Comparison of different multifunctional reactors for hydrogen production from bioethanol

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Highlights

- Renewable hydrogen production from bioethanol
- Performance comparison of different processes including ESR, SESR, SECLR and Modified SECLR with TRCL concept
- Hydrogen from modified SECLR with TRCL concept showed high productivity and purity as well as low energy requirement.

1. Introduction

Renewable hydrogen is an attractive energy source. It can be derived from bioethanol. The well-known process of H_2 production is steam reforming (SR) process which suffers from several disadvantages and therefore various multifunctional reactors have been proposed. A sorption enhanced steam reforming (SESR) process with addition of CO_2 sorbent offers in situ CO_2 capture, driving the equilibrium shifting to product side. A chemical looping reforming (CLR) concept was proposed by adding solid oxygen carrier (OC) for transferring oxygen to fuel for partial oxidation reaction. The re-oxidation of OC in a regeneration reactor can provide heat for highly endothermic reaction in the fuel reactor. The CL concept has been studied both of two and three reactors loop. The three reactors loop of chemical looping is called three-reactor chemical looping (TRCL) [1]. The combination between SESR and CLR concept becomes an intensified process called sorption enhanced chemical looping steam reforming (SECLR) process. In this study, various ethanol-derived H_2 production processes including conventional ESR, SESR, CLR and SECLR were simulated and compared their performance. The effect of operating conditions (temperature, pressure, *S*/*E* ratio, solid circulation) on H_2 productivity, purity and CO_2 capacity and thermal requirement were determined. CaO and NiO were used as CO_2 adsorbent and OC, respectively. In addition, the comparison also included the case of the TRCL concept in SECLR using CaO as CO_2 adsorbent and Fe_2O_3 as OC.

2. Methods

The processes for H_2 production were simulated by using ASPEN Plus program. The SOLIDS model with modified vapor phase of ESSRK was used as prediction property method. The RGibbs units based on minimizing Gibbs free energy were selected for all reactors and cyclone units were used for solid separation.

Sensitivity analysis was performed for range of temperature 350-750°C, pressure 0-20 bar, *S*/*E* ratio 0-10, CaO/EtOH ratio 0-1 (for SESR), NiO/EtOH ratio 0-3 (for CLR).

3. Results and discussion

The simulation was firstly validated the SECLR of methane employed by Rydén and Ramos [2] and the results showed good agreement under the same conditions. The effect of operating conditions was performed by parametric sensitivity analysis. The results as shown in Table1 indicated the process performance and thermal requirement with complete ethanol conversion under the studied conditions.

Table 1. Process performance and thermal requirement for hydrogen production

Section 1	H_2 productivity (kmol/hr)	%H_2 purity	%CO_2 capacity	Thermal requirement (MW)
CLR	2.15	51.8	-	0.065
SESR	5.27	96.7	81.8	0.12
SECLR	5.16	96.8	83	0.06
Section 2				
SECLR	5.18	96.6	81.5	0.065
modified SECLR	5.42	98.6	92.7	0.059

*T_{Ref} = 500°C, $T_{Cal,Air,Reg}$ = 900°C, T_{Steam}=300°C, *P*=1 bar, *S/E* ratio=4, CaO/EtOH=1, NiO/EtOH=1

The SECLR was found to be an appropriate technology to produce hydrogen with high H_2 productivity, purity and low thermal requirement. The modified SECLR with TRCL concept by using CaO and Fe_2O_3 as CO_2 adsorbent and OC indicates the better performance than the unmodified SECLR because the modified SECLR has steam reactor that can produce hydrogen with high purity. Moreover, the modified SECLR requires lower energy as it provides better heat management in the system.

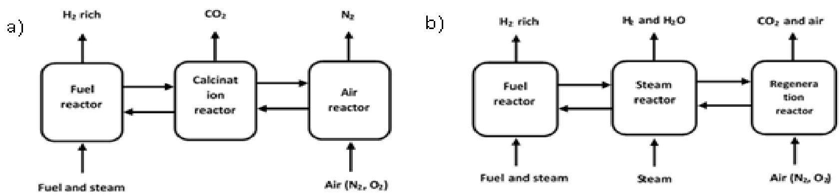

Figure 1. Block flow diagrams of (a) SECLR and (b) modified SECLR with TRCL for hydrogen production.

4. Conclusions

In this study, the hydrogen production processes from bioethanol (conventional ESR, SESR, CLR and SECLR) were simulated. The thermodynamic analysis was performed to determine the appropriate technology. The SECLR offers the best performance. To further improve this SECLR process, the TRCL concept was applied and the results showed significant advantages to obtain higher H_2 productivity, purity and low energy requirement.

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Keywords
Hydrogen production; Sorption enhanced chemical looping reforming; Process simulation; Ethanol steam reforming.