CO_2 ACTIVATION VIA REVERSE WATER GAS SHIFT (RWGS) PROCESSES: A COMPARATIVE THERMODYNAMIC ANALYSIS

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Abstract

The conventional gas phase reverse water gas shift (RWGS) process is compared to the RWGS chemical looping process for syngas production from CO_2 by thermodynamic analysis. For the analysis, an idealized process system is defined, which includes all steps from water electrolysis to product separation. The energy consumption for the product separation is approximated by an empirical formula based on available, realistic information for gas separation processes (House et al. (2011)). The power-to-fuel (PtF) efficiency was defined to evaluate both processes with regard to their energy efficiency toward syngas production. The influence of various process parameters on the process efficiency is investigated. The analysis indicates that the RWGS chemical looping process has a significantly higher PtF efficiency, based mainly on the reduced energy consumption for the product separation. Especially for syngas with a low H_2/CO ratio, the RWGS chemical looping process possesses clear advantages over the conventional RWGS process.

Keywords

Chemical Looping, Reverse Water Gas Shift, Thermodynamic Analysis

Introduction

Using sustainable energy sources, the reverse water gas shift (RWGS) reaction offers an attractive way to produce syngas from CO_2. Syngas is a major chemical intermediate, which is used widely in the chemical industry. Moreover, it can be used to produce sustainable fuels by Fischer-Tropsch synthesis. The conventional RWGS reaction is described by Equation (1):

$$H_2 + CO_2 \rightleftharpoons H_2O + CO \quad (1)$$

Using an oxygen carrier material (e.g. modified iron oxide, see Galvita et al. (2007)) the reaction can be split into Equations (2) and (3), resulting in separate streams of CO and water. This process is called RWGS chemical looping, as first mentioned by Daza et al. (2014):

$$H_2 + Fe_3O_4 \rightleftharpoons H_2O + Fe \quad (2)$$

$$CO_2 + Fe \rightleftharpoons CO + Fe_3O_4 \quad (3)$$

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The main advantage of RWGS chemical looping is the inherent gas product separation. Thus, energy consumption for the separation can be significantly reduced and undesired side reactions (e.g. methanation) can be effectively avoided.

Figure 1 illustrates schematically both processes. After conventional RWGS, a mixture of four components has to be separated, while in RWGS chemical looping, two streams with only two components each must be separated.

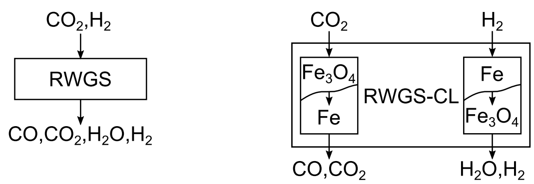

Figure 1. Conventional RWGS process (left) and RWGS chemical looping (RWGS-CL, right).

Thermodynamic Analysis

Although RWGS chemical looping has been addressed in the literature, a systematic analysis of this approach in comparison to competing processes is still lacking and the advantages are not quantified yet. For the comparison of the processes, idealized process systems were developed. Figure 2 shows the simplified process system for the conventional RWGS. The idealized system for the RWGS chemical looping is constructed in a similar way to allow a systematic comparison.

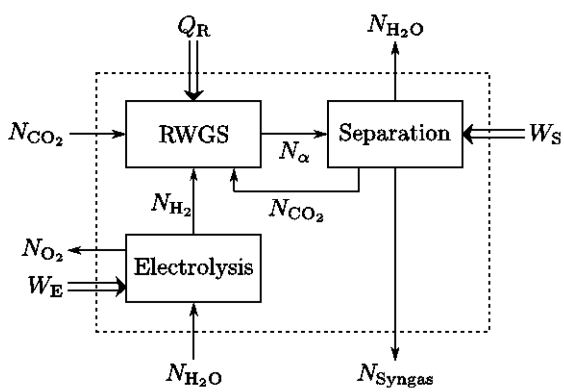

Figure 2. Simplified process system for the conventional RWGS process.

The Power-to-Fuel (PtF) efficiency is defined as the ratio of the higher heating value of the produced syngas to the sum of energy inputs, according to Equation (4):

$$\eta_{PtF} = \frac{N_{Syngas} \cdot HHV_{Syngas}}{\sum \text{Energy input}} \quad (4)$$

The energy consumption for product separation is approximated based on published data for typical gas separation processes (House et al. (2011)).

The PtF efficiency η_{PtF} was calculated for syngas production with different H_2/CO ratios as presented in Figure 3. It can be seen, that the RWGS chemical looping process is superior to the conventional RWGS process in terms of energy efficiency, especially for syngas with low H_2/CO ratios.

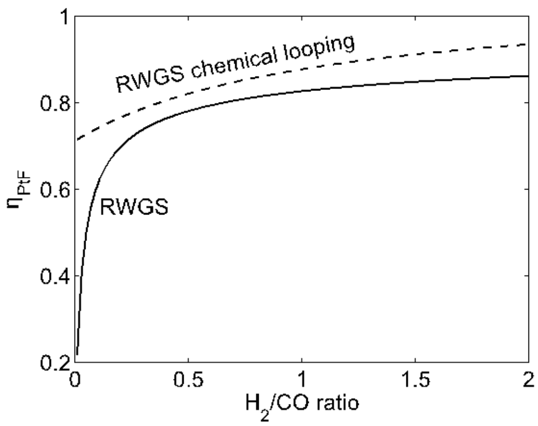

Figure 3. PtF efficiency η_{PtF} for conventional RWGS and RWGS chemical looping as a function of the H_2/CO ratio in the product syngas.

Conclusions

A thermodynamic analysis of the idealized process systems for syngas production demonstrated clearly, that the RWGS chemical looping process achieves higher PtF efficiency than the conventional RWGS process, especially for the production of syngas with low H_2/CO ratio.

Outlook

The presented methodology can be applied to other competing syngas production systems as well, e.g. thermo-chemical looping.

The influence of various operating parameters, e.g. temperature and pressure level of each unit or heat recovery effectiveness will be investigated in the next step.

References

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