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Marcus Wenzel, Liisa Rihko-Struckmann, Kai Sundmacher

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Continuous Production of CO from CO_2 by RWGS Chemical Looping in Fixed and Fluidized Bed Reactors

Marcus Wenzel[a,*], Liisa Rihko-Struckmann[a], Kai Sundmacher[a,b]

[a] *Max-Planck-Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany*
[b] *Otto-von-Guericke-University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany*

Abstract

A fixed bed and a fluidized bed reactor design for the reverse water-gas shift chemical looping (RWGS-CL) process with 80 wt% $Fe_2O_3 - Ce_{0.5}Zr_{0.5}O_2$ as oxygen storage material (OSM) are analyzed and compared by process simulation. The influence of gas inlet flow velocity on the the reaction regime is investigated and feasible regions of operation for continuous CO production are identified. Two performance indicators are defined for the process: 1) the average CO concentration and 2) the OSM utilization. Optimization problems are solved to maximize the performance indicators and analyze their mutual dependency. The results are discussed in a Pareto plot. It is shown that a fixed bed reactor design is advantageous for the RWGS-CL process because of more degrees of freedom for operation compared to the fluidized bed reactor design. A quasi-continuous production of CO is demonstrated for both reactor designs. A steady CO production with an average CO mole fraction of $\bar{x}_{CO} = 0.64$ and an OSM utilization of 83.9% can be realized with two fixed bed reactors. The fluidized bed reactor configuration can potentially minimize problems associated with material sintering but the average CO concentration and OSM utilization are significantly lower compared to the fixed bed due to the limited operational freedom. The results indicate the importance of dynamic simulations for understanding and exploiting the kinetic and thermodynamic aspects of inherently dynamic processes like RGWS-CL to maximize process performance.

Keywords: Reverse water-gas shift, Chemical looping, Fixed bed reactor, Fluidized bed reactor, Dynamic simulation, Optimization

1. Introduction

Syngas is widely used in industry as a building block for the production of many bulk chemicals and chemical intermediates. The H_2/CO-ratio of the syngas is determined by its production method. Low H_2/CO syngas is required in the Monsanto process for acetic acid production and for hydroformylation processes. High H_2/CO syngas is used for alcohol synthesis. Today, syngas is produced almost exclusively

*Corresponding author