An Integrated Kinetic Model to Estimate the Quality and Composition of Syngas from the Supercritical Water Gasification of Biomass

S.McGarvey[1], A.Carruthers[1]* , Jun Li[1] , Leo Lue[1]

[1] CPE dept, The University of Strathclyde, 75 Montrose Street ,Glasgow, G1 1XJ
*e-mail: a.carruthers@strath.ac.uk

Supercritical Water Gasification

Supercritical Water Gasfication (SCWG) of biomass is a method of producing potentially carbon neutral fuel and chemical feedstock from waste biological material. In this process water is used as a reacting medium which makes it well suited for very wet biomass and so is a promising alternative to standard gasification processes which would require extensive drying in these cases[1].

Model Methodology

A kinetic model to provide estimates on product quality and quantity was developed by taking model compounds to represent the more complicated long-chain components in biomass: Cellobiose for Cellulose, D-Xylose for Hemicellulose, Guaiacol for Lignin, and Alanine for the various proteins. The impact of supercritical water on these reactions was then taken into account using a H_2/O_2 reaction mechanism, called the San Diego (SD) Mechanism[2], which involves reactions of radical species and short-chain hydrocarbons.

This kinetic model was written in MATLAB for a 2-reactor setup with sub- and supercritical conditions, recreating the experimental conditions of Lu et al[3]. It uses simple Arrhenius rate equations for the kinetics. The key results used to validate the model were mass analyses of major product species, Carbon Conversion Efficiency (CCE) and Gasification Efficiency (GE). A table comparing the model and its predecessor to the experimental results can be seen in Table 1.

	H_2 (mol/kg)	CO_2 (mol/kg)	CH_4 (mol/kg)	CCE (%)	GE (%)
Decomp reactions[4]	-6.4	-1.9	4.6	-10.3	-6.9
Decomp with SD Mechansim	-3.1	-0.6	4.3	-9.9	-0.1

After the successful model validation, the impact of varying biochemical composition was investigated by using different feedstock compositions typical to materials like: micro-algae, pig-cow manure, and paper pulp. Furthermore, operational parameters such as the residence time for the reactor with subcritical conditions (t_{sub}), the temperature of the reactor with supercritical conditions (T_{sup}), and dry biomass content was altered to observe the optimal SCWG environment.

Major Findings

The optimal condition

1 D. Macri, Ecatizzone, A. Molino and Migliori. *Renewable Energy,* 2020, 150, 624-636

2 UC San Diego, http://web.eng.ucsd.edu/mae/groups/combustion/sdmech/sandiego20011105/sandiego20011105.pdf, (accessed March, 2021).

3 Lu, Y. J.; Guo, L. J.; Ji, C. M.; Zhang, X. M.; Hao, X. H.; Yan, Q. H. *Int. J. Hydrogen Energy* 2006, 31, 822.

4 6 O. Yakaboylu, G. Yaper, M. Recalde, J. Harinck, K. Smit, E. Martelli and W. de Jong, *Ind. Eng. Chem. Res.*, 2015, 54, 8100-8112