Optimization for Improving Efficiency on Membrane Reactor for WGS Reaction

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Introduction: In previous study, the modeling for WGSR-MR has been performed with reference to Chein paper[1] and effects of various operating conditions were evaluated for conversion for carbon monoxide and hydrogen flux. In this continuous study, sensitivity analysis is performed for operating conditions to improve efficiency for carbon monoxide and hydrogen removal in reactor and the reactor is optimized through parametric study with selected conditions.

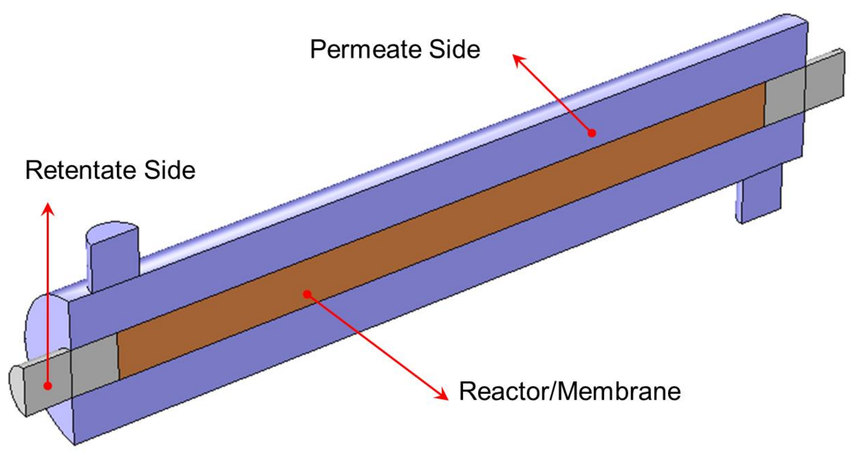

Figure 1. Geometry of Membrane reactor for WGSR

Computational Methods: For this work, COMSOL Multiphysics® and Chemical Reaction Engineering Module are used : "Transport of Concentrated Species", "Free and Porous Media Flow", and "Heat Transfer in Fluid" interface are used to study mass, momentum, and heat balance for mixture of gas. These physics interfaces are coupled with each other.

The objective function of sensitivity model is set for improving CO conversion and hydrogen removal at outlet of sweep gas. Reference condition is T=450℃ P=15bar, and S/C=1.

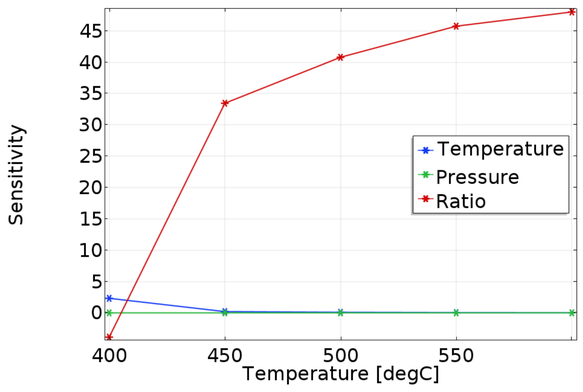

Fig 2. Sensitivity results with respect to temperature

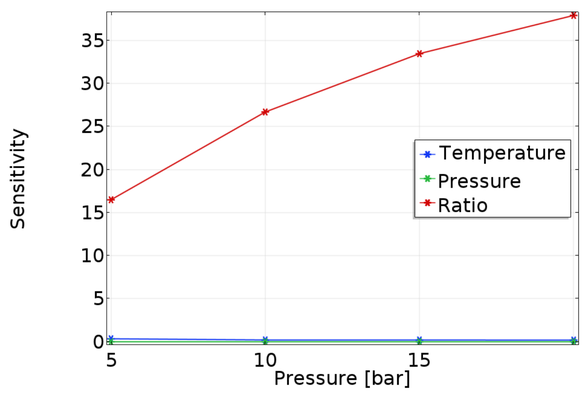

Fig 3. Sensitivity results with respect to pressure

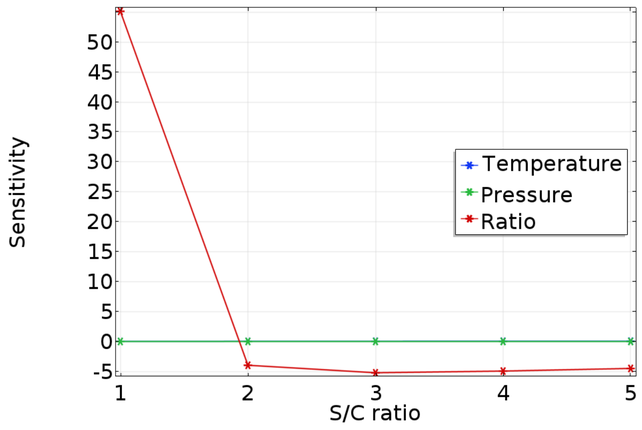

Fig 4. Sensitivity results with respect to ratio

Results: Through the sensitivity analysis, we can see that the S/C ratio is a dominant variable for improving efficiency of the reactor. Being based on it, we conducted parametric study to find optimal condition with respect to S/C ratio.

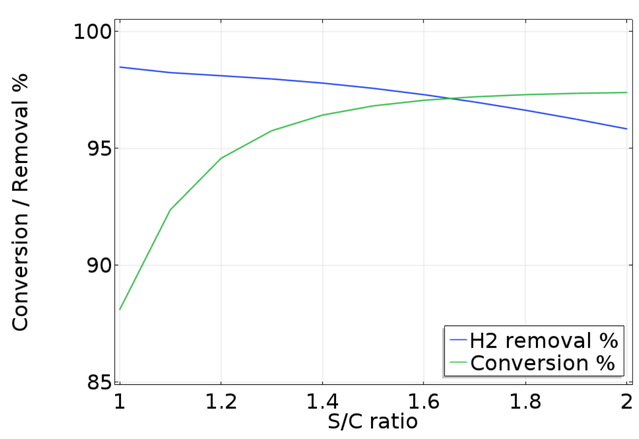

Fig 5. Conversion and H_2 removal as S/C Ratio (T=600℃, P=20bar)

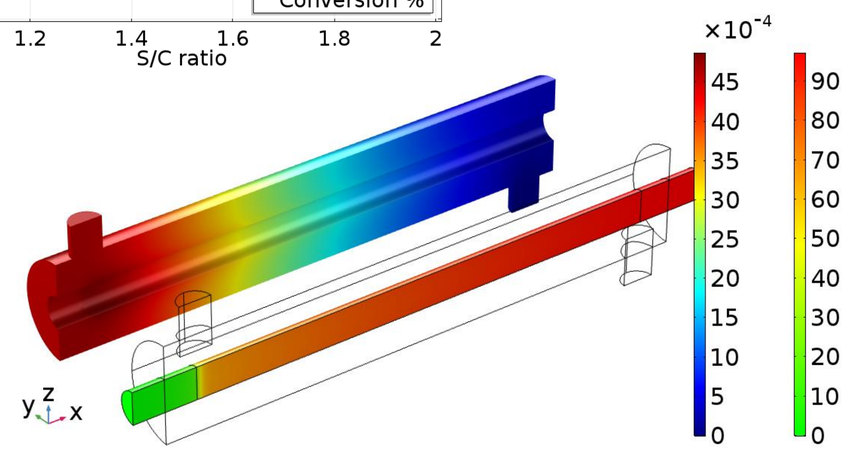

Fig 6. H_2 mass fraction in permeate (Left) CO conversion in reactant (Right) at S/C = 1.7

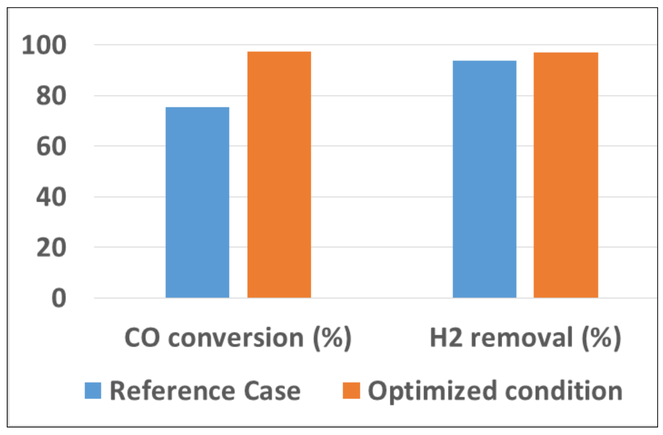

Fig 7. Comparison with reference case and optimization condition

Conclusions: In this study, we have conducted sensitivity analysis and parametric study for improving efficiency of WGSR-MR . Through these simulation, we could increase CO conversion and H_2 removal at outlet each for 21.85%, 3.16%.

References:

1. R.Y. Chein et al., Sweep gas flow effect on membrane reactor performance for hydrogen production from high-temperature water-gas shift reaction, J Membrane Sci, Vol 475, p. 193 (2015)
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3. Adams and Barton, A dynamic two-dimensional heterogeneous model for water gas shift reactors, J Hydrogen Energy, Vol 34, p. 8877 (2009)
4. Augustine et al., High pressure palladium membrane reactor for the high temperature water-gas shift reaction, Vol 36, p.5350 (2011)