Towards more accurate and reliable mathematical model for steam gasification

Nutchapon Chiarasumran[1], Richard Blanchard[1], Brahim Benyahia[1*]

[1]Department of Chemical Engineering, Loughborough University, LE11 3TU, UK
b.benyahia@lboro.ac.uk

INTRODUCTION

Over the last decade, renewable energy has undergone unprecedented growth and development because of the increasing need for cleaner and more environmental friendly technologies. Hydrogen is one of the most important renewable energy that can be employed in many applications e.g. fuel cell technologies. Biomass, including municipal solid waste, is also a potential option for producing hydrogen and they can be converted through the thermochemical process particularly gasification, which is a technology that can produce H_2 on both small and large scales using just air or steam as the oxidizing agents. Developing accurate and highly predictable model for the gasification is essential for process design and optimization. In order to predict the product gas composition and the amount of hydrogen produced from the gasification process precisely, the simulation of the mathematical models to present the behaviors and properties of gases is needed to be developed. Different types of gasification models are used to predict the maximum yield of the product gases based on thermodynamic equilibrium[1]. In addition, different simulators have been developed, such as Aspen Plus model type, but still not predictable enough compared to the experimental data[2]. The objective of this work is to develop more precise equilibrium model for the biomass steam gasification using Gibb's energy minimization and Lagrange multiplier method. A rigorous and systematic procedure was developed to improve parameter estimation, using global optimization approach, which enhances the prediction capabilities of the mathematical model.

SIMULATION METHOD

The non-stoichiometric equilibrium model of the steam gasification based on Gibb's energy minimization using Lagrange multiplier method was simulated in MATLAB software in order to predict four species of the gas product: hydrogen, carbon monoxide, carbon dioxide, and methane. The minimum value of Gibb's energy can be obtained when the partial derivative with respect to each species (x_i) is equal to zero:

$$\frac{\partial G^t_{T,P}}{\partial x_i} = 0 \qquad (1)$$

This term can be calculated from Gibbs energy as follows:

$$\frac{\partial G^t_{T,P}}{\partial x_i} = \Delta G_{fi} + RT \ln\left(x_i / n_{total}\right) + \lambda_j \qquad (2)$$

where x_i is the mass fraction of the species *i* and λ_j is Lagrange multiplier. The model also requires the mass balance equations and can predict the mole fractions of each species in the product.

RESULTS AND DISCUSSION

The mole fraction of each gas species obtained from the steam gasification of the wood residue ($CH_{1.65}O_{0.67}N_{0.03}$) at different steam-per-biomass ratio (S/B) is shown in figure 1. The results are more accurate when compared to the results from the previous model[2]. The highest hydrogen yield was obtained at 52 g and 68 g H_2 per 1 kg biomass when S/B ratio = 1 at 700 °C and 900 °C respectively.

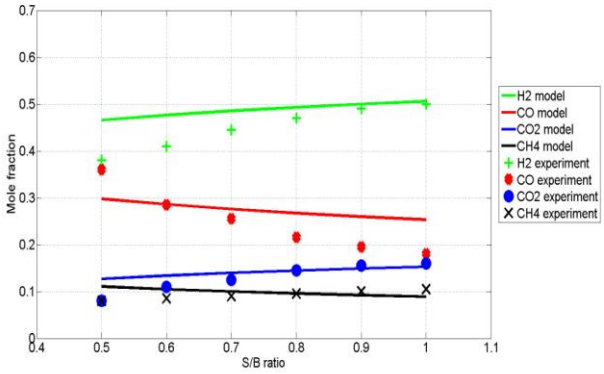

Fig. 1 Model predicted vs experimental gas products mass fraction obtained for wood residue at 700 °C [3].

CONCLUSION

The developed model was proved to be more reliable to predict the gas product composition from the biomass steam gasification at different steam-per-biomass (S/R) ratios and temperatures. It can also be extended to predict the gas composition other biomass types.

REFERENCES

1. T.K. Patra et. al, Ren. Sus. Ener. Rev. 50, 583-593 (2015).
2. L.P.R. Pala et. al. Ren. Ener. 101, 484-492 (2017).
3. S. Fremaux et. al., Ener. Con. Manag. 91, 427-432 (2015).