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Experimental Study and Mathematical Modelling of Straw Co-Firing with Peat

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The gasification/combustion characteristics of biomass pellet mixtures were experimentally studied and mathematically modelled by co-firing wheat straw with peat with the aim to assess the effect of straw addition to peat on the mixture thermal decomposition, on the formation and combustion of volatiles, and to optimize the mixture composition and to provide more intensive use of straw for energy production. The results of the experimental study show that the co-firing of straw with peat pellets enhances the thermal decomposition of peat pellets at the primary stage of the flame formation ($t < 500$ s). This leads to more intensive release of the combustible volatiles entering the combustor, to faster ignition of volatiles and faster formation of the flame reaction zone. Analysis of the effect of wheat straw co-firing with peat has shown that the thermal interaction between the components completes the combustion of the mixture, increasing so the heat output from the device, the produced heat energy, the volume fraction of CO_2, whereas the air excess in the products decreases, with the maximum co-firing effect on the main combustion characteristics at 10-20 % of the straw mass load. A mathematical model for volatiles (CO, H_2) combustion downstream the combustor has been developed using the environment of MATLAB package and two exothermic reactions for H_2 and CO combustion with account of variations in CO:H_2 supply into the combustor by varying the mass load of straw in the mixture.

1. Introduction

In accordance with the EU 2020 strategy targets on climate change and energy, the main aim of the current research is to reduce greenhouse gas (GHG) emissions by 20 % to 2020 compared to 1990 levels with a target of 20 % of gross final energy consumption from the renewable energy resources (harvesting and agriculture residues). Because of the rapidly increasing consumption of harvesting residues for residential heating, there is a growing need for wider use of alternative fuels, e.g., agriculture residues for energy production (Glithero, 2013), which are the more problematic fuels than harvesting residues (wood) and can cause the lower heat energy production per mass of burned fuel, the enhanced release of polluting NO_x emission and the enhanced formation of ash (Vasilev, 2012). To minimize these negative effects, co-combustion of straw with renewable (Nordgren, 2013) or fossil fuels (Demirbas, 2003) is proposed which could provide the wider use of straw for cleaner heat energy production with reduced ash formation and fossil CO_2 emissions. In fact, multi-fuel firing is becoming a common practice of heat energy producers when co-firing of different fuels in different proportions (Hupa, 2005). However, the results of the previous experimental study suggest (Barmina, 2017) that the main gasification/combustion characteristics of fuel mixtures and the composition of emission are influenced by differences in the elemental and chemical composition of the components, and small variations of the mixture composition can cause variations of the thermal decomposition of components, the formation and ignition of volatiles with direct influence on the combustion conditions, composition of emissions and produced heat energy. With this account, the main aim of the current study is to provide the detailed experimental study and mathematical modelling of the processes developing at co-combustion of straw with peat pellets to assess the main effects which affect the thermo-chemical conversion of the mixture.

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2. Experimental

The effects of wheat straw co-gasification/co-combustion with peat pellets were studied using a batch-size pilot device, combining a biomass gasifier and the water-cooled sections of the combustor, and the methodology described in Abricka et al., 2015. The gasifier was filled with a mixture of straw and peat pellets, with the varying the mass load of straw in the mixture from 0 up to 100 %. The thermal decomposition of the biomass mixture was initiated by a propane flame flow with the average heat input 1 kW and 350 s duration. The gasification/combustion characteristics at thermo-chemical conversion of the mixtures are studied experimentally at the average air excess ratio in the flame reaction zone $\alpha \approx 1.6\text{-}1.7$. The experimental study involved joint measurements of the main characteristics (elemental composition, heating values) of the biomass pellets and their mixtures, DTG and DTA analysis of their thermal decomposition (Barmina, 2013), complex measurements of the mixture weight loss rate (dm/dt), measurements of the composition of volatiles entering the combustor and the products composition by a gas analyser Testo 350, and calorimetric measurements of the cooling water for the gasifier and combustor.

3. Results and discussion

The results of the DTG and DTA analysis of wheat straw and peat pellets show a significant difference in their thermal decomposition, which can be related to the difference in chemical composition of wheat straw and peat. The thermal decomposition of wheat straw pellets results in the formation of the dominant weight loss and temperature peaks at T = 560 K (-9 %) with a comparatively less increase of the weight loss (3.16 %) and temperature at 650 K and at around 710 K (2.09 %). In accordance with data (Yang, 2009), the wheat straw thermal degradation below 630 K can be related to the thermal decomposition of hemicelluloses and cellulose, whereas at T > 630 K the thermal decomposition of lignin dominates which is highly responsible for the char formation and combustion. On the contrary, the most intensive thermal decomposition of peat pellets (up to 7.1 %) with the correlating increase of the temperature is observed during the char conversion stage with (T = 684 K), when the thermal decomposition of lignin promotes the char formation and conversion (Figure 1-a, b).

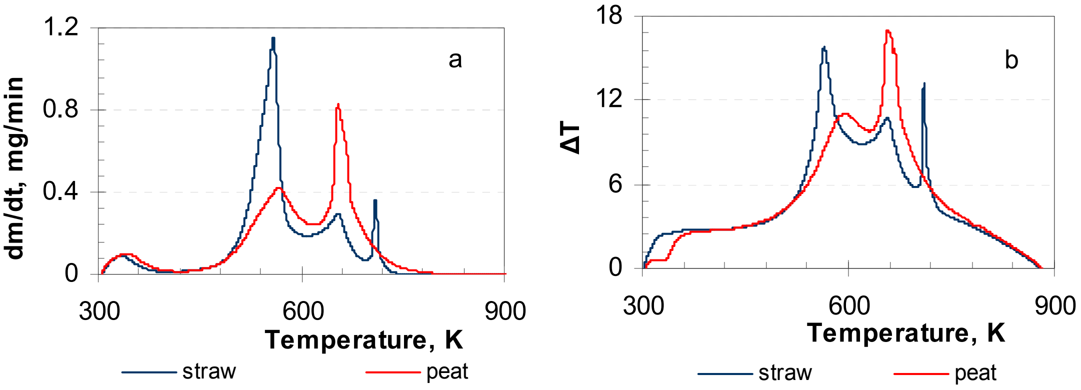

Figure 1. DTG (a) and DTA (b) analysis of the thermal decomposition of wheat straw and peat pellets in oxidative atmosphere.

The kinetic study of the thermal decomposition of the biomass samples (straw, peat and their mixtures) has shown that in accordance with the results of the DTG and DTA analysis the thermo-chemical conversion of biomass pellets and their mixtures develops as a two stage processes with the primary stage of the thermal decomposition and flaming combustion of volatiles followed by the gradual transition to the char conversion stage. At the primary stage of the thermal decomposition (t < 1000 s), a higher weight loss rate (up to 0.135 g/s) with the faster formation and ignition of volatiles was observed for wheat straw pellets with a delay of the weight loss and ignition of volatiles for peat pellets (Figure 2, a-d). The difference between the weight loss rates, the formation and ignition of volatiles for straw and for peat pellets promotes the thermal interaction between the components. The faster thermal decomposition of straw with the faster ignition and faster heat release at the combustion of volatiles activates the thermal decomposition of peat pellets promoting the faster transition to the flaming combustion of volatiles, with the correlating increase of the weight loss rates of biomass mixtures, flame temperature, heat output from the device and CO_2 volume fraction in the products up to their peak values, and with the faster transition from the flaming combustion of volatiles to the end stage of char conversion (t > 2000 s).

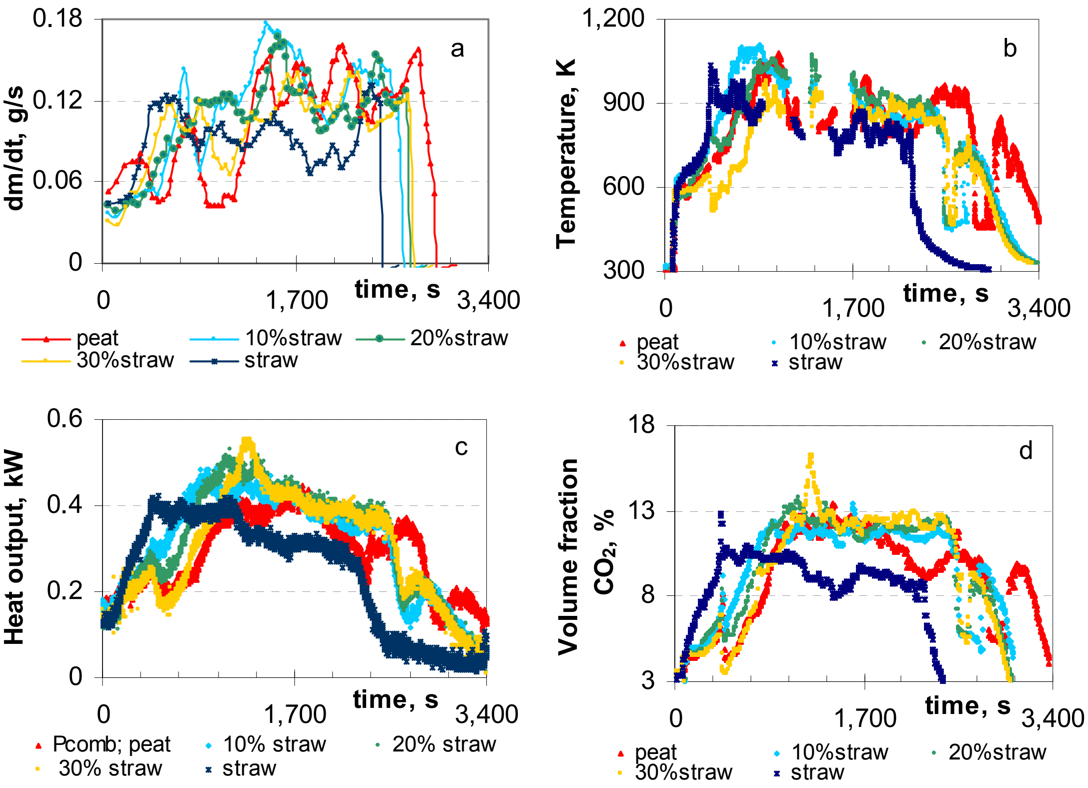

Figure 2. Kinetics of the thermal decomposition (a), flame temperature (b), heat output (c) and the CO_2 volume fraction in the products (d) at co-combustion of straw with peat.

To determine the optimal mass load of straw in the mixture, the average values of the weight loss rate, the composition of volatiles entering the combustor, the main flame characteristics and the composition of the products were estimated for different values of the mass load of straw. The results suggest that at the primary stage of the thermo-chemical conversion of the biomass mixtures, when increasing the mass load of straw in the mixture up to the 10-20 % activates the thermal interaction between the components, the average values of the weight loss rates and the mass fraction of volatiles entering the combustor increase up to their peak values, decreasing to the minimum the air excess ratio in the flame reaction zone and improving so the combustion conditions (Figure 3, a-b). The enhanced thermal decomposition and the improvement of the combustion conditions promote an increase of the average values of the flame temperature, heat output from the device and CO_2 volume fraction in the products. With the further increase of the mass load of straw in the mixture the thermal decomposition of pellets is influenced by the variations of the mixture elemental composition and heating values (Table 1) determining the correlating linear decrease of the weight loss rate, volume fraction of volatiles at the bottom of the combustor, heat output from the device, flame temperature and the CO_2 volume fraction in the products.

Table 1: The elemental composition and heating values (HHV) of straw pellets, peat pellets and their mixtures (dry mass)

Biomass	C, %	H, %	O, %	N, %	Moisture, %	Ash, %	HHV, MJ/kg
Wheat straw	46.62	5.09	42.72	1.31	9.10	4.26	18.50
Peat	53.83	5.12	36.93	1.11	11.40	3.02	21.20
Straw 10 % + peat	53.11	5.12	37.51	1.13	11.17	3.14	20.93
Straw 20 % + peat	52.39	5.11	38.09	1.15	10.94	3.27	20.39
Straw 30 % + peat	51.67	5.11	38.67	1.17	10.71	3.39	20.32

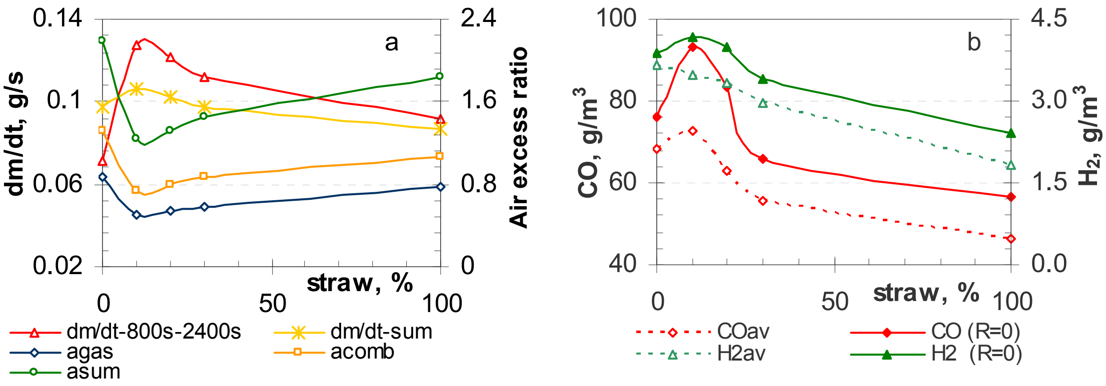

Figure 3. The effect of the mass load of straw in the mixture on the thermal decomposition (a) and on the formation of volatiles (b).

4. Results of mathematical modelling and numerical simulation

For a more detailed analysis of the processes developing when co-combusting straw with peat, mathematical modelling and numerical simulation of the processes were carried out considering two dominant second-order chemical reactions of the volatiles combustion:

$H_2 + OH \rightarrow H_2O + H$; $E_1 = 14{,}360\ J{\cdot}mol^{-1}$; $A_1 = 216\ m^3{\cdot}mol^{-1}{\cdot}s^{-1}$
$CO + OH \rightarrow CO_2 + H$; $E_2 = 30{,}787\ J{\cdot}mol^{-1}$; $A_2 = 0.96{\cdot}10^6\ m^3{\cdot}mol^{-1}{\cdot}s^{-1}$

Accordance to the results of the experimental measurements, the average values of C_1 (H_2) and C_5 (CO) depend on the mixture composition and are as follows: for peat H_2 = 1.8 $mol{\cdot}m^{-3}$, CO = 2.4 $mol{\cdot}m^{-3}$; for 10 % of straw in the mixture H_2 = 1.7 $mol{\cdot}m^{-3}$; CO = 2.6 $mol{\cdot}m^{-3}$; for 20 % of straw – H_2 = 1.7 $mol{\cdot}m^{-3}$; CO = 2.2 $mol{\cdot}m^{-3}$; for 30 % of straw – H_2 = 1.5 $mol{\cdot}m^{-3}$; CO = 2.0 $mol{\cdot}m^{-3}$; for 100% of straw – H_2 = 0.9 $mol{\cdot}m^{-3}$; CO = 1.6 $mol{\cdot}m^{-3}$. These values (10 times decreased) were used in a mathematical model, where C_2 is the mass fraction for OH and $C_1 + C_2 + C_3 = 1$.

The production rate for k-th species can be expressed as (Smooke, 1987):

$$\Omega_k = \sum_{j=1}^{2} [(\nu''_{jk} - \nu'_{jk}) R_j(T) \prod_{n=1}^{6} (\frac{\rho C_n}{m_n})^{\nu'_{jn}}],\ k \in [1,6], \quad (1)$$

with $R_j(T)$ being a rate constant modified by the Arrhenius temperature dependence for the forward path of the chemical reaction (ρ , $kg{\cdot}m^{-3}$ is the mixture density)

$$R_j(T) = A'_j T^{\beta_j} \exp(-E_j / RT), \quad (2)$$

where A'_1= 216, A'_2= $0.96{\cdot}10^6$ ($m^3{\cdot}mol^{-1}{\cdot}s^{-1}$) are the reaction rate pre-exponential factors, R = 8.314 ($J{\cdot}mol^{-1}{\cdot}K^{-1}$) is the universal gas constant, $\nu'_{jk} = 1, \nu''_{jk} = 1$ are the stoichiometric coefficients of the k-th species (reactants) in the j-th reaction, $\beta_j = 0$ is the order for temperature, $m_1 = 2$, $m_2 = 17$, $m_3 = 18$, $m_4 = 1$, $m_5 = 28$, $m_6 = 44$ ($g{\cdot}m^{-3}$) are the molecular weights of species. In the equation for the mass fractions of concentration C_k the source term is – $m_k{\cdot}\Omega_k{\cdot}\rho^{-1}$ ($1{\cdot}s^{-1}$), but in the equation for temperature

$$\frac{1}{m\rho c_p} \sum_{k=1}^{6} h_k m_k \Omega_k \ (K{\cdot}s^{-1}), \text{ where } m = \frac{1}{6} \sum_{k=1}^{6} m_k\ , \quad (3)$$

$h_1 = 0$; $h_2 = 39.46$; $h_3 = -242$; $h_4 = 218$; $h_5 = -111$, $h_6 = -394$ ($kJ{\cdot}mol^{-1}$) are the enthalpy of species, $c_p = 1000$ ($J{\cdot}kg^{-1}{\cdot}K^{-1}$) is the specific heat at a constant pressure.

For the mathematical modeling, a system of dimensionless parabolic type partial differential equations was used to describe the formation of the 1D compressible reacting swirling flow, the mass fractions of the flame species and the flame temperature:

$$
\begin{cases}
\dfrac{\partial \rho}{\partial t}+\dfrac{\partial (w\rho)}{\partial x}=e\dfrac{\partial^2 \rho}{\partial x^2}, \\
\dfrac{\partial w}{\partial t}+w\dfrac{\partial w}{\partial x}=-\dfrac{\partial p}{\partial x}+\mathrm{Re}^{-1}\dfrac{\partial^2 w}{\partial x^2}, \\
\dfrac{\partial T}{\partial t}+w\dfrac{\partial T}{\partial x}=\dfrac{P_0}{\rho}\dfrac{\partial^2 T}{\partial x^2}+q_1\rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right)+q_2\rho A_2 \exp\left(-\dfrac{\delta_2}{T}\right)C_2C_5, \\
\dfrac{\partial C_1}{\partial t}+w\dfrac{\partial C_1}{\partial x}=P_1\dfrac{\partial^2 C_1}{\partial x^2}-\rho A_1 C_1 C_2 \exp\left(-\dfrac{\delta_1}{T}\right), \\
\dfrac{\partial C_2}{\partial t}+w\dfrac{\partial C_2}{\partial x}=P_2\dfrac{\partial^2 C_2}{\partial x^2}-\rho A_1 C_1 C_2 \dfrac{m_2}{m_1}\exp\left(-\dfrac{\delta_1}{T}\right)-\rho A_2 C_2 C_5 \exp\left(-\dfrac{\delta_2}{T}\right) \\
\dfrac{\partial C_3}{\partial t}+w\dfrac{\partial C_3}{\partial x}=P_3\dfrac{\partial^2 C_3}{\partial x^2}+\rho A_1 C_1 C_2 \dfrac{m_3}{m_1}\exp\left(-\dfrac{\delta_1}{T}\right), \\
\dfrac{\partial C_4}{\partial t}+w\dfrac{\partial C_4}{\partial x}=P_4\dfrac{\partial^2 C_4}{\partial x^2}+\rho A_1 C_1 C_2 \dfrac{m_4}{m_1}\exp\left(-\dfrac{\delta_1}{T}\right)+\rho A_2 C_2 C_5 \dfrac{m_4}{m_2}\exp\left(-\dfrac{\delta_2}{T}\right), \\
\dfrac{\partial C_5}{\partial t}+w\dfrac{\partial C_5}{\partial x}=P_5\dfrac{\partial^2 C_5}{\partial x^2}-\rho A_2 C_2 C_5 \dfrac{m_5}{m_2}\exp\left(-\dfrac{\delta_1}{T}\right), \\
\dfrac{\partial C_6}{\partial t}+w\dfrac{\partial C_6}{\partial x}=P_6\dfrac{\partial^2 C_6}{\partial x^2}+\rho A_2 C_2 C_5 \dfrac{m_6}{m_2}\exp\left(-\dfrac{\delta_2}{T}\right),
\end{cases}
\tag{4}
$$

where: C_k – mass fractions of the species (H_2, OH, H_2, H CO, CO_2) entering the combustor k = 1(1)6, $x = z/r_0$, $w = u_z/U_0$ are the axial coordinate and the velocity, $P_k = D_k/(U_0 \cdot r_0) = 0.01$, $P_0 = \lambda/(c_p \cdot \rho_0 U_0 \cdot r_0) = 0.05$, $(m_1h_1 + m_2h_2 - m_3h_3 - m_4h_4) / (m_1 \cdot m \cdot c_p \cdot T_0)$, $q_1 = Q_1/ c_p \cdot T_0) = 437$, $q_2 = Q_2/ c_p \cdot T_0) = 157$, $Q_1 = (m_1h_1 + m_2h_2 - m_3h_3 - m_4h_4) /(m_1 \cdot m) = 131 \cdot 10^6$ [J/kg], $Q_2 = (m_2h_2 - m_4h_4 + m_5h_5 - m_6h_6) / (m_2\, m) = 47 \cdot 10^6$ [J/kg] are heat releases for each reaction, $\delta_k = E_k/(R \cdot T_0)$, ($\delta_1 = 5.76$, $\delta_2 = 12.34$) are the scaled activation-energy, $\lambda = 2.5 \cdot 10^{-1}$ [J/(s·m·K)] is the thermal conductivity, $D_k = 2.5 \cdot 10^{-4}$ [m^2/s] is molecular diffusivity of species, $A_1 = A'_1 \rho_0 \cdot r_0 / (U_0\, m^2)$, $A_2 = A'_2 \cdot \rho_0 \cdot r_0/(U_0 \cdot m_5)$, ($A_1 = 6,353$, $A_2 = 1.7143 \cdot 10^7$) are the scaled reaction-rate pre-exponential factors, $\mathrm{Re} = U_0 \cdot r_0 \cdot \rho_0 / \mu = 1,000$ is the Reynolds number, $\mu = 5 \cdot 10^{-6}$ [kg/m· s] is the viscosity, $e = 10^{-5}$ is the factor of the artificial viscosity for approximation of the density. The scaled values are: for the inlet temperature and density $T_0 = 300$ [K], $\rho_0 = 1$ [kg/m^3], for the axial velocity $U_0 = 0.1$ [m/s], for the length $r_0 = 0.05$ [m] (the combustor radius), for time $t_0 = r_0/U_0 = 0.5$ [s].

For the dimensionless pressure p, we use a model for perfect gas: $p = \rho \cdot T$. The boundary conditions at the inlet (x= 0): $\rho = w = T = 1$, $C_3 = C_4 = C_6 = 0$, $C_1 = C_{10}$, $C_2 = C_{20}$, $C_5 = C_{50}$ (depending on pellets). These values are used for the initial conditions at t=0. At the outlet the zero derivatives conditions are used.

The numerical results depending on (x, t) were obtained for $0 < x < 2$, $0 < t < 1$. At the thermo-chemical conversion of the biomass pellets and their mixtures the maximum values of the temperature T_{Max}, axial flow velocity w_{Max}, the mass fractions of the species CO_2, H_2, and the minimal value of the mass fraction of H_2O, CO were obtained during the co-combustion of the 10 % of straw with peat (Figure 4-a,b), where $w_{end} = w(2,1)$, $T_{end} = T(2,1)$. To express the temperature and velocity as the dimensionless values, the multipliers T_0 = 300 K and U_0 = 0.1 m/s were used. In accordance with the data of the experimental study, the increase of the flame temperature, flow velocity and CO_2 mass fraction correlates with the enhanced thermal decomposition of the mixture, indicating the formation of the peak values at 10 % of straw mass load, when the enhanced release of the volatiles was observed (Figure 3). With the constant primary and secondary air supply rates, this led to a decrease of the air excess ratio in the reaction zone from 1.8 to 1.4, with improved the combustion conditions and promoted the complete combustion of volatiles, that is confirmed by the results of mathematical modeling: the mass fraction of the reactants CO, OH decreased to zero at t = 0.5 s. It should be stressed that the enhanced thermal decomposition with the enhanced release of volatiles results in an increase about 12 % of the produced heat energy during the burnout of the mixture.

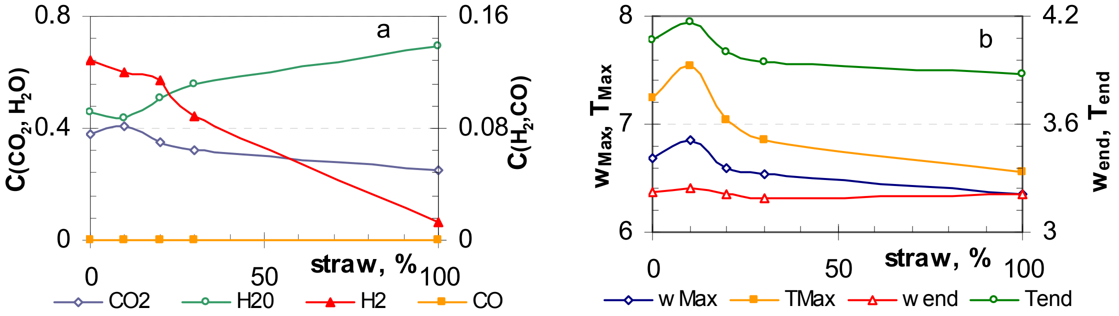

Figure 4. Mathematically calculated effect of the straw mass load at co-combustion with peat on the mass fraction of volatiles (CO, H_2) and main products (CO_2, H_2O) (a), maximum and end values of the axial velocity (w_{Max}, w_{end}), maximum and end values of the temperature (T_{Max},T_{end}) (b).

5. Conclusions

With the aim to achieve a more effective use of straw as a fuel for energy production, the complex experimental study and mathematical modelling of the processes developing at co-combustion of straw with peat were performed.

The results of the experimental study suggest that the development and efficiency of the processes of thermo-chemical conversion at co-combustion of straw with peat are highly influenced by the variations of the mass load of straw in the mixture.

At a mass load of straw up to 20 %, the thermal decomposition of the mixtures and the formation of volatiles are determined by the activation of the thermal interaction between the components, thus improving the combustion conditions, with the positive effect on the main combustion characteristics, heat output from the device and on the products composition.

With a higher mass load of straw in the mixture the thermal decomposition of the mixture and the formation of the volatiles are predominately influenced by the linear decrease of the mixture HHV with the correlating linear decrease of the biomass weight loss rate, volume fraction of the volatiles entering the combustor determining thus the negative effect of straw on the combustion characteristics.

Acknowledgments

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