resulting effect on the performance is assessed. The sensitivity results have helped identify key factors to consider prior to pilot-scale implementation and further improvement for agile designs; a one third reduction in tube length reduced pressure drop by as much as 50% but reduces methane conversion by 15% points, neglecting slag deposition on tubes over-predicts performance only by 3%, and a 10% change in gas emissivity calculations affects model prediction of performance by less than 1%.

1. Introduction

Synthesis gas (commonly referred to as “syngas”) is a gaseous mixture where the major constituents are hydrogen and carbon monoxide. It is a key feedstock in the production of hydrogen, electricity, methanol, ammonia, synthetic fuels by the Fischer–Tropsch (FT) process, and commodity chemicals such as di-methyl ether (DME). Gasification and reforming are the two primary industrial routes available to produce syngas. The gasification path employs high temperature partial oxidation of solid fossil fuels like coal, biomass or carbon intensive waste products like petcoke and municipal solid waste. For reforming, a variety of hydrocarbons can be used as feedstock, but methane is the preferred feedstock in many of the hydrogen production facilities in the world [1]. Steam reforming of methane is an endothermic catalytic process where the heat required is supplied by combustion of fuel (usually natural gas) to the reactant gases (steam and methane) within multiple tubes that are placed inside a furnace. Though the product from both gasification and reforming is syngas, the quality of syngas varies widely between them. Moreover, each of these processes has unique advantages and disadvantages which are exploited depending upon the industry they are applied in.

One of the main advantages of gasification technology is that it allows for the consumption of vast available resources of solid fossil fuel reserves to produce fuels, chemicals and electricity, thereby reducing the reliance on oil, especially for nations that import crude oil but have large reserves of coal. The major disadvantage in using gasification for fuels and chemicals synthesis is the low H_2/CO molar ratio in the product synthesis gas. The H_2/CO molar ratio usually ranges from 0.7–1.1 depending upon the type of feed (coal/biomass) [2], which generally needs to be upgraded to a higher H_2/CO ratio depending on the application (for example, Fischer–Tropsch (FT) synthesis requires a feed ratio of 2 [2] but some DME synthesis routes require a feed ratio of 1.2–1.5 [3]). The gas is usually upgraded by employing a Water Gas Shift (WGS) reactor that converts carbon monoxide and steam to hydrogen and carbon dioxide. This process, however, leads to a loss in the plant-wide carbon efficiency (ratio of total carbon atoms in products to total carbon atoms in the input to the plant), increased carbon dioxide emissions and higher capital and processing costs. Alternatively, reforming is an established technology especially in petroleum refineries, and the resulting syngas is hydrogen rich with a molar H_2/CO ratio of greater

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than 3. However, the disadvantage is that the Steam Methane Reforming (SMR) process is highly endothermic necessitating combustion of natural gas to supply the heat required resulting in CO_2 emissions. Clearly, there is an opportunity to improve performance of syngas production processes using synergistic options with reduced emissions. Bhat and Sadhukhan [4] present an excellent review on the possibilities for improving SMR technology using different process intensification strategies, one of which involves using heat integration with exothermic or high temperature systems to supply heat to the endothermic reactions. Considering the need to find more efficient plants that incorporate sustainable designs, the advantages of each of these independent technologies can be harnessed by integrating them together in one unit that will result in efficiency improvements, flexible capability to meet different H_2/CO molar ratios for downstream processes and reduced emissions.

One such application was studied by Adams and Barton [2] who explored integrating natural gas steam reforming with coal based entrained-bed gasifiers as shown in Fig. 1. The integrated design resulted in an increase in the total system efficiency (compared to non-integrated equivalent processes) by up to 2 percentage points and an increase in net present value of up to $100 million for a polygeneration plant of 1711 MW (equivalent to 227 TPH of coal feed). The concept was centred on the need to cool the high temperature coal-derived synthesis gas exiting the gasifier at 1600 K to 1020 K (conventionally done using steam generation in a radiant cooler with tubes) and the steam methane reforming process requiring heat to drive the endothermic reactions. The heat integration strategy involves placing tubes in the radiant cooler filled with SMR catalyst. The proposed integrated configuration resolves the issue of meeting the desired H_2/CO ratio without WGS reactors or external reformers. The proposed configuration also envisioned dynamic operational capability. It is attractive because there are significant potential economic advantages if the products of downstream processes can be changed periodically to respond to market demands and prices [5]. Currently, this is difficult to do in part because the gasifier which forms the upstream part of the plant exhibits poor dynamic operability. However, by integrating gasification and steam methane reforming into one unit, it is possible to change syngas production quality and rate dynamically while keeping the gasifier itself at steady state.

Though Adams and Barton [2] showed that this integrated system was attractive from a systems-level techno-economic perspective, the feasibility of such a device itself was never studied in any level of detail. The authors acknowledged the need to develop and study the integrated device in order to determine key design parameters, product yields and qualities, conversion efficiencies, costs, controllability, dynamic operating envelopes, and other performance criteria. Therefore, the primary focus in this work is to develop first-principle based multi-scale, dynamic, heterogeneous model to address these issues and propose an initial base-case design. To the best of our knowledge, this is the first work to propose a specific design for the integrated concept, develop a corresponding model, and study its performance in detail.

2. Materials and methods

The development of the multi-scale, dynamic, heterogeneous model for the integrated system is explained in this section. The model consists of five sub-models that are coupled to simulate the hybrid system. The five sub-models include the (1) refractory lining of the RSC, (2) coal-derived syngas inside the RSC, (3) tube wall of the SMR tubes, (4) gas phase inside the tubes and (5) catalyst particles that are packed within the tubes. Both co-current and counter-current configurations for the tube gas flow have been analyzed and presented. It should be noted that the gasifier, that precedes the RSC, has not been modelled in this work as the key idea behind the proposed configuration is to operate the gasifier at steady-state and not subject it to the dynamic transients of a polygeneration plant.

2.1. RSC shell model

The RSC shell model includes mass balances, energy balances, and a pseudo-momentum balance for the shell syngas phase. The model accounts for the spatial and temporal variations in concentration and

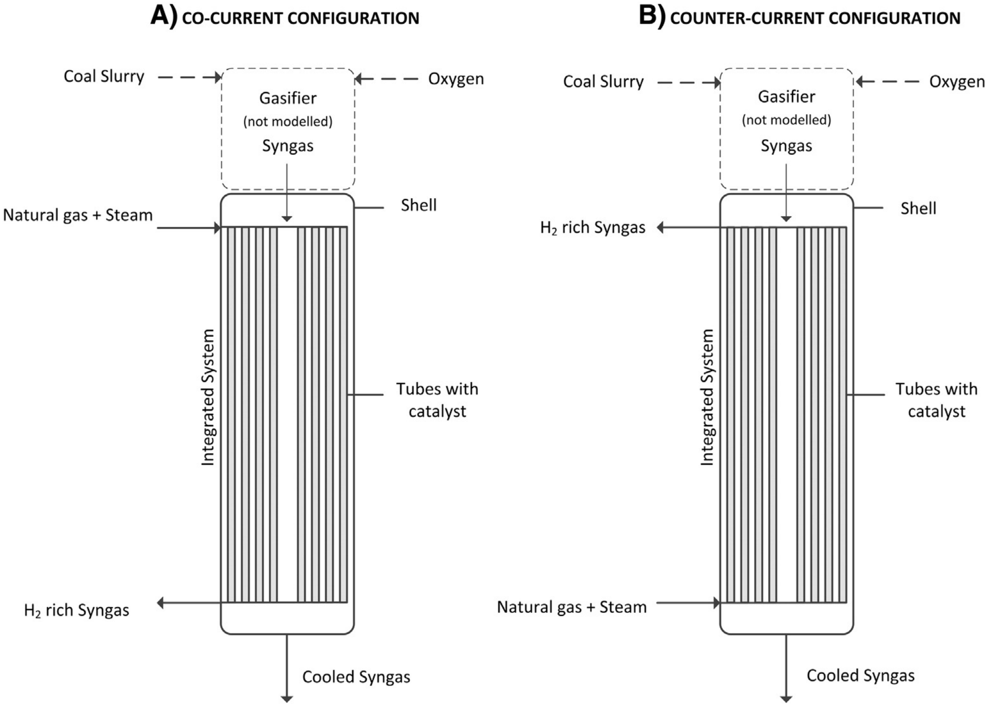

Fig. 1. Proposed concept of integrating RSC of an entrained-bed gasifier with SMR.