THE MODEL FOR DETERMINATION OF THE TEMPERATURE AND THE GAS COMPOSITION OF BIOMASS GASIFICATION PRODUCTS BY THE USE OF MATERIAL AND ENERGY BALANCES

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Abstract:
The paper presents the model for the analytical determination of the temperature and the gas composition of biomass gasification products in downdraft gasification reactors at atmospheric pressure. The temperature and the gas composition were determined by the use of material and energy balances.
Key words: biomass, gasification, gasification temperature.

INTRODUCTION

The main disadvantage of the existing models for prediction of downdraft gasification gas composition is only applying the material balance equations. Analytically gained results for the temperature and the gas composition by the use of material balance equations are acceptable only for the precise relation between moisture content of the biomass and the amount of carbon that is used as a heat source for occurring of gasification reactions, apropos for the definite heat loss through sensible heat of gasification products.

The model modification, presented in this paper, is done by applying the equation of energy balance and the homogeneous reversal equation:

$$CO_2 + H_2 \Leftrightarrow CO + H_2O$$

MODEL FOR DETERMINATION OF THE BIOMASS GASIFICATION TEMPERATURE

The assumption made for determination of the temperature and the gas composition of biomass gasification products is that in the reduction zone of downdraft gasification reactor these reactions take place:

$$C + 2 H_2 \Leftrightarrow CH_4 \quad (1.1)$$
$$C + CO_2 \Leftrightarrow 2 CO \quad (1.2)$$
$$C + H_2O \Leftrightarrow CO + H_2 \quad (1.3)$$
$$CO_2 + H_2 \Leftrightarrow CO + H_2O \quad (1.4)$$

The difference between this and other models is that this model includes the fourth homogeneous reaction (1.4).
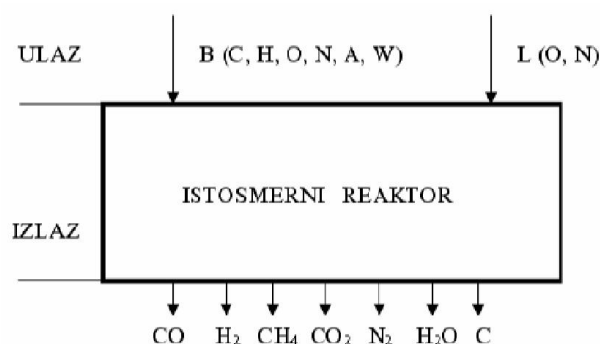

Figure 1.1. Downdraft reactor scheme

B (kg) – the amount of the fuel that enters in the reactor
W (kg/kgB) – the moisture content of the fuel
L (kg/kgB) the amount of air that enters in the reactor
X_{CO}, X_{H2}, X_{CH4}, X_{CO2}, X_{N2}, X_{H2O}, X_C (kmol/kmol) – the mole fractions of the reactions products at the equilibrium mixture.

This is a complex mathematical problem that requires solving the system of eight equations with eight unknowns. The seven unknowns are the mole fractions (X_{CO}, X_{H2}, X_{CH4}, X_{CO2}, X_{N2}, X_{H2O}, X_C) and the eighth is the gasification temperature.

The additional assumption, which states that whole amount of the biomass hydrogen, is used as the heat source for the reactions in the reduction zone is introduced.

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The chemical equilibrium constant of the assumed homogeneous reaction (1.4) depend on temperature, and is determined with equation:

$$\log K_4 = 1.6945 - \frac{1855.6}{T} \qquad (1.5)$$

Determination of the gas composition and the gasification temperature is done for the different values of fix carbon that comes into the reduction zone, and for the different biomass moisture content.

The equations for determination of the mole fractions in equilibrium mixture and the temperature of biomass gasification are:

$$X_{CO} + X_{H_2} + X_{CH_4} + X_{CO_2} + X_{N_2} + X_{H_2O} + X_C = 1 \quad (1.6)$$

$$\frac{\sum O_2}{\sum H_2} = \frac{\frac{1}{2} \cdot X_{CO} + X_{CO_2} + \frac{1}{2} \cdot X_{H_2O}}{X_{H_2} + 2 \cdot X_{CH_4} + X_{H_2O}} = A \qquad (1.7)$$

$$\frac{\sum C}{\sum N_2} = \frac{X_{CO} + X_{CO_2} + X_{CH_4} + X_C}{X_{N_2}} = \frac{1}{B} \qquad (1.8)$$

$$\left(12635 \cdot X_{CO} + 10785 \cdot X_{H_2} + 35880 \cdot X_{CH_4}\right) \cdot$$
$$\cdot \left(\frac{\frac{22.4}{12} \cdot (C - C_g)}{12 \cdot (X_{CO} + X_{CO_2} + X_{CH_4})} \right) = H_{dB}(1 - q_g) \qquad (1.9)$$

$$K_1 = \frac{X_{CH_4} \cdot (1 - X_C)}{p \cdot X_{H_2}^2} \qquad (1.10)$$

$$K_2 = \frac{p \ X_{CO}^2}{(1 - X_C) \cdot X_{CO_2}} \qquad (1.11)$$

$$K_3 = \frac{X_{CO} \cdot X_{H_2} \cdot p}{X_{H_2O} \cdot (1 - X_C)} \qquad (1.12)$$

$$K_4 = \frac{X_{CO} \cdot X_{H_2O}}{X_{CO_2} \cdot X_{H_2}} \qquad (1.13)$$

The dimensions in the above equations of material and energy balances are:

$C_g \ \left[\dfrac{kJ}{kgB} \right]$ - the mass fraction of carbon in the ash

$q_g \ \left[\% \right]$ - the entire heat loss through sensible heat, and conduction and radiation

$H_{dB} \ \left[\dfrac{kJ}{kg} \right]$ - the biomass heating value.

$$H_{dB} = 33900 \cdot C + 117000 \cdot \left(H - \frac{O}{8} \right) - 2500 \cdot W \quad \left[\frac{kJ}{kg} \right]$$

➤ The amount of carbon:

$$\sum C = \frac{1}{12} \cdot C \quad \left[\frac{kmolC}{kgB} \right]$$

➤ The amount of oxygen:

$$\sum O_2 = \frac{1}{32} \cdot \left(\frac{16}{18} \cdot W + \frac{8}{3} \cdot R \cdot C + 8 \cdot H \right) \quad \left[\frac{kmolO_2}{kgB} \right]$$

➤ The amount of hydrogen:

$$\sum H_2 = \frac{1}{2} \cdot \left(H + \frac{1}{9} \cdot W \right) \quad \left[\frac{kmolH_2}{kgB} \right]$$

➤ The amount of nitrogen:

$$\sum N_2 = \frac{1}{28} \cdot \left(N + \frac{77}{23} \cdot \left(\frac{8}{3} \cdot R \cdot C + 8 \cdot H - O \right) \right) \quad \left[\frac{kmolN_2}{kgB} \right]$$

In equations (2.6), (2.8), (2.10), (2.11) and (2.12) there is unburned carbon (Xc). The equations are derived on this way:

$$X_{CO} + X_{H_2} + X_{CH_4} + X_{CO_2} + X_{N_2} + X_{H_2O} + X_C = 1 \quad (1.14)$$

$$\frac{X_{CO}}{1 - X_C} + \frac{X_{H_2}}{1 - X_C} + \frac{X_{CH_4}}{1 - X_C} + \frac{X_{CO_2}}{1 - X_C} + \frac{X_{N_2}}{1 - X_C} + \frac{X_{H_2O}}{1 - X_C} = 1$$

$$p \frac{X_{CO}}{1 - X_C} + p \frac{X_{H_2}}{1 - X_C} + p \frac{X_{CH_4}}{1 - X_C} + p \frac{X_{CO_2}}{1 - X_C} + p \frac{X_{N_2}}{1 - X_C} + p \frac{X_{H_2O}}{1 - X_C} = p$$

According to Dalton's law:

$$p_{CO} + p_{CO_2} + p_{H_2} + p_{H_2O} + p_{CH_4} + p_{N_2} = p \qquad (1.15)$$

By using the partial pressures determined in the equation (1.14), the equilibrium constants of chemical reactions can be calculated by following equations:

$$K_1 = \frac{P_{CH_4}}{P_{H_2}^2} = \frac{X_{CH_4} \cdot (1 - X_C)}{p \cdot X_{H_2}^2}$$

$$K_2 = \frac{P_{CO}^2}{P_{CO_2}} = \frac{p \ X_{CO}^2}{(1 - X_C) \cdot X_{CO_2}}$$

$$K_3 = \frac{P_{CO} \cdot P_{H_2}}{P_{H_2O}} = \frac{X_{CO} \cdot X_{H_2} \cdot p}{X_{H_2O} \cdot (1 - X_C)}$$

$$K_4 = \frac{X_{CO} \cdot X_{H_2O}}{X_{CO_2} \cdot X_{H_2}} \cdot$$

The equilibrium constants K_1, K_2, K_3, and K_4 of the chemical equations were determined by laboratory measurements, when the full equilibrium was reached (homogeneous temperature, pressure, and concentration fields after sufficient reaction time). These conditions can not exist in a real process.

The system of equations was solved by the software MATLAB R12, and the results are illustrated on the figures (1.2), (1.3) and (1.4).

TABLE 1.1 GAS COMPOSITION

Gasification temperature (^{0}C)		703	681	662	645	630	615
The amount of injected moisture W_1(kg/kgB)		0.25	0.25	0.25	0.25	0.25	0.25
The amount of burned carbon R		0.36	0.36	0.36	0.36	0.36	0.36
Heat loss J		0.05	0.08	0.11	0.14	0.17	0.2
Gas composition	xCO(%)	24.36	22.26	19.63	17.84	15.79	13.66
	xH$_2$(%)	19.00	19.11	18.81	19.13	19.01	18.49
	xA(%)	0.19	0.13	0.63	0.005	0.15	0.34
	xCH$_4$(%)	0.45	0.60	0.78	0.95	1.14	1.33
	xCO$_2$(%)	5.39	7.18	8.82	10.61	12.13	13.18
	xH$_2$O(%)	2.73	3.68	4.57	5.68	6.76	7.77
	xN$_2$(%)	27.88	27.04	26.76	25.78	25.02	25.23
	xW$_G$(%)	20.00	20.00	20.00	20.00	20.00	20.00

TABLE 1.2 GAS COMPOSITION

Gasification temperature (^{0}C)		719	701	687	675	663	653
The amount of injected moisture W_1(kg/kgB)		0.1	0.15	0.2	0.25	0.3	0.35
The amount of burned carbon R		0.35	0.35	0.35	0.35	0.35	0.35
Heat loss J		0.08	0.08	0.08	0.08	0.08	0.08
Gas composition	xCO(%)	26.74	24.60	23.15	21.44	20.01	18.46
	xH$_2$(%)	18.59	19.01	19.52	20.00	20.28	20.54
	xA(%)	0.15	0.07	0.08	0.04	0.08	0.08
	xCH$_4$(%)	0.36	0.46	0.58	0.69	0.81	0.99
	xCO$_2$(%)	4.62	5.81	6.99	7.94	8.91	9.82
	xH$_2$O(%)	2.25	2.86	3.52	4.21	4.91	5.62
	xN$_2$(%)	38.20	24.15	29.50	25.68	21.93	18.57
	xW$_G$(%)	9.09	13.04	16.66	20.00	23.07	25.92

Applying the energy balance equation with the definite losses through sensible heat allows determination of gas composition as a function of biomass moisture content and an assumed amount of burned carbon at reduction zone.

With the use of the homogeneous reaction can be seen the difference between the model prediction and real gas composition at lower gasification temperatures. At higher gasification temperatures, the predicted gas composition coincides with a real gas composition.
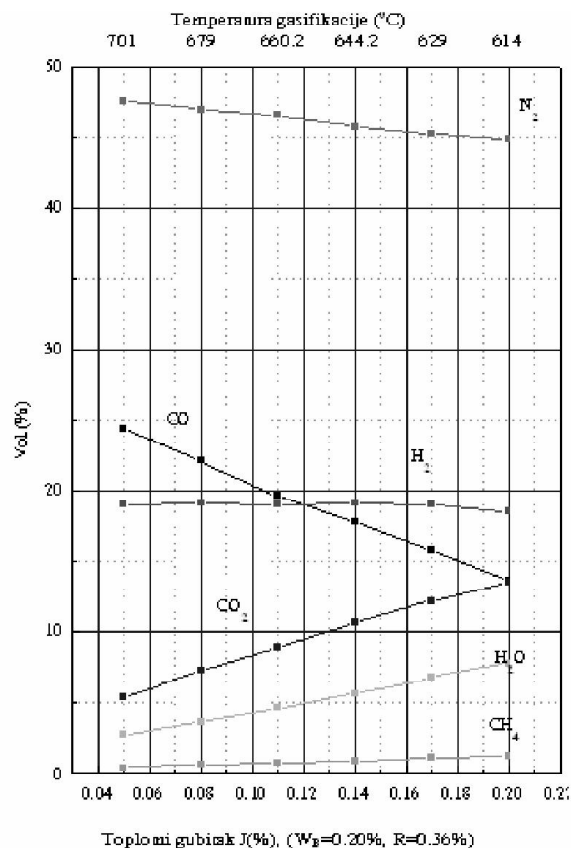

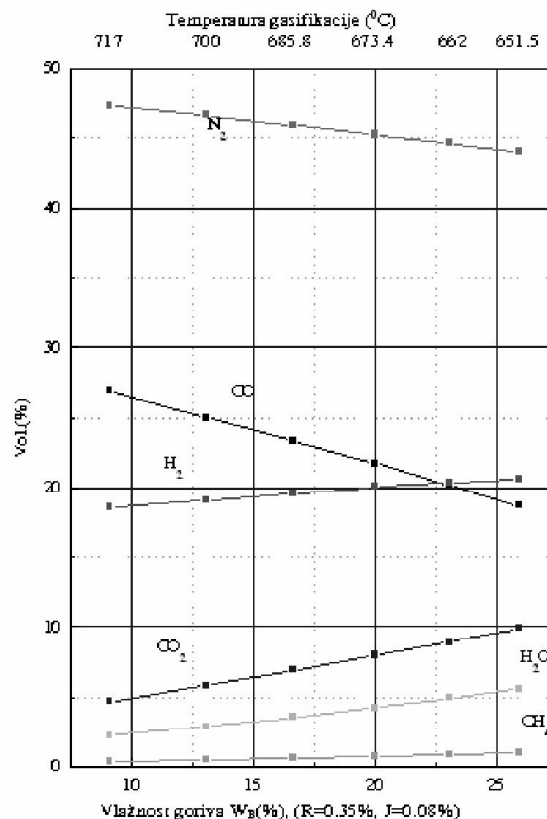**Figure 1.2 Gas compositions as a function of biomass moisture content**

Figure 1.3 Gas compositions as a function of biomass moisture content

TABLE 1.3 GAS COMPOSITION

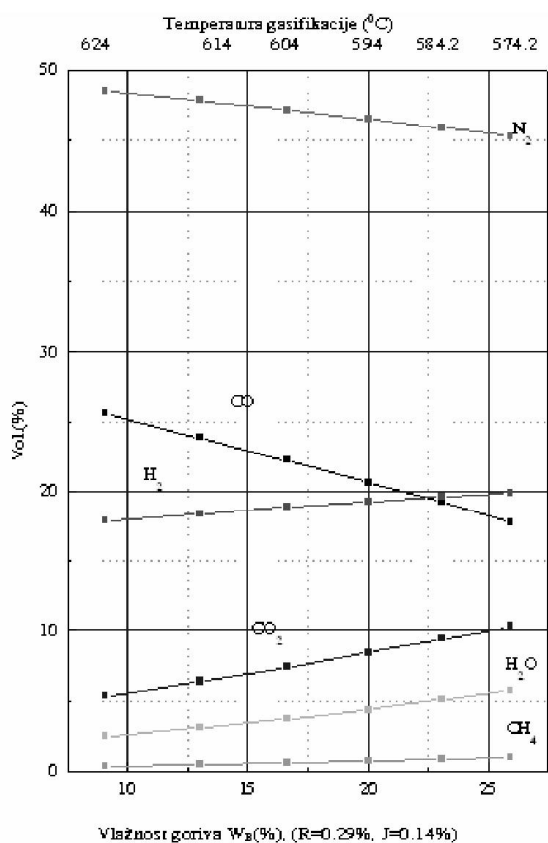| Gasification temperature (°C)		624	614	604	594	584.2	574.2
The amount of injected moisture W_1(kg/kgB)		0.25	0.30	0.35	0.40	0.45	0.50
The amount of burned carbon R		0.29	0.29	0.29	0.29	0.29	0.29
Heat loss J		0.14	0.14	0.14	0.14	0.14	0.14
Gas composition	xCO(%)	15.70	13.90	12.40	11.0	10.00	8.81
	xH_2(%)	21.94	21.56	21.35	21.17	20.94	20.76
	xA(%)	0.49	0.14	0.11	0.24	0.06	0.09
	xCH_4(%)	1.40	1.72	1.94	2.13	2.48	2.81
	xCO_2(%)	13.08	14.10	14.61	15.44	16.16	16.88
	xH_2O(%)	7.90	9.30	10.0	11.10	12.14	13.22
	xN_2(%)	19.49	15.58	13.67	10.35	7.19	4.10
	xW_G(%)	20.00	23.70	25.92	28.57	31.03	33.33

Figure 1.4 Gas compositions as a function of biomass moisture content

CONCLUSION

Comparing the model and experimental results of biomass gasification gas composition one can notice the same tendencies of some components, and some differences at the different biomass moisture content and the different amount of available carbon for endothermic reactions occurring. In a real gasification reactor the reactions equilibrium does not exist and it is the reason why the difference between model prediction and experimental results occurs. The values for equilibrium constants which are used for analytical determination of the gas composition, were obtained in laboratory measuring where chemical equilibrium does exist (homogeneous temperature, pressure and concentration fields after sufficient reaction time) that is, the condition which does not occur in a real process.

Comparing experimental results with the model prediction of the gas composition can be concluded that the model can be used for determination of the temperature and the gas composition of biomass gasification.

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