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Membrane assisted WGSR – Experimental study and reactor modeling

Jan Galuszka [a,*], Terry Giddings [a], Gaetano Iaquaniello [b]

[a] Natural Resources Canada, CanmetEnergy – Ottawa, 1 Haanel Drive, Ottawa, Ontario, Canada K1A 1M1
[b] Tecnimont KT S.p.A, V.le Castello della Magniana 75, 00148 Rome, Italy

HIGHLIGHTS

- Langmuir–Hinshelwood (LH) equation parameters determined for conventional WGS reactor.
- WGS membrane reactor data simulated using LH parameters for same catalyst.
- H_2O permeance through silica membrane and CO_2 inhibition of catalyst accounted for.
- Catalyst amount needed to bring system to equilibrium in membrane reactor resolved.
- Operating parameters of WGS membrane reactor for complete CO conversion at 450 °C projected.

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ABSTRACT

An experimental program on membrane assisted WGSR and a membrane reactor (MR) modeling aimed at finding a sensitivity envelope of the key parameters controlling MR performance was carried out using bitumen and coke–coal gasification streams at 450 °C. It was determined that a Langmuir–Hinshelwood (LH) model of the kinetics fit adequately the conventional reactor (CR) experimental data. To simulate the MR performance the LH kinetic parameters were applied to MR data that showed a 7% enhancement of CO conversion over the CR. The model predicted that by adjusting the MR operating parameters within reasonable limits, the CO conversions in the range of 98% could be reached, at least 15% over the thermodynamic equilibrium conversion of a conventional system.

1. Introduction

The catalytic conversion of CO to hydrogen and carbon dioxide through the water–gas shift reaction (WGSR), discovered more than two centuries ago [1], is currently of great importance in many industrial processes, such as hydrogen and ammonia production, Fischer–Tropsch and methanol synthesis.

The WGSR is a pressure neutral, reversible, moderately exothermic reaction. Consequently, CO conversion is limited by thermodynamic equilibrium at higher temperatures while the rate of reaction is low at lower temperatures. In order to achieve high CO conversion, a two-step catalytic process is usually employed in the industry, i.e. the high temperature (350–420 °C) shift (HT) using a Fe–Cr based catalyst and the low temperature (180–250 °C) shift (LT) using a Cu–Zn based catalyst [2]. Addition of greater than stoichiometric quantities of steam improves CO conversion.

More recently the WGSR has gained additional significance as it forms an essential step in the emerging Integrated Gasification Combined Cycle (IGCC) technology. The IGCC is considered as the most viable technology that would allow utilization of low-cost, opportunity feed-stocks such as coal, petroleum coke, bitumen, biomass or municipal waste for clean energy or clean hydrogen production with zero CO_2 emissions [3,4]. However, the current high cost of IGCC technology is the biggest obstacle to its integration in the power or hydrogen market to achieve the much needed diversification.

It is considered that combining the IGCC and hydrogen membrane reactor technology could radically improve the commercial outlook for the IGCC scheme. The expected significant process simplification and intensification capitalizes on a new industrial paradigm offered by membrane reactors that allows combining reaction and separation in one step. Hydrogen membrane reactors can circumvent the thermodynamic limitation of WGSR as they can separate H_2 as it is produced. Effectively, the products of gasification of low-cost opportunity feed-stocks could be converted in a membrane assisted, one step WGSR process to a clean hydrogen

* Corresponding author. Tel.: +1 613 995 1585; fax: +1 613 996 9400.
E-mail address: janga@pioneerwireless.ca (J. Galuszka).

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