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An Exergetic Life Cycle Assessment for Improving Hydrogen Production by Steam Methane Reforming

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Hydrogen is expected to play a significant role in the future energy system. An efficient production of hydrogen with minimum cost and in an environmentally acceptable way is crucial for the development of our hydrogen-based economy. As recent technological progress has made hydrogen a realistic long-term energy option with little or no pollution, the developments of new methods for hydrogen production and the improvement of conventional technology are of a permanent importance. However, on a shorter time perspective, there will be a transitory period, during which large-scale hydrogen production will be based on optimization and improvement of current technologies. Actually, Steam Methane Reforming (SMR) is one of the most important and commonly used processes of hydrogen production. The SMR technology is the oldest, the cheapest, and the most widely used.

Recent years have seen an upsurge of interest in life cycle assessment (LCA) as a tool for evaluation, with a cradle to grave approach, of potential environmental impacts of a product, process, or activity. During the past decade several researchers have tried to enhance LCA methods by considering exergy rather than or in conjunction with energy flows. Such an extension of LCA is referred to as exergetic life cycle assessment (ELCA). Exergy is defined as the maximum amount of work that can obtained when a thermodynamic system or flow (e.g., matter, heat, work) is brought into equilibrium with a reference environment. ELCA determines the depletion of natural resources, while the other environmental effects are calculated with the LCA.

The purpose of this study is to demonstrate how the results of an Exergetic Life Cycle Assessment (ELCA) can be used to improve the performances of an SMR process. The methodology opted in this work contain three main steps.

In the first step, the SMR process is simulated using Aspen Plus™ software. The thermodynamic data and phase behavior predictions of the material stream are achieved using the Soave-Redlich-Kwong equation of state and the component list was restricted to CH_4, O_2, N_2, H_2O, CO, H_2 and CO_2. The SMR process studied consists of four sections: natural gas pretreatment, synthesis gas generation, water gas shift and gas purification.

The first section, which is natural gas pretreatment, consists of removing the impurities present in the natural-gas feedstock to avoid poisoning the catalysts.

In the second section called the reforming ((1) and (2)), natural gas - steam mixture is catalytically converted to hydrogen, carbon monoxide and carbon dioxide. The reforming reaction is highly endothermic and a large amount of heat is provided by external burners.

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \qquad \Delta H^0_{298} = 206\ kJ.mol^{-1} \qquad (1)$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \qquad \Delta H^0_{298} = 165 \text{ kJ.mol}^{-1} \qquad (2)$$

These reactions are typically carried out at a temperature of 800–1000°C and a pressure of 14-20 atm over a nickel based catalyst.

The syngas exiting the reformer is passed through a water–gas shift (WGS) reactor that converts the CO in the syngas to CO_2 and H_2 using the available H_2O in the syngas or from additional H_2O added to the system. Herein, the following reaction occurs:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H^0_{298} = -41 \text{ kJ.mol}^{-1} \qquad (3)$$

In practice, the shift reaction takes place over two reactors that operate between 200- 400 °C and 125–180 °C, respectively.

The last section is the purification of hydrogen. It consist of producing high end stream H_2 purity (>99%).

In the second step an energetic and exergetic analyses are performed for the SMR process as following: (1) Determination of the process stream exergy (physical, chemical and mixing exergies) (2) Performing the exergy balance for the process element. (3) Calculation of the process energetic and exergetic efficiencies.

The results indicate that the thermal and the exergetic efficiencies of the SMR process are respectively 70% and 65.5%. It shows that 26.67% of exergy reaching the process are destroyed due to the thermodynamic imperfections. The main part of the destroyed exergy is located in the reformer with à contribution of 65.81% of the whole process destroyed exergy. The exhaust exergy represents 7.86% of process inlet exergy, this attributed to the smoke physical exergy. The improvement of the process energetic and exergetic performances will be by reducing its exhaust exergy. This is performed by incorporating, in the original process, a third economizer for a smoke calories recovery. Consequently a new process is build (SMR2).

In the third step, the processes performances comparison is achieved using ELCA approach. The life cycle assessment is done according to the ISO 14040 series. The LCA process is a systematic approach that consists of four stages: goal definition and scoping, inventory analysis, impact assessment and interpretation. The SimaPro LCA Version 7.1 software's Eco-indicator 99 method is used to investigate the following three environmental impact categories: human health, ecosystem quality and resources. The ultimate goal of this ELCA is to compare the environmental impacts of two SMR processes for hydrogen production. The functional unit is one mole of hydrogen produced by each process. The construction and dismantlement of SMR equipments and the catalyst production are assumed equivalent for each process. Therefore they are neglected in this study. The systems have three stages:

- Hydrogen production plant.
- Production and distribution of natural gas.
- Production and distribution of electricity.

The required data to conduct the impact analysis for production and distribution of natural gas and electricity are taken from the SimaPro 7.1 database, while the SMR operating parameters are obtained by using Aspen Plus™ software.

The results obtained indicate that by incorporating a new heat exchanger in the original process (SMR1) we obtain multiple benefits:

- The thermal and the exergetic efficiencies of the new process are respectively 74% and 69.1%. However, for the original process they are 70% and 65.5%.
- The un-used exergy is reduced by 9.3% from 125.9 to 114.2 kJ per mole of H_2 produced. One mole of methane in the new process is more hydrogen productive. It produces 2.48 mole H_2 against 2.35 mole H_2 for the original process.
- The figure 1 shows a reduction in all the process categories impacts. Thus we observe theses reductions: 5% in human health indicator, 3% in ecosystem quality and 5% in resources.
- The figure 2 shows 5.2% as reduction in the process' single score.

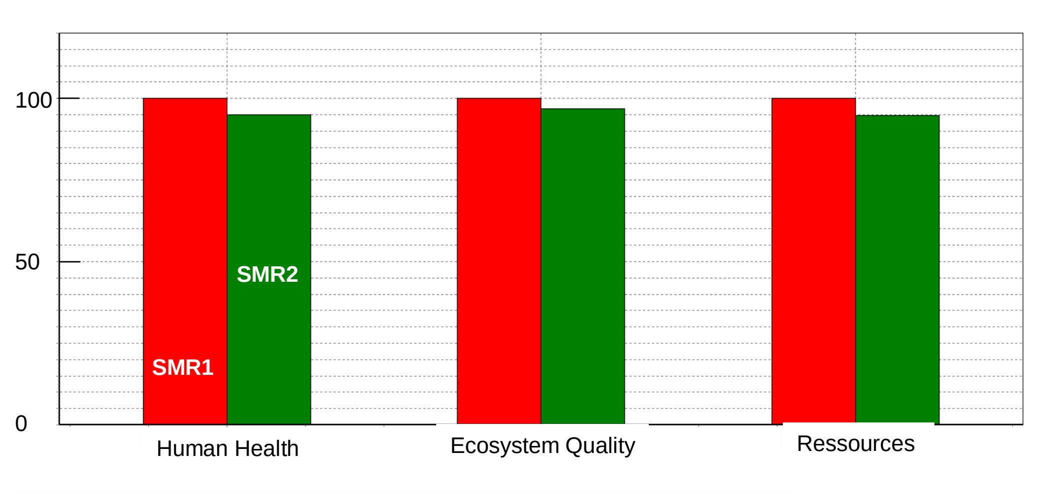

Figure 1: SMR damage assessment result in bar chart (EcoIndicator 99).

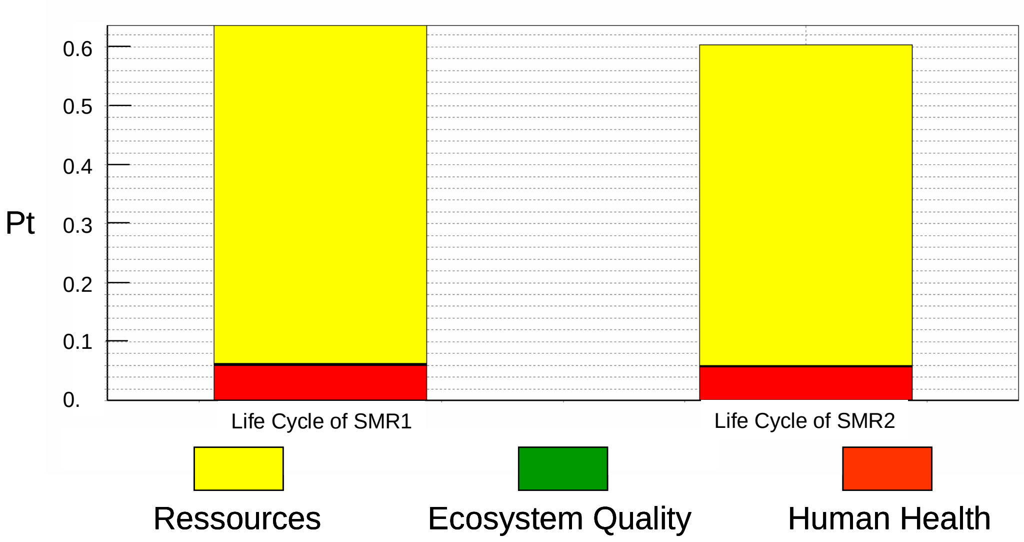

Figure 2: SMR Single score in bar chart (EcoIndicator 99).