Modeling steam gasification of biomass with Mathcad 15 via two reaction stages

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1. Introduction

The use of biomass as renewable fuel gives an opportunity to decrease the carbon footprint of the energy sector. Novel gasification technologies ensure the flexible and efficient utilization of different biogenic fuel types. Dual fluidized bed (DFB) gasification is a fast progressing technology for allothermal steam gasification of biomass, developed at TU Wien. [1]

To enable technology scale-up, a model is beneficial, which can deliver reliable process data for reactor design. Therefore, the authors propose a model of biomass steam gasification for a DFB reactor system. The developed model predicts the process gas composition and gasification product yields based on fuel ultimate and proximate analysis and process conditions. The model bases on a closed mass and energy balance. The algorithm was written in Mathcad 15 [2]. It allows for the calculation of heat demand of the gasification reactor and serves as a tool for predicting performance indicating key parameters of the gasification process. The model is validated by experimental results of gasification test runs conducted with the advanced 100 kW_{th} DFB pilot plant at TU Wien [3].

In the DFB reactor system, chips or pellets of biomass are rapidly heated after entering the steam blown gasification reactor. Before the fuel particles reach the reactor's temperature, they undergo drying and pyrolysis. The pyrolysis process of biomass typically occurs within the temperature range of 250-650 °C. In any case, pyrolysis is already finished when biomass reaches the typical operation temperature of the fluidized bed gasification reactor (ca. 850 °C). The degassed fuel particles end up as solid char. At the same time, the tar produced during pyrolysis starts to decompose with higher temperatures [4]. Gasification of the char from the pyrolysis with steam is the rate-limiting reaction of the entire process in gasification reactor. Steam gasification of char occurs preferably at higher temperatures [5]. In addition, the water-gas-shift reaction and steam reforming of hydrocarbons take place. In a fluidized bed reactor operating at steady-state conditions, all kind of single sub-reaction pathways take place in parallel and influence each other. The overall gasification process inside a fluidized bed is highly complex. Thus, it was aspired to develop a chemical model as simple as possible, nevertheless enabling meaningful results.

2. Model development

The developed model approach of DFB steam gasification of biomass is presented in Figure 1. The proposed model involves two subsequent stages: i) pyrolysis of fuel particles considered as a non-isothermal process with very high heating rate in the order of thousands of Kelvins per minute, and ii) gasification of the pyrolysis products (char, tar and gaseous components) considered as an isothermal process occurring at the temperature of the gasification reactor. The total heat demand for the process in gasification reactor (Qt) is the sum of heat demand for the pyrolysis stage (Qp) and the heat demand for steam gasification of pyrolysis products (Qg). The oxidation of unconverted residue char in the combustion reactor, serves as the heat source for the overall process in the gasification reactor. The two reactors are connected via circulating solid heat carrier (bed material).

Pyrolysis of biomass is described according to first order devolatilization reaction kinetics extended to describe particular pyrolysis products formation. The pyrolysis model also covers a secondary decomposition of produced tar components. Products of the pyrolysis reactions include pyrolytic gases, steam, benzene, toluene and xylene (BTX), tar and residue char including ash. The model of biomass pyrolysis was based on algorithm for coal pyrolysis developed by Sciazko M. [6].

Primary and secondary pyrolysis products are inputs for the **second stage of gasification**, during which unreacted char, remaining tar, and reactive gaseous components (CO, CO_2, H_2O, H_2) together with steam are involved in gasification reactions. Three gasification reactions are taken into account: water gas reaction, water gas shift reaction and tar steam reforming according to arbitrary assumed stoichiometry. A pseudo-equilibrium model is applied for calculations – the expressions for equilibrium constants of chosen reactions are corrected by using empirical coefficients accounting for the difference between equilibrium and the actual state in the reactor. This approach can be considered as an analysis of quasi stationary states. For the sake of model simplicity all other compounds not considered in gasification reactions are assumed to be inert and they are bypassed around the gasification reactions stage. The final process gas is a physical mixture of gaseous components released during pyrolysis and bypassed around gasification reactions stage and those formed or transformed during gasification reactions.

The heat demand for the gasification reactor is calculated as a difference between the total enthalpy of products and the total enthalpy of substrates.

3. Results

Table 1 presents simulation results. The calculated values are validated by measurement results from a gasification test run with a 100 kW dual fluidized bed steam gasifier, wood pellets as fuel, and a catalytic active olivine-limestone mixture as bed material. The relative errors between the simulation and the measurements are below 10% in most cases. The model has a higher error in predicting the tar and BTX contents in the process gas. Nevertheless the main process gas composition is predicted with good accuracy. Moreover, model can serve as a tool for quick and accurate estimation of key parameters indicating process performance (e.g. process gas yield, H_2O conversion, cold gas efficiency, H_2 to CO ratio) for given fuel and process conditions. In addition to the presented validation, also results with other bed material types and gasification temperature were investigated.

4. Conclusion

The proposed model of DFB steam gasification of biomass comprising combination of non-isothermal, kinetic pyrolysis stage and isothermal pseudo-equilibrium stage of pyrolysis products gasification with bypass for some gaseous components presents innovative approach to biomass gasification modeling. It allows for obtaining meaningful results with relatively simple model structure which corresponds to actual process pathway in DFB gasification reactor. The model gives an insight into the process flow by delivering mass and energy balance of all considered stages.

The pyrolysis phase of the model can be used autonomously and serves to predict biomass pyrolysis products yields and the process energy balance.

The pseudo-equilibrium approach in the gasification reactions stage is a good compromise between more detailed but also tedious and complex kinetic models and easy to apply but limited due to divergence between equilibrium state and the actual state in gasification reactor equilibrium models.

Choosing Mathcad 15 as a simulation tool gives an advantage of flexibility and good control over each step of modeling process. It also favors better understanding of the applied approach, since the entire calculation algorithm has to be introduced equation after equation.

The developed model has a high potential for practical applications. It is a good tool for quick and accurate prediction of yields and compositions of gasification products and estimation of key parameters indicating process performance based on fuel ultimate and proximate analysis and process conditions. However it has limitations regarding prediction of BTX and tar compounds in the process gas stream.

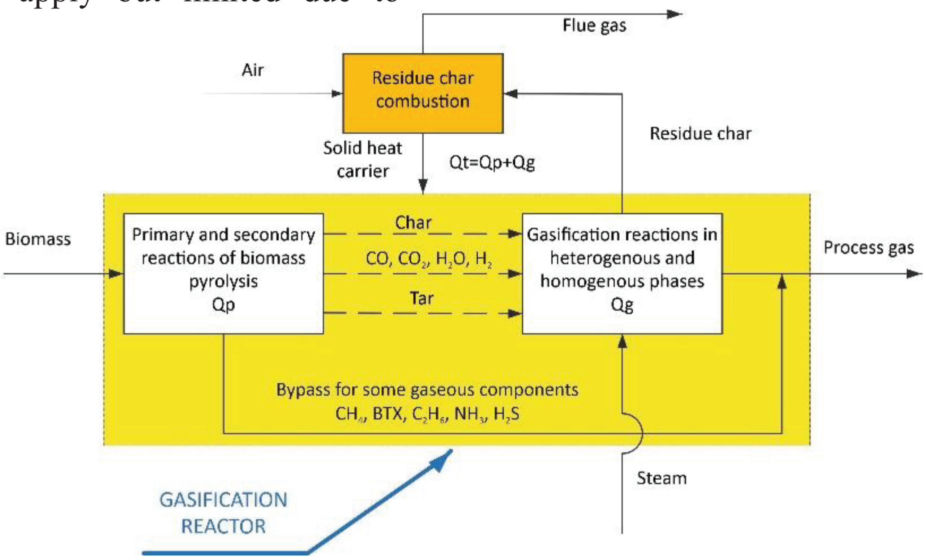

Fig. 1: Model approach of dual fluidized bed steam gasification of biomass (modified from [2])

Table 1 Comparison of experimental and simulation results generated for gasification of soft wood using a mixture (50/50 wt. %) of olivine and calcite as bed material.

Parameter	Unit	Experiment	Simulation	Relative error (%)
H_2	vol. % $_{dry}$	43.8	45.1	3.0
CO	vol. % $_{dry}$	20.9	22.1	5.7

CO_2	vol. % $_{dry}$	20.8	22.4	7.7
CH_4	vol. % $_{dry}$	9.43	9.13	-3.2
C_xH_y	vol. % $_{dry}$	1.03	1.05	1.9
Water in the gas stream	vol. %	31	32	3.2
Dry process gas volume flow	Nm^3/h	28	28	0.0
Dry process gas yield	$Nm^3/kg_{bio,\ daf}$	1.42	1.40	-1.4
Steam-related H_2O conversion	$kg_{H2O}/\ kg_{H2O}$	0.32	0.35	9.4
Fuel-related H_2O conversion	$kg_{H2O}/\ kg_{bio,daf}$	0.24	0.28	16.7
Dry process gas lower heating value	MJ/Nm^3	11.4	11.6	1.8
Process gas power	kW	89	89	0.0
Cold gas efficiency	%	87	86	-1.1
Process gas H_2 to CO ratio	-	2.1	2.0	-4.8
Tar content in the dry gas stream	g/Nm^3	3.6	4.0	11.1
BTX content in the dry gas stream	g/Nm^3	15.2	6.8	-55.3
Heat demand for gasification reactor	kW	-	19.34	-

5. References

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