

WOOD PYROLYSIS USING ASPEN PLUS SIMULATION AND INDUSTRIALLY APPLICABLE MODEL

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Abstract

Over the past decades, a great deal of experimental work has been carried out on the development of pyrolysis processes for wood and waste materials. Pyrolysis is an important phenomenon in thermal treatment of wood, therefore, the successful modelling of pyrolysis to predict the rate of volatile evolution is also of great importance. Pyrolysis experiments of waste spruce sawdust were carried out. During the experiment, gaseous products were analysed to determine a change in the gas composition with increasing temperature. Furthermore, the model of pyrolysis was created using Aspen Plus software. Aspects of pyrolysis are discussed with a description of how various temperatures affect the overall reaction rate and the yield of volatile components. The pyrolysis Aspen plus model was compared with the experimental data. It was discovered that the Aspen Plus model, being used by several authors, is not good enough for pyrolysis process description, but it can be used for gasification modelling.

Keywords: Pyrolysis, Spruce sawdust, Modelling, Aspen Plus

1 INTRODUCTION

Pyrolysis is a thermochemical decomposition process at elevated temperature in absence of oxygen. The pyrolysis gas contains mainly H₂, CO, CO₂, CH₄, and others light hydrocarbons such as C₂H₂, C₂H₄, C₂H₆, C₃H₆, C₃H₈. Pyrolysis of biomass yields gases, liquids (so-called bio-oils), and a carbonaceous residue (so-called bio-char). The obtained yields depend on the feedstock composition and pyrolysis conditions. There are three types of pyrolysis: fast pyrolysis with a typical maximum bio-oil yield of around 60-80 wt. % at very short residence times, convectional pyrolysis with equal yields of product at middle residence time (minutes), and as the last, slow pyrolysis with a maximum solid yield of around 60-80 wt. % at very long residence time (hours) [1]. Cellulose, hemicelluloses, and lignin are typical main compounds of wood. The amounts of these compounds are dependent on the type of wood. Water and inorganic elements are further components of wood.

The pyrolysis of wood is typically initiated at 200 °C (so-called torrefaction) and lasts till the temperature of 450-550°C is achieved, depending on the species of wood and required product [2]. Pyrolysis plays an important role in the thermal treatment of wood sawdust, since the products of this stage, namely gas and char combustion, respectively, release thermal energy. The sawdust is not combustible directly, because its particle size distribution is not suitable. Therefore, it is necessary to use the briquetting, but that is another input energy and loss of money. The next possibility is to use it as a build material in OSB tables. Recently, the market is oversaturated with sawdust and thus its use for pyrolysis can be acceptable. In order to design a sawdust treatment process, a techno-economical model can bring interesting information [3]. The primary objectives of these models are to provide a diagnostic tool for evaluating the importance of various system parameters and identify system characteristics useful for experimentalists and comparisons between them. The pyrolytic decomposition of wood involves a complex series of reactions, and consequently, changes in experimental heating conditions or sample composition, and preparation may affect not only the rate of reaction, but also the actual course of reactions. The conversions of wood materials to liquids and gaseous products were the processes of great interest in many experiments [4]. Second-generation biofuels are seen as a solution for further increasing the share of renewable energies in the transport sector while reducing the negative impacts associated with conventional biofuels. In fact, there is an important potential of lignocellulosic biomass from forest residue, agricultural waste, and energy crops which is still unused and potentially suitable for bioenergy production with low environmental impact. Maximizing the use of residual biomass is necessary in order to fulfil the targets for biofuel share and greenhouse gas emission reduction set up in the proposal for renewable energy directive. Nevertheless, converting wood and biomass into liquid fuels is not an easy task and adequate technologies are needed [5].

2 EXPERIMENTAL PART

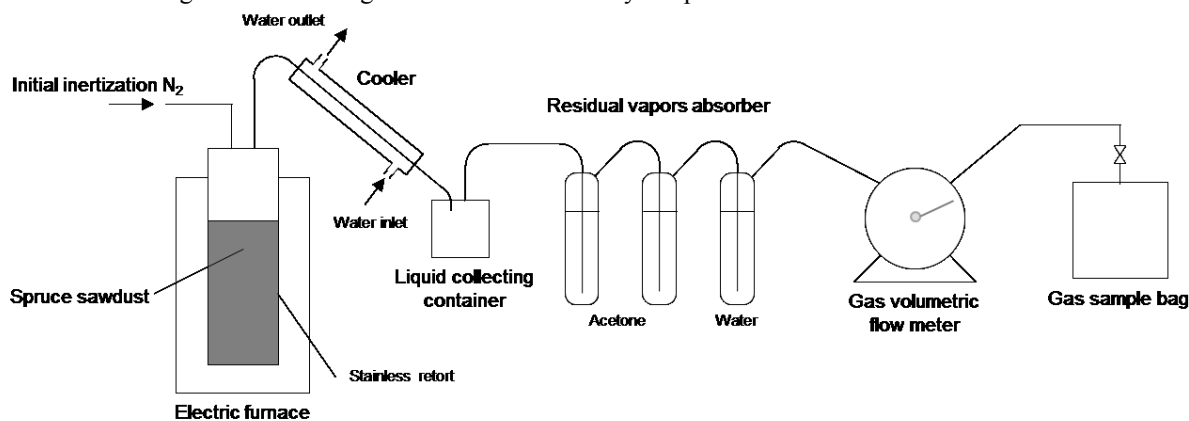
The spruce sawdust was used as a pyrolysis material. The ultimate and proximate analyses were made based on the elemental analysis and thermogravimetric analysis. The results of the analyses are listed in Table 1.

Table 1: Ultimate analysis and proximate analysis of spruce sawdust

Ultimate analysis		Proximate analysis	
component	wt. %	component	wt. %
C	51.75	Moisture	17.30
H	6.09	Volatiles	77.51
N	0.96	Fixed C	21.89
O*	40.60	Ash	0.60

* oxygen was calculated to 100 wt. %

A stainless steel reactor was used for thermal treatment of the waste spruce sawdust. The schema of the experimental apparatus is shown in Figure 1. The sawdust sample, 100 g in weight, was used as FEED in the reactor which was heated at a heating rate of 5 °C/min, and samples of gases were collected between 20 °C and 800 °C at an interval of approximately of 50 °C. The liquid phase is collected in the cylindrical container in the middle of the equipment and a continuous flow of cold water is passed through to maintain the heating effect of the equipment. Acetone and Water are used as absorbents of volatile products, which were not collected in the container after the cooler. While the gas is passing through these samples, the colour of the absorbent changes with a change in the composition of gases. The solid residue remained in the reactor (stainless retort) and was removed and weighed after cooling the reactor to laboratory temperature.

**Figure 1: Flow sheet of Experimental Setup**

The samples of gases were collected in the Tedlar bags and analysed on chromatography to find the composition of CH₄, CO, H₂, and CO₂. The compositions of gas samples were determined by the gas Chromatography Agilent 7890A with a flame ionization detector and a thermal conductivity detector. A Micropacked column (2 m x 0.53 mm) was used in the chromatograph to separate gaseous components. The result of all the sampling is elaborated in the graphs below (Figures 2 and 3). The gas composition was measured at different intervals of temperatures. The liquid and solid products were weighed, and the mass balance of pyrolysis was created.

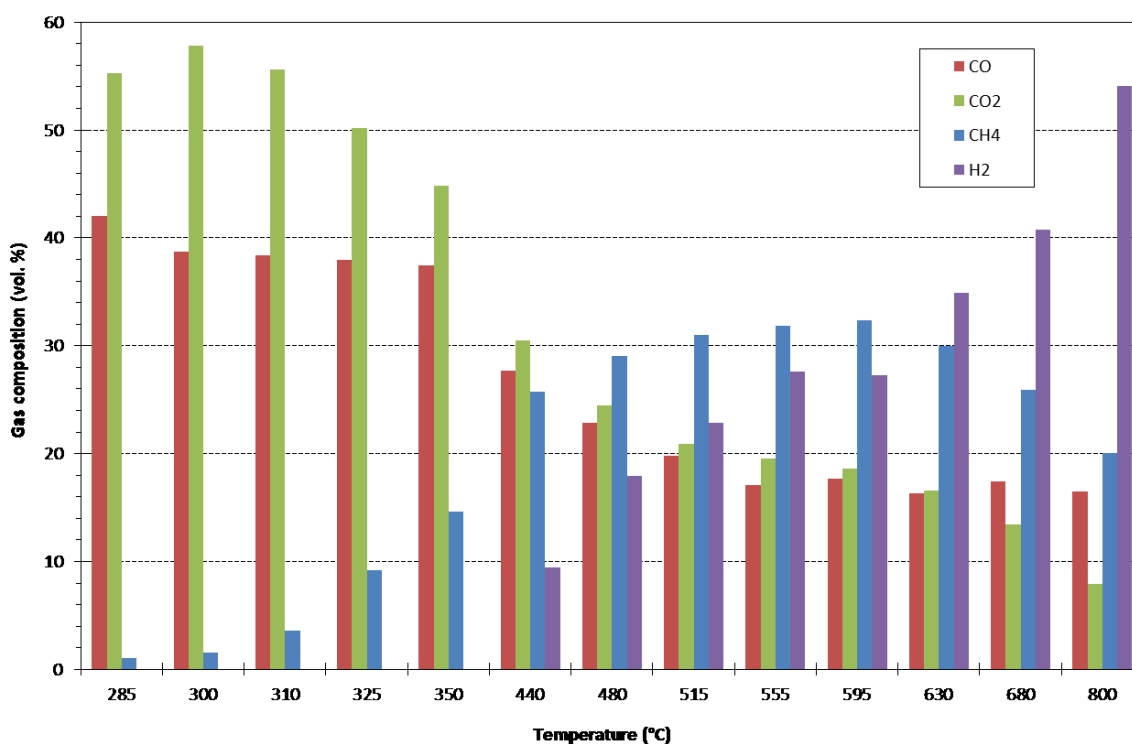


Figure 2: Change in gas composition (CO, CO₂, CH₄, and H₂) during pyrolysis

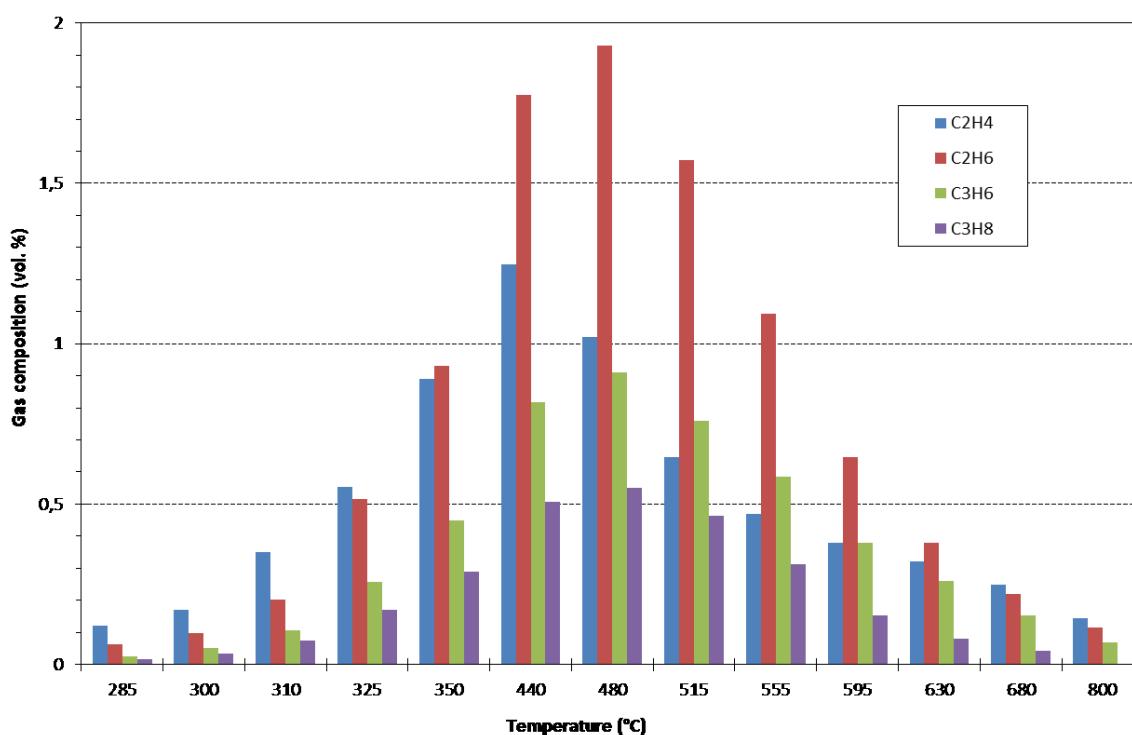


Figure 3: Change in gas composition (light hydrocarbons) during pyrolysis

3 SIMULATION OF PYROLYSIS

This work presents a model of a pyrolysis reactor based on an equilibrium model approach implemented in Aspen Plus[®]. Unlike other works, which implement the pyrolysis reactor as a black box unit giving an a priori defined pyrolysis product composition, the use of an equilibrium approach permits a really predictive simulation, which estimates yields and compositions of pyrolysis products depending on reactor conditions. Aspen Plus[®] has advanced and dedicated functionalities, such as detailed heat exchanger design, dynamic simulation, batch and reactor process modelling. It also provides the option to use an equation-based approach in some of its routines,

which permits convenient use of design. External FORTRAN files are used in the Aspen Plus[®] user subroutine for the description of complex mechanisms. Property methods: PENG-ROB is used as a base property method for the whole system. Spruce sawdust and char components were defined as non-conventional components based on their ultimate analysis including C, H, O, N, S; Cl and Ash elements, and proximate analysis (see Table 1). The syngas production from the spruce sawdust was done at temperatures in a range of 300-800 °C and atmospheric pressure (101325 Pa) was used.

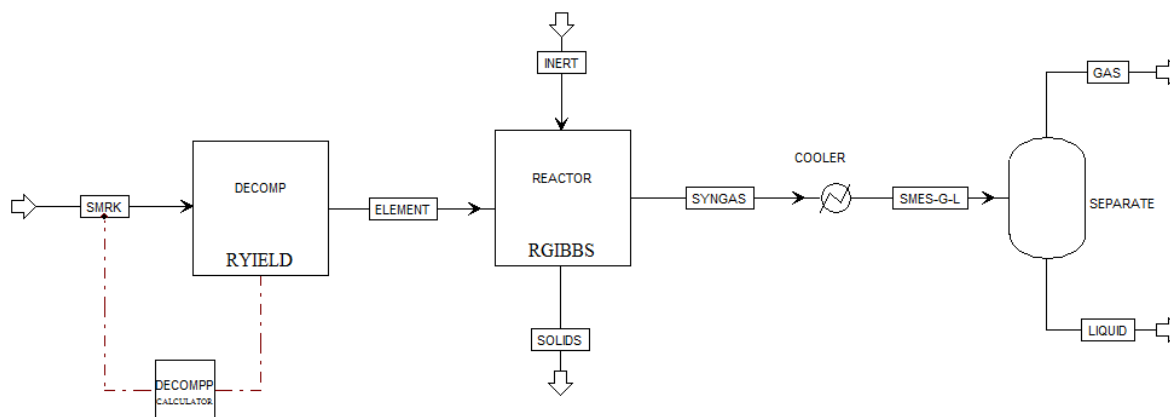


Figure 4: Flowsheet of decomposition and pyrolysis of spruce wood

The flowsheet of syngas production is shown in Figure 4. The spruce wood was decomposed in the RYIELD reactor (a reactor where stoichiometry and kinetics are unknown parameters) to the elements by the ultimate analysis. These elements passed to the RGIBBS reactor (a reactor with a phase equilibrium or simultaneous phase, and a chemical equilibrium in vapour-liquid-solid systems) where syngas was created by thermodynamics equilibrium for a given temperature and pressure. The solid residue was divided in the RGIBBS reactor. The vapour mixture was cooled to 20 °C by a cooler and divided in a separator (FLASH2) to gases and liquid (represented by water only). The gas composition produced by pyrolysis was important as those gases are created from elements by the thermodynamic equilibrium at given temperature and pressure.

4 RESULTS

The yields of pyrolysis products (gas, liquid, and solid) are shown in Figure 5. The amount of solid residue was around 25 wt. % at 600 °C, and relates to the content of fixed carbon. At higher temperatures, the water gas shift reaction started, carbon monoxide and hydrogen were created, and the amount of carbon began to decrease. This part significantly differs from the experimental one. Water was evaporated below 200 °C and collected after the cooler in a condensate container, so it could not react with carbon in the reactor at higher temperature. The amount of gas product increased with increasing temperature, which was observed by many authors [6, 7]. The gas composition of pyrolysis product is shown in Figure 6. The concentration of CO and H₂ increased with increasing temperature. The increases in the CO, H₂ content relate to the decreasing concentrations of CO₂, H₂O, and CH₄. The concentrations of light hydrocarbons were in a range on 400-500 °C, after that, light hydrocarbons were decomposing, which resulted in increases of H₂ concentrations. On the other hand, a half of the volume of produced gas was created below 400 °C that means without H₂.

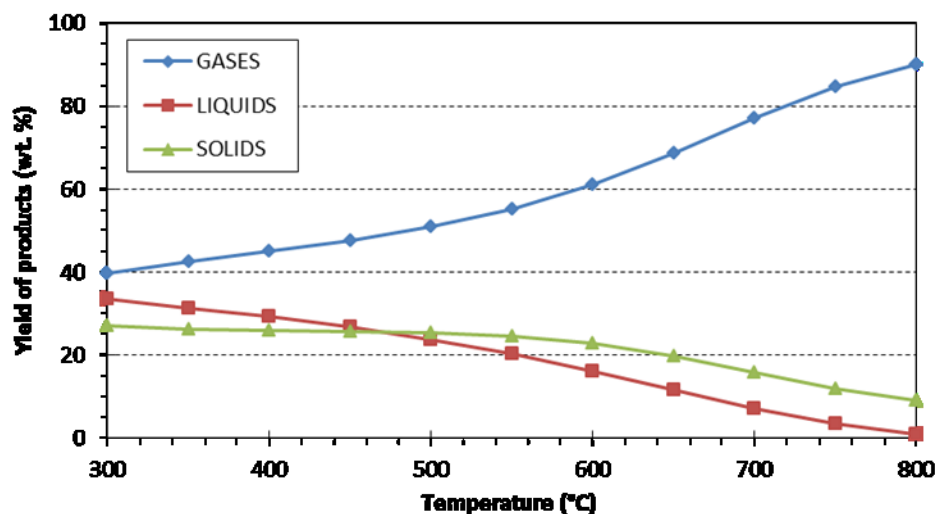


Figure 5: Yields of products from simulation of spruce sawdust pyrolysis

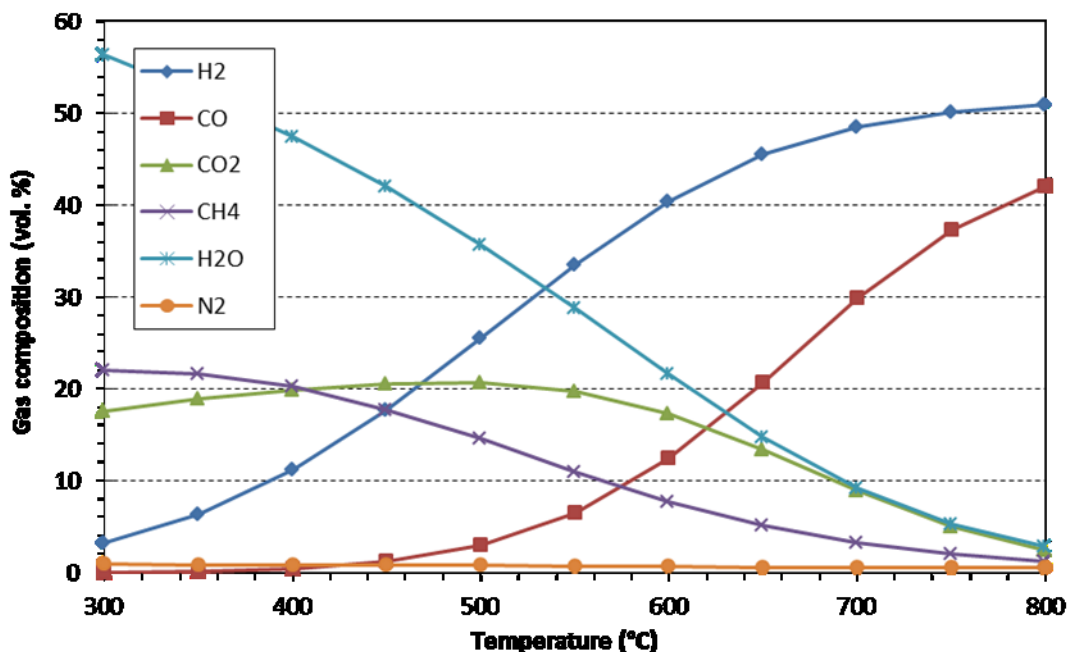


Figure 6: Gas compositions from simulation of spruce sawdust pyrolysis

This increasing content of CO, H₂ had a huge effect on the low heating value of the produced syngas (shown in Figure 7). When multiplying the low heating value and the volume of produced syngas, we will get the energetic potential of produced syngas related to 1 kg feed of spruce sawdust; it is more energy than in the raw wood (approximately 14 MJ/kg). The heating value of solid residue was not calculated, because the biochar is better to use as bio-fertilizer than the solid fuel.

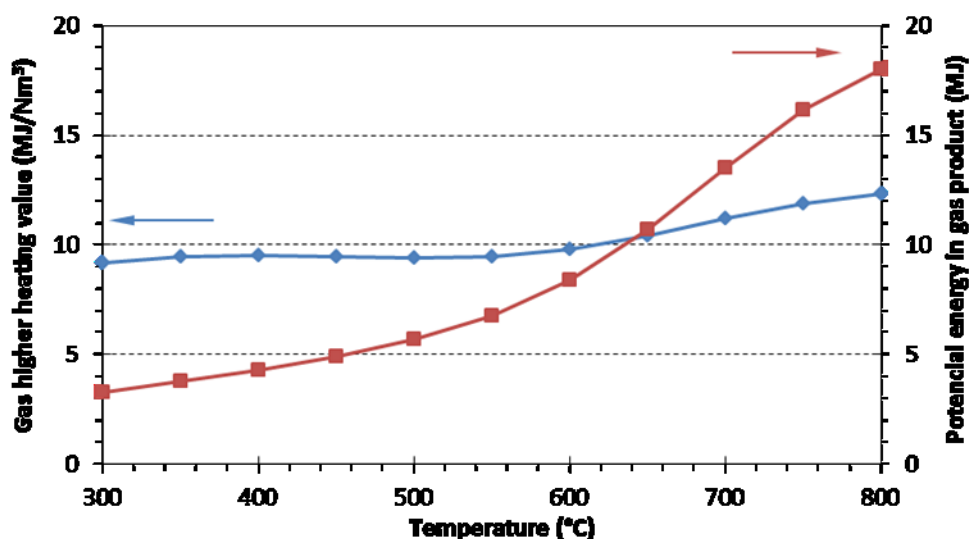


Figure 7: Gas lower heating value and total amount of energy in produced syngas

5 CONCLUSION

The process of spruce sawdust pyrolysis in the laboratory was compared with the model created in the AspenPlus software. Figures 2, 3 and Figure 5 show great differences between the aspen plus model and experiments. It is obvious that the modelling through the decomposition and subsequent formation of gas based on the thermodynamics equilibrium is not appropriate for the modelling of pyrolysis process. There are articles where authors [8] used only a model without comparative experiments, and those results are misleading. The industrial application of the spruce sawdust pyrolysis model can be used, but only for the gasification process, not for the pyrolysis process. The pyrolysis model must contain a chemical reaction of individual wood compounds (cellulose, hemicellulose, and lignin) which is highly dependent on temperature and chemical composition of ash (catalytic effect). One of pyrolysis products is a liquid condensate, which contains hundred organic oxygenate compounds (phenol, cresols, organic acids, etc.), and creating these products is impossible to model without knowledge of chemical reactions kinetics.

Aspen Plus is a suitable tool for creating a techno-economic performance analysis of the pyrolysis or gasification processes [9, 10]. However, it is necessary to create a suitable model, which will reflect the experimental conditions, duration and progress of process.

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