Effects of Geometry and Operating Conditions on Membrane Reactor for Water Gas Shift Reaction

D. Shin[1], T. Kim[1], J. Lee[1]
1. Altsoft Inc., Seoul, South Korea.

Introduction: Recently, to enhance the overall coal to hydrogen thermal efficiency and cost effective design, the water gas shift reaction in membrane reactor(WGSR-MR) has been developed. In this study, mass, momentum, and heat balance in WGSR-MR are simulated. Effects of geometry and operating conditions are evaluated.

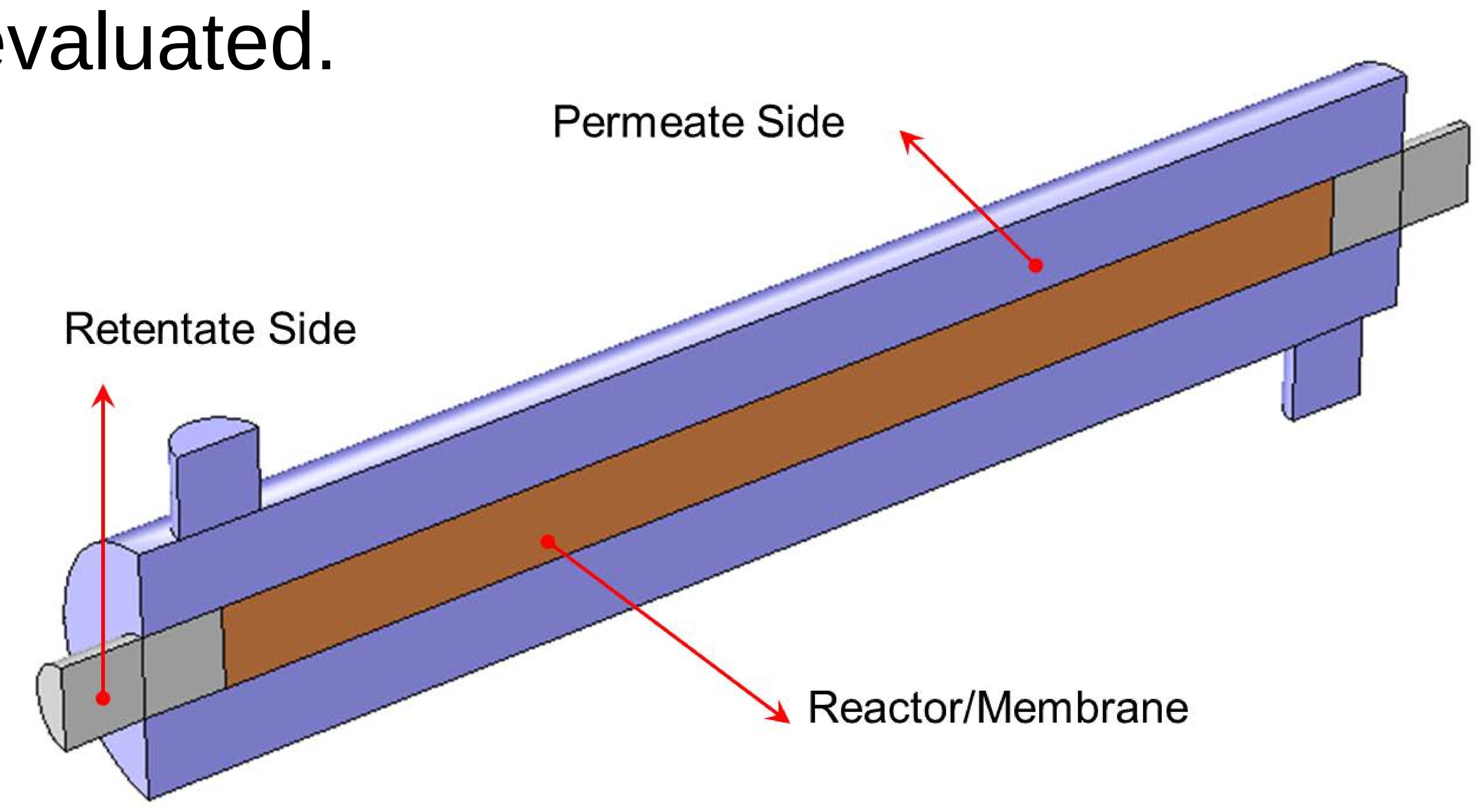

Figure 1. Geometry of Membrane reactor for WGSR

Computational Methods: To simulate the WGSR-MR, momentum, mass, heat balance equations are used and coupled with each other. In Chemical Reaction Engineering Module of COMSOL Multiphysics®, “Transport of Concentrated Species”, “Chemistry”, “Free and Porous Media Flow”, and “Heat Transfer in Fluids” interfaces are used. This model is referred from Chein et al[1].

✓ Kinetics

$$r_{WGS} = \rho_{cat}(1-\varepsilon)F_{\text{press}}(1.69\times 10^{7}\ \text{mol/g}\cdot\text{h})\exp\left(-\frac{88{,}000}{RT}\right)$$
$$\times\, x_{CO}^{0.9}x_{H_2O}^{0.31}x_{CO_2}^{-0.156}x_{H_2}^{-0.05}\left(1-\frac{x_{CO_2}x_{H_2}}{x_{CO}x_{H_2}K_{eq}}\right)$$

$$K_{eq} = \exp\left(\frac{4577.8}{T} - 4.33\right) \qquad F_{press} = P_R^{0.5-P_R/250}$$

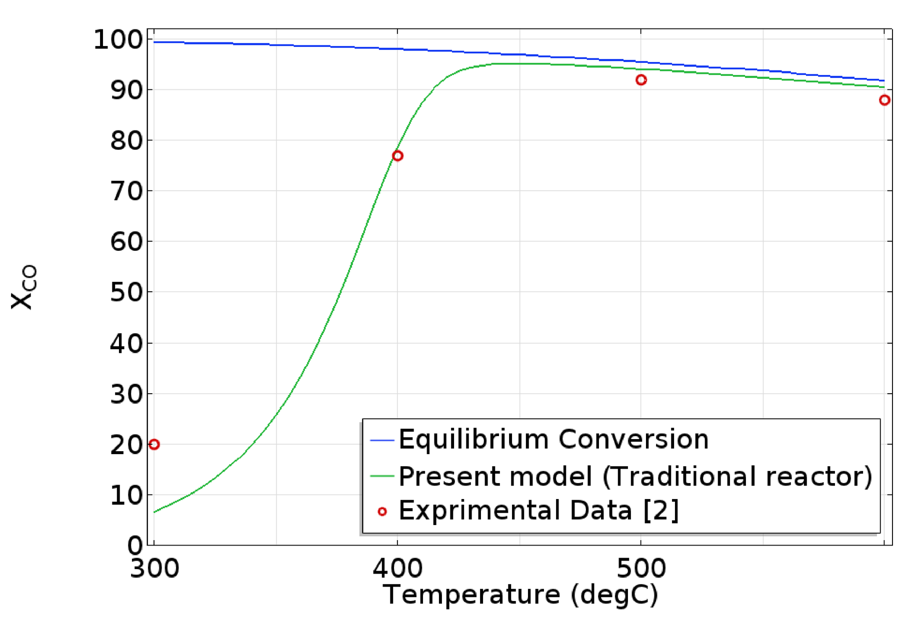

Figure 2. Comparison between present model and experiment. (S/C ratio = 5)

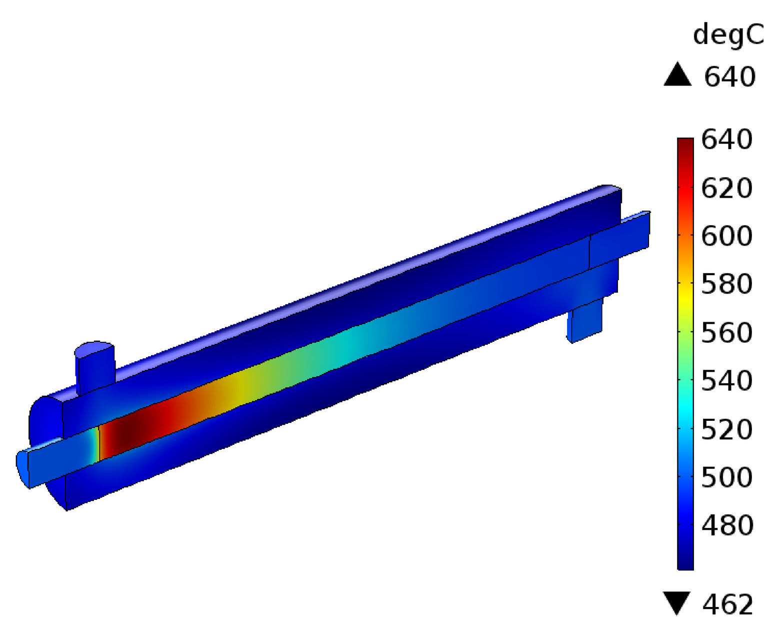

Figure 3. Temperature profile on WGS reactor at 500 ℃

Results: WGS reactions are affected by streamline, flow rate of coolant or temperature, S/C ratio and flow rate of reactant. As Table 1, various conditions are simulated in this study.

Variable	Value	Units
Temperature of Reactant	450 - 600	℃
CO flow rate ratio	1 - 5	-
N_2 flow rate ratio (Coolant)	1 - 5	-
Flow pattern	Counter-current Co-current	

Table 1. Simulation conditions for effect of conditions

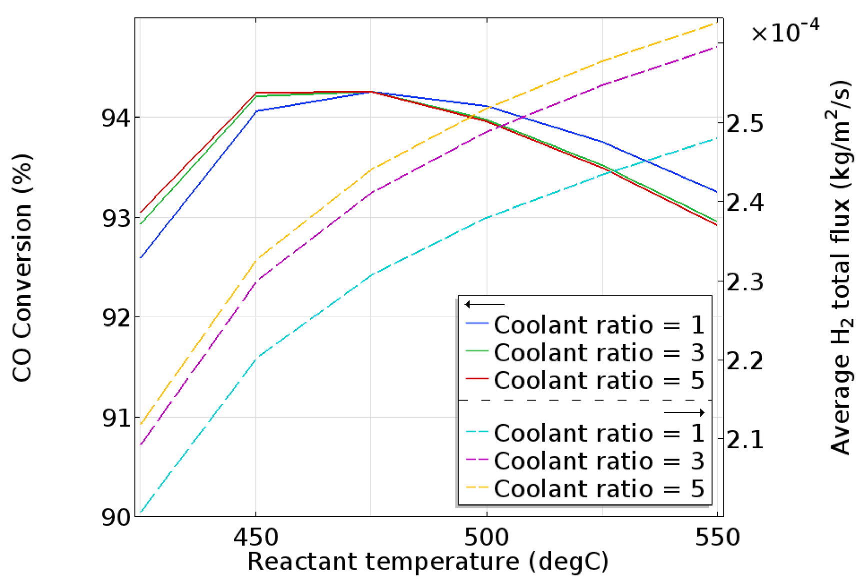

Figure 4. CO conversion and H_2 total flux on CO flow rate ratio = 1

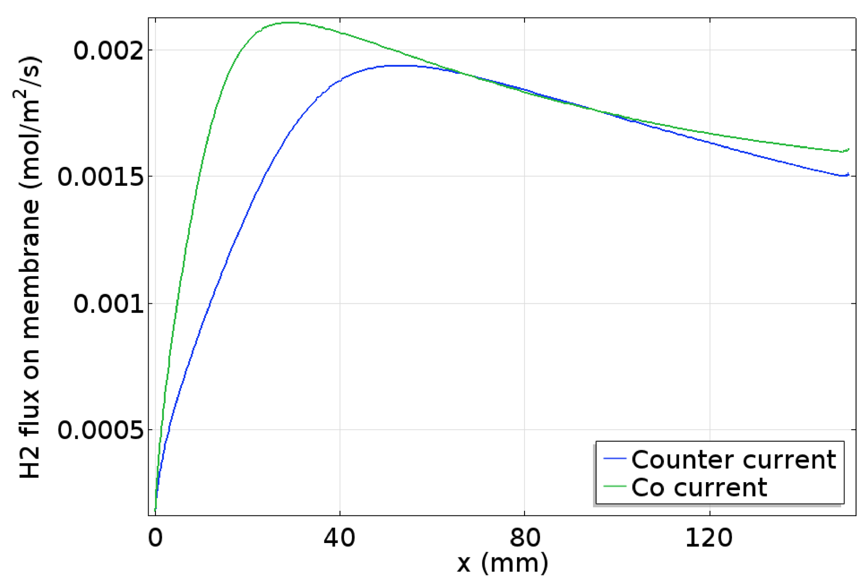

Figure 5. Comparison between Counter and Co current for H_2 flux on membrane

Conclusions: Simulation results are shown H_2 flux at outlet has better efficiency at the higher flow rate ratio and temperature of coolant, but CO conversion has maximum efficiency at optimal temperature. This model will simulate the effect of S/C ratio change and geometry change for efficiency.

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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