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A steady state model for predicting performance of small-scale up-draft coal gasifiers

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HIGHLIGHTS

- Fixed-bed gasification process is simulated through an Aspen Plus-based model.
- Syngas composition and process parameters are assessed in different conditions.
- An Alaskan lignite has been considered as reference fuel for the reported simulations.
- Model results are compared with experimental results from a pilot-scale unit.
- The comparison shows that the model well represents the experimental results.

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ABSTRACT

Small-scale fixed-bed coal and biomass gasifiers represent an attractive option for distributed combined heat and power generation. As known, gasification phenomena are very complex, involving drying, devolatilization, pyrolysis, heterogeneous and homogenous reactions, with a large number of intermediate and final products. Gasification processes are also influenced by reaction kinetics and fluid-dynamical effects, such as temperature and concentration gradients. For this reason, simulation models are able to predict gasifiers performance under the assumption of thermodynamic equilibrium only if the gasification process takes place at a known temperature and the reaction time is lower than the reactants residence time. As a consequence, for fixed-bed gasifiers equilibrium models must consider drying and devolatilization taking place at lower temperature in the heat transfer zone, where solid feed is heated by syngas. Therefore, moisture and volatiles are not involved in the gasification reactions since they are released before reaching the reaction zone.

Several models based on steady-state and one-dimensional representations have been developed to reproduce gasification processes in fixed-bed reactors. These models have been found adequate to provide information for engineering design and process optimization. In this framework a steady-state simulation model has been developed at the Department of Mechanical Chemical and Materials Engineering (DIMCM) of the University of Cagliari by using the Aspen Plus computer code for predicting performance of small-scale up-draft fixed-bed coal gasifiers. The model can be used to evaluate the mass and energy balance in each zone of the gasifier and the main characteristics of the syngas produced by the gasification process (composition, mass flow, temperature, heating value, etc.).

This paper describes the model and presents the main results of a parametric analysis, which shows how the gasification process is influenced by the main operating parameters. Moreover, the results of the model have been compared with the experimental results of an up-draft gasifier fed with an lignite from Alaska. The above-mentioned gasifier is part of a pilot gasification and gas treatment plant built at the Sotacarbo Research Centre in Sardinia, Italy. The comparison shows that the model well represents the performance of the pilot-scale unit.

1. Introduction

Coal gasification is an increasingly attractive option both for power generation and for the production of hydrogen, methanol, dimethyl-ether and other chemicals and clean fuels. In the future

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coal gasification processes integrated with high efficiency energy conversion systems, such combined cycles based on new generation gas turbine and high temperature fuel cells, will allow to achieve efficiencies as high as 50–55% [1]. Other clean coal technologies (CCT), such as, for example, advanced fluidized-bed combustion (FBC) plants are available today, but coal gasification, especially when integrated with combined cycle power plants (IGCC) and carbon capture and storage (CCS) systems is, for several specific applications, the most attractive one [2]. For technical and economic reasons, IGCC plants are currently used chiefly for large-scale power generation (300–600 MW), and already achieve efficiencies as high as 43–46%, with very low pollutant emissions. However, research and development activities are now also focussing on small- and medium-scale applications, based on fixed- and fluidized-bed gasifiers, using air as oxidant instead of pure oxygen [3–5].

Among fixed-bed gasification processes, up-draft gasifiers have the advantages of high reliability, high efficiency, low specific emissions and feedstock flexibility, but they typically produce a syngas with a high tar content [6]. In addition, air-blown gasification is more available and simple than the oxygen-blown one [7], with significant advantages in particular for small-scale applications.

The DIMCM and Sotacarbo are engaged in a long time cooperation concerning CCT, with an emphasys on small and medium scale coal gasification systems for combined heat and power (CHP) generation. Within this cooperation, DIMCM has developed a zero-dimensional, steady-state, fixed-bed gasification model (SFBG), implemented by using the Aspen Plus simulation tool, with the aims to investigate the gasification process in different operating conditions and to support the design of experiments in pilot gasification units. In particular, it was applied to design the recent experimental campaigns performed in the Sotacarbo gasification pilot plant.

After a description of the model, this paper presents the results of a simulation analysis performed to determine the effects of the main assumptions and process parameters on the gasifier's performance. Moreover, a comparison between the simulation and some corresponding experimental results obtained in the Sotacarbo pilot unit is reported.

2. Simulation of fixed-bed gasification processes

In general, a gasification process includes a wide series of chemical and thermochemical reactions, occurring in different operating conditions depending on the geometry and the fluid dynamic of the reactor. The most significant reactions are summarized in Table 1 [8].

Table 1
Gasification main reactions.

Reaction	Reaction name	Heat of reaction (kJ/mol)
$C + O_2 = CO_2$	Carbon combustion	−393
$2C + O_2 = 2CO$	Carbon partial combustion	−221
$C + CO_2 = 2CO$	Boudouard reaction	+173
$C + H_2O = CO + H_2$	Steam gasification	+131
$CO + H_2O = H_2 + CO_2$	CO-shift conversion	−412
$CO + 3H_2 = CH_4 + H_2O$	Steam reforming	−206
$CO_2 + 4H_2 = CH_4 + 2H_2O$	Metanation	−165
$S + O_2 = SO_2$	Sulphur combustion	−297
$SO_2 + 3H_2 = H_2S + 2H_2O$	Hydrogen sulphide formation	−207
$CO + S = COS$	Carbonyl sulphide formation	+63
$COS + H_2O = H_2S + CO_2$	Carbonyl sulphide hydrolysis	−34
$N_2 + 2O_2 = 2NO_2$	NO_2 formation	+66
$N_2 + 3H_2 = 2NH_3$	Ammonia formation	−46

As well known, autothermal gasification is generally carried out by injecting substoichiometric air or oxygen (just to promote the combustion of a portion of fuel to provide heat for the endothermic reactions) and eventually steam. In general, an increasing of air (or oxygen) injection promotes fuel combustion, thus involving an increasing temperature of the process, higher CO_2 concentrations and lower CO concentrations in raw syngas. On the other hand, an increasing in steam injection involves a temperature reduction and promotes shift conversion equation, with a subsequent increasing in H_2 and CO_2 concentrations in raw syngas despite a reduction of CO content.

Thermodynamic equilibrium models are barely able to accurately predict performance and syngas composition in fixed-bed gasification processes. The temperature inside the gasifier is not constant and the overall process is very complex, involving drying, devolatilization, pyrolysis, combustion, heterogeneous (solid–gas phase) and homogenous (gas phase) reactions, with a large number of intermediate and final products. Besides, gasification processes are also influenced by reaction kinetics and fluid-dynamic effects such as temperature and concentration gradients, which depend on reactor characteristics and gasification technology [9, 10]. For this reason, equilibrium models are able to predict more accurately the performance of entrained-flow and fluidised-bed gasifiers, since temperature is almost uniform throughout the reactor [11–14]. On the contrary, when applied to fixed- or moving-bed gasifiers, equilibrium models lead to large uncertainties in the reaction temperature, even though reactants residence time inside the gasifier is higher than reaction time, insofar as coal is heated by syngas, through countercurrent heat transfer [9,10,15–17]. Therefore, in fixed- and moving-bed gasifiers, coal drying, devolatilization and pyrolysis processes take place in the heat transfer zone at a lower temperature than in the gasification zone; consequently, moisture and volatiles are not generally involved in the gasification reactions since they are released before reaching the reaction zone.

Since the 70s of the last century, several models have been developed for studying fixed-bed gasifiers. First models were zero-dimensional [18–21] or one-dimensional [9,13,16,22,23], considering steady-state [18,20,24,25] or transient [23,26,27] operation. Some of these models are listed as homogenous [9,13,19,21,28], some as heterogenous [10,16,22,23], which implies separate solid and gas temperature [29]. A detailed and complete description of these models is summarized by Hobbs et al. [29]. During the 90s, more complex fixed-bed gasifier models were developed. Starting from MBED-1 model by Hobbs et al. [16], Radulovic et al. [30,31] developed the FBED-1 model including an advanced devolatilization sub-model. This model was later modified and improved by Monazam and Shadle [32]. More recent models were developed by Morea-Taha [33], Brundu et al. [34,35], Grana et al. [36], De Souza-Santos [37] and Kulkarni and Ganguli [38]. In recent years more complex CFD (computational fluid dynamics) models were also developed for evaluating fixed-bed gasifier performance, for example, by Murgia et al. [39], Rogel and Aguillon [40] and Yang et al. [41].

3. The steady-state fixed-bed gasification (SFBG) model

As mentioned, a computer simulation model for predicting performance of fixed-bed coal gasification processes has been developed over the past few years at the DIMCM [42,43] and implemented through the Aspen Plus® commercial software package. The model provides an accurate evaluation of chemical and physical properties of both coal and syngas evolving into the