Simulation of methanol synthesis from syngas obtained through biomass gasification using Aspen Plus®

M. Puig-Gamero¹, J. Argudo-Santamaria¹, J.L. Valverde¹, P. Sánchez¹, L. Sánchez-Silva¹

¹Department of Chemical Engineering, University of Castilla-La Mancha, Ciudad Real, Castilla-La Mancha, 13071, Spain

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The current environmental problem has forced the search of new and more sustainable alternatives as the biomass to face the continuous energy demand. Biomass can be used to obtain high value products and power, contributing to the reduction of greenhouse emissions. However, at the present, the technologies required for biomass transformation are not mature enough.

Nowadays, the most common technique to obtain clean syngas is through the steam reforming of natural gas. Natural gas can be also used directly as an alternative fuel (Susmozas et al., 2015). In this sense, the steam gasification of biomass for producing clean syngas could be an interesting alternative from the environmental and economical point of view. The syngas quality determines if it can be used to produce high-added value products such as methanol, ethanol or liquid hydrocarbons through the Fischer-Tropsch process. Among of them, methanol is one of the most attractive due to its wide variety of applications. Methanol can be used directly as a clean fuel or can be mixed with other conventional fuels. Furthermore, many chemicals products as formaldehyde, methyl tertiary butyl ether, acetic acid or gasoline can be obtained from it.

On the other hand, the process simulation is an increasingly important tool for the chemical industry that allows to scale up a process which requires a knowledge of the influence of the operating conditions on the plant performance. In addition, the process simulation also allows to reduce costs and time (Couto et al., 2015). There are many commercial simulators of chemical processes, being Aspen Plus® one of the most used. In the present work, the commercial software Aspen Plus® was used to simulate the gasification process of biomass, the subsequent syngas purification and the further methanol synthesis. In addition, the tar produced in the gasification process was also simulated. Figure 1 shows the Aspen Plus® flowsheet of the mentioned process.

Figure 1. Aspen Plus® process flowsheet.
Firstly, the gasification process was simulated using a thermodynamic equilibrium model which is based on the minimization of the Gibbs free energy of the system. A double chamber gasifier, which allows the separation of the gasification and combustion zones to obtain a high-quality gas, was considered. Furthermore, part of the char was burnt in the combustion chamber increasing the bed temperature and generating all the energy needed in the process. The simulation model was validated with data obtained from a double chamber gasifier pilot plant owned by the British Columbia University (Canada) (Hejazi et al., 2017). On the other hand, the influence of the steam to biomass (S/B) mass ratio and the temperature on the gas product composition was studied. The S/B mass ratio and the temperature were varied from 0.5 to 1 and 800 and 1000 ºC, respectively. The objective was to obtain a H2/CO ratio as close as possible to 2.4, which is needed to perform the synthesis of methanol. The best calculated operational condition of the process was 900ºC and a S/B mass ratio of 0.9.

One of the main technical barriers for the syngas production is the presence of tar coming from the gasification process. According to the simulation performed, tar production was hindered with increasing temperatures and steam flowrates. Dolomite was used as the catalyst in the decomposition of tar because its low cost.

Then, a pressure swing adsorption (PSA) process was considered to clean the syngas and simultaneously capture the greenhouse gases. This way, about 80% of the CO2 and 95% of the CH4 were sequestered.

Once the H2/CO molar ratio of the clean syngas was fitted, the methanol synthesis proceeded. The pressure was varied from 40 to 100 atm, whereas the temperature was varied from 220 to 280ºC. Although the methanol production is favoured at high pressures, a pressure of 55 atm was chosen in order to avoid operational issues observed at higher pressures. On the other hand, it is well known that low reaction temperatures improves the methanol yield. This way, 220ºC and 55 atm were selected as the optimal operation conditions for the methanol synthesis. Finally, the methanol synthesis waste stream was recycled to the combustion chamber in order to analyse its effect on the process performance.

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References