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Introduction of a ternary diagram for comprehensive evaluation of gasification processes for ash-rich coal

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ABSTRACT

The present paper addresses the development of a comprehensive thermodynamic approach for the evaluation of gasification processes. A ternary diagram is introduced for a South African coal with an elevated ash content of 25.3 wt.%(wf). The ternary diagram allows the evaluation of most of the commercially applied gasification technologies depending on the three variables O_2, H_2O and coal mass flow. Cold gas efficiency, dry CH_4 yield, specific syngas production, H_2/CO ratio, CO/C and CH_4/C selectivity as well as temperature and carbon conversion were selected as performance measures. Based on literature data, generic models of the commercial Shell, Siemens, ConocoPhillips, HTW and GE coal gasifications systems were developed enabling an integration into the ternary diagram at standardized boundary conditions. The graphical approach indicates the existence of optimum configurations for the specific gasifier types and leads to an individual potential assessment. At a typical gasification pressure of 30 bar, a theoretical maximum cold gas efficiency of 87.4% was identified at a temperature of 980 °C for the above mentioned coal, whereas the maximum syngas yield of 2.09 m^3(H_2 + CO STP)/kg(waf) was located at 1135 °C. It is shown that only fluid-bed or two-stage processes have the potential to achieve these global maxima. The sensitivity of these maxima to varying ash contents from 5 to 45 wt.% and to coal rank is investigated as well. The study is concluded by the introduction of a simplified user diagram which was derived in order to drive a process towards the identified maxima.

1. Introduction

Due to midterm depletion of oil and gas, coal gains importance not only as energy carrier but as feedstock for various chemical syntheses [1]. The available commercial gasification processes which have been presented earlier [2] must be evaluated if they are capable for such conversion strategies. The main challenge is the increasing ash content of the coal as reported from South Africa [3], India [4], Japan [5], and China [6].

The comprehensive assessment of gasification processes is difficult due to lots of independent variables such as coal composition and reactivity, temperature, pressure, H_2O supply and other varying boundary conditions. A well-known approach, which was suggested first by Grout [7], is to split coal in its molar C–H–O composition plotting a ternary diagram. While Ghosh [8] used the diagram for coal rank indication, Stephens [9] and Battaerd and Evans [10] incorporated reacting gases and hydrocarbons as well. Recently, Li et al. [11] used the same diagram to illustrate carbon deposition isotherms for a gasification system. However, regarding performance parameters, technology comparison and optimum identification, the C–H–O plot has not been used, although it has a significant potential to illustrate basic relations. It should be noted that in a C–H–O molar plot, the region of gasifier operation in the range of the triangle O_2–H_2O–$C_xH_yO_z$ would be very small. However, if the same O_2–H_2O–$C_xH_yO_z$-system is used as corner points for a new molar based ternary diagram, recalculations of the coal flow eliminating sulfur, nitrogen, moisture and ash as well as recalculations of the technical oxygen flow eliminating nitrogen and argon will be necessary.

In the present paper, we introduce a novel approach of plotting O_2–H_2O–coal mass flow in wt.% in a ternary plot. It allows the assessment of temperature, carbon conversion, cold gas efficiency, dry methane yield, specific synthesis gas production, H_2/CO ratio as well as CO/C and CH_4/C selectivity of the converted carbon in an easy way without recalculations of the input flows.

With the disengagement from molar fractions, a distinct atomic ratio is not longer necessary for each stream. Hence, $C_xH_xO_z$ can be replaced by coal containing all impurities (e.g. mineral matter) and oxygen may include nitrogen as well. Consequently, the diagram is easy to use because the mass flows into a technical gasifier from practice can be applied directly.

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2. Theoretical and technological background

2.1. Ternary diagram setup

The O_2–H_2O–coal ternary diagram is developed by means of equilibrium modeling applying minimization of Gibbs free enthalpy, e.g. in the software Aspen Plus [12]. Fig. 1 indicates the principal scheme of the ternary gasification diagram setup. It can be seen that the mass flow rates into the gasification systems are normalized to unity and treated as mass fractions in wt.% which serve as input parameters for the diagram. In order to concentrate information and maintain applicability, reasonable combinations of output parameters are identified leading to four types of ternary diagrams as presented in Fig. 1.

1. Temperature and carbon conversion in equilibrium are combined offering a general overview and an easy location of gasifier domains.
2. Cold gas efficiency on lower heating value (LHV) basis and dry methane gas yield are fitted together because the high LHV of methane contributes significantly to the cold gas efficiency but limits gas quality in terms of synthesis applications or pre-combustion CO_2 separation.
3. Syngas yield and H_2/CO ratio are combined since the expected carbon utilization as well as the CO shift conversion efforts for a desired downstream process can be derived directly.
4. The selectivity of carbon gasified to CO, CH_4 and CO_2 permits carbon management, illustrating to which species the carbon is converted. In order to normalize the sum to 100%, the isolines refer only to the converted part of the carbon. Higher hydrocarbons (tars) are neglected.

A pressure of 30 bar is selected due to the suitability for various chemical syntheses [13] and integrated gasification combined cycle (IGCC) power generation including CO_2 capture as well [14].

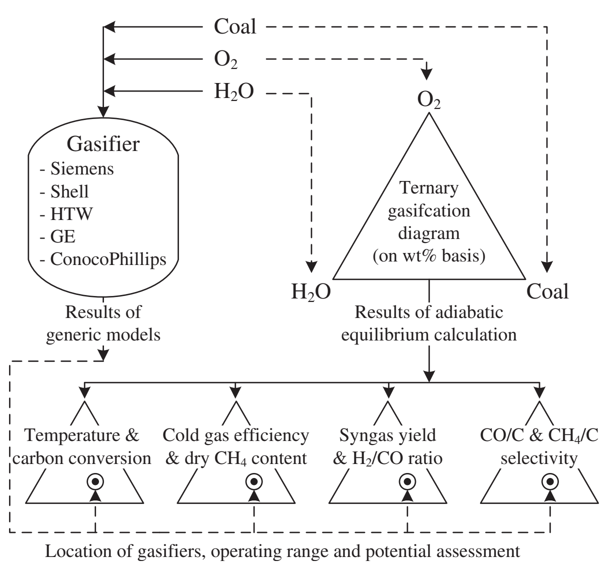

Fig. 1. Schematic overview of the ternary gasification diagram setup.

An ash-rich South African coal was selected for the investigation since elevated ash contents pose a challenge to most of the commercial gasification processes. Table 1 presents the coal composition and LHV showing an ash content of 25.3 wt.%.

Since all diagrams are based on isobar, adiabatic equilibrium calculations, all figures represent the maximum achievable values of the distinct parameters. In the next step, technical gasifiers are incorporated in the diagram according to their O_2–H_2O–coal consumptions.

2.2. Location of technical gasifiers

Higman and van der Burgt [13] provide detailed descriptions for the ConocoPhillips (E-Gas), General Electric (GE), Shell, Siemens, HTW (high-temperature Winkler) and Lurgi fixed-bed dry bottom (Lurgi FBDB) gasification technologies, which are selected to be integrated in the diagram. In a first step, for each entrained-flow and fluid-bed process a generic thermodynamic Aspen Plus model is developed. Deviations from equilibrium are included using user defined functions. Verification data for the models are given by Woods et al. [15] for ConcoPhillips, by McDaniel [16] for GE, by Rich et al. [17] for Shell, by Deutsche Babcock [18] for Siemens, and by Bellin et al. [19] for HTW. In a second step, unified boundary conditions were applied to the models to maintain comparability. From the two types of Lurgi fixed-bed gasifiers, the low-temperature Lurgi fixed-bed dry bottom (Lurgi FBDB) system was integrated in the study, because Modde and Krzack [20] provide data which was gained from operating experiences for a similar coal (German bituminous coal from Dorsten with 22.0 wt.%(wf) ash). For the high-temperature slagging British Gas/Lurgi (BGL) fixed-bed gasifier, no data for ash-rich coal was available. Table 2 shows all the operating conditions and the physical states of all entering streams serving as boundary conditions for the models.

In order to simplify the location of gasifiers and the analysis of the diagrams, four different domains **A**, **B**, **C** and **D** are introduced. These four domains apply for single stage processes and their boundaries are given mostly by technical limitations. For entrained-flow gasifiers, an upper temperature limit of 2000 °C and a lower temperature limit of 1440 °C (ash fluid temperature) must be maintained to ensure material lifetime and slag discharging conditions. In case of dry feeding systems, moderator steam can vary between 0 and 6 wt.%. Hence, the domain **A** for dry feed

Table 2
Unified boundary conditions for gasification modeling (LHV – lower heating value, IP – intermediate pressure).

Parameter	Value	Comment/reference
Pressure	30 bar	[13,14]
Temperature	1550 °C	>100 K above ash fluid temperature for slagging systems
Thermal capacity	500 MW	LHV basis, equivalent to 2066 t/d
Coal/N_2	25 °C	+3 bar above reactor pressure
Coal/transport gas	350 kg/m^3(eff.)	[13]
Solids in slurry	65 wt.%	[21]
Slurry temperature	120 °C	[25]
O_2 purity	95 vol.%	Residual: 3 vol.% Ar and 2 vol.% N_2
O_2 temperature	240 °C	+3 bar above reactor pressure
Moderator steam	37 bar/246 °C	Saturated from IP level
Quench water	37 bar/175 °C	Preheated for high gas moisture

Table 1
Ultimate analysis of South African high-volatile bituminous coal (waf – water and ash free, wf – water free, ar – as received, LHV – lower heating value).

C wt.%(waf)	H	O	N	S	Ash wt.%(wf)	Moisture wt.%(ar)	LHV MJ/kg(wf)
79.6	4.1	13.3	2.1	0.9	25.3	6.0	22.39