MATHEMATICAL MODELING OF GASIFICATION AND COMBUSTION OF BIOMASS IN MATLAB

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Abstract

This paper deals with the mathematical modeling of biomass gasification and combustion. It begins with an analysis of biomass as an alternative fuel; e.g. its distribution, composition, caloric value etc., and as processes taking place with the biomass gasification and combustion.

The programming environment for the modeling of technological processes is also analyzed. There are various programming environments with which the tasks can be examined and the results visualized. MATLAB is among the most suitable environments for the creation of simulation models. It allows the implementation of various data types; it also provides the right environment for model formation and also provides a library for the solution of various mathematical tasks for example calculating a system of differential equations. MATLAB provides a refined input/output graphical interface for the creation of simulation environments.

The idea for a complex model for the gasification and combustion of biomass is derived from the initial process analyses, which was suggested as a synthesis of elementary process models. The synthesis is possible because of the basic thermal exchange between biomass and gas elements. It is based on the accumulation of heat which is relative to the difference between input and output heat flow created by the source or heat consumption. In the case of elementary models the following models are described; heating model, drying model, thermal breakdown model, oxidation of the solid element model and oxidation of gas element model. The heating model is based on the process of heat accumulation and the transfer of heat by convection. The basis of the evaporation model is the model for the transformation of liquid water into steam. This process requires heat consumption relative to the rate of evaporation. The remaining three models include thermal breakdown of biomass, release of gasses and the burning of the solid by product.

Elementary process models were independently implemented and verified in a MATLAB environment as individual m-functions. The result of which is the m-function library.

The results from the simulation of elementary processes are also stated in this paper. The results are analyzed and further possible uses and methods are suggested for the utilization of model gasification and combustion.

1 Introduction

Energy consumption has increased because of the growth of the Earth's population. It is for this reason that we need to find new energy resources that will have less impact on the environment and the population. One such resource is biomass. Biomass is a renewable resource produced by the Sun which makes it infinite. It can be divided into plant mass (wood biomass – woods and phytomass – young plants) and animal mass (zoomass). By biomass we mean wood, straw, organic farm waste, parts of communal waste as well as artificially grown energetic plants [2].

Among the elements found in biomass are nitrogen, phosphor, sulphur, kalium, sodium, chlorine, calcium, magnesium, iron, copper, arsenic, lead and other elements which make their way into the biomass during its growth as it absorbs nutrients from the soil and air. From a physical point of view the water contained in biomass can be divided into free water and locked water. The quality of the fuel as a resource depends on the quality combustibles and the ballast content – moisture and ash.

Wood biomass is characteristic with a high moisture content and volatile fuel, low coal content, low ash content and low sulphur content. This means that the heating capacity of wood biomass by combustion depends on the amount of moisture, the more moist the less the heating power. The heating power of relatively dry and healthy wood is very high, with deciduous trees it is 18 MJ.kg^{-1}, with coniferous trees it is 19 MJ.kg^{-1}. This relation of heating power and moisture is demonstrated in Fig. 1 [1, 2]:
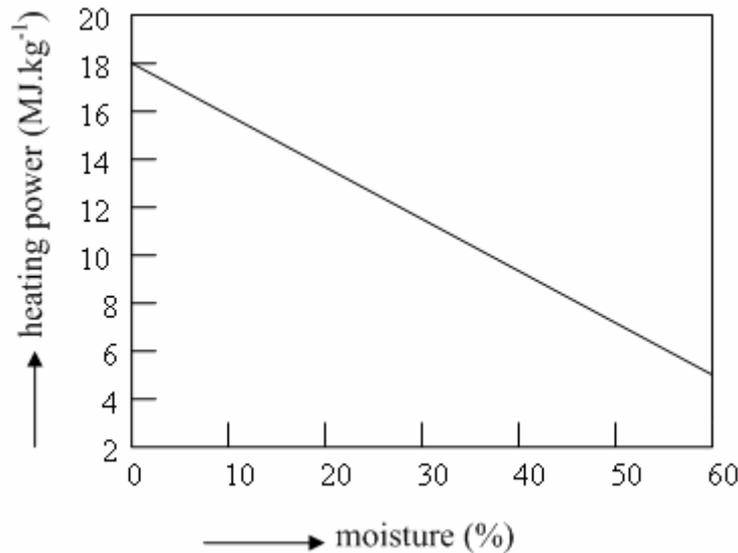
Figure 1: Dependence of the heating power of wood biomass and moisture content [1]

The mathematical model is based on the similarities between real and abstract systems which enable the study of real systems using abstract systems with mathematical relations. We can describe the system using mathematical relations

Various programming environments or languages can be used for the implementation of mathematical models with which it is possible to express the mathematical relations of the system with a mathematical model. After evaluating many of the programming environments MATLAB was chosen for its complexity and suitability for the creation of a mathematical model [4, 11, 14, 15].

2   Gasification process of biomass

Gasification is a process in which flammable gasses like hydrogen, carbon monoxide, methane and some inflammable products are produced. The whole process takes place with the incomplete combustion and heating of biomass with the heat produced during combustion. The resulting mixture of gasses has a high energy value and can be used as a gas fuel both in the production of heat and electricity and in automobiles.

Gasification of biomass is a process during which the chemical energy of a solid fuel transforms the biomass into a chemical and heat energy gas fuel. The gasification of biomass is an automatic process during which heat for endothermic gas reactions is obtained from the combustion of some of the biomass with a deficiency of combustible air at a certain temperature. Oxygen, water vapour or carbon dioxide can also be used as a medium. Any type of biomass that does not have very high moisture content can be used in the gasification process. This means that the amount of heat to evaporate the moisture in 1kg of biomass is less than the heating power of 1kg of fuel. The main product from the gasification of biomass is synthesis gas – wood gas, made up mainly of carbon monoxide and dioxide, hydrogen, methane, water vapour, nitrogen and contaminants. The composition of this synthesis gas depends not only on the type of biomass gasification used but also on the type of combustion.

During the gasification of biomass chemical reactions are produced identical to those produced with the gasification of coal, the following process take place in the reactor [1]:

- drying,

- pyrolysis (dry destillation),
- oxidation – combustion,
- reduction.

3 Combustion process of biomass

Combustion is an oxidation process in which flammable components of fuel are oxidized by oxygen whereby the energy content of the fuel is changed into heat. Biomass combustion products are ash, tar, and burnt gases.

The technology of direct combustion of biomass is the most common way its energy is used. It is a verified method and commercially available on a high level. The heat generated is used as a resource in technological processes (process heat) or for the production of electrical energy. For effective combustion a sufficiently high temperature must be present, enough air and enough time for complete combustion of the biomass [1].
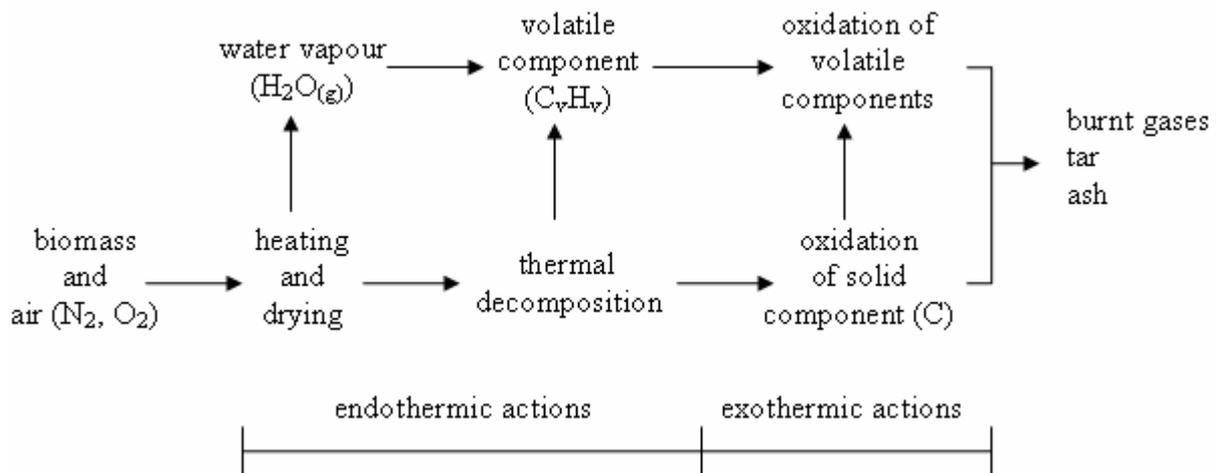
Figure 2: Processes occurring during the combustion of biomass

4 Suggestion of mathematical model

During the initial creation of a mathematical model an analyses of individual partial models was performed and the processes occurring in them. Each of the models were assigned input and output parameters.

An input and output for the model of heating wood biomass is the wood biomass itself and the burnt gases resulting from the combustion used for heating wood biomass. The heating model is based on processes of accumulation of heat and heat transfer by convection.

The following equation is a valid example for the process of heat transfer by convection

$$I_Q = k_S.S.\left(T_{den} - T_{sp}\right) \quad \text{(W)} \tag{1}$$

where I_Q is heat flux (W), k_S – exchange coefficient (W.m^{-2}.K^{-1}), S – wall surface (m^2), T_{den} – wood biomass temperature (K), T_{sp} – burnt gases temperature (K).

In the case of the process of heat accumulation the amount of accumulated heat is proportional to the temperature change according to this equation

$$\frac{dQ}{d\tau} = m.c.\frac{dT}{d\tau} \quad \text{(W)} \tag{2}$$

where Q is the volume of thermal energy (J), m – weight (kg), c – specific heat capacity (J.kg^{-1}.K^{-1}), T – temperature (K), τ – time (s).

The water evaporation model immediately follows on the model of heating because the evaporation can take place or intensively take place only after prior heating.

The basis for the water evaporation model is the process of transforming liquid water into water vapour according to the equation

$$H_2O_{(l)} \rightarrow H_2O_{(g)} \tag{3}$$
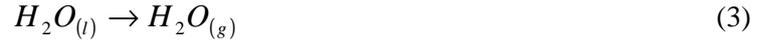
The thermal decomposition model of wood biomass follows on the heating model and water evaporation model. Thermal decomposition occurs after the evaporation of water and subsequent increase of temperature to 300 °C.

Combustion models of volatile components and of solid components are based on the thermal decomposition model of wood biomass. Volatile components are released in a range of temperature from 260 to 410 °C. The combustion of solid components occurs in a temperature range from 400 to 500 °C.

Due to the suggested solution it was also necessary to create a static combustion model, which included the following calculations, e.g. the calorific value of fuel (wood biomass), theoretical, respectively, minimum amount of air needed for combustion of fuel based on the chemical composition of the fuel or from the given calorific value of the fuel, subsequently the calculation of the amount of dry and moist smoke gases. The static model included in addition to these calculations also other auxiliary calculations such as the calculations of atmospheric humidity of the air, the pressure of saturated water vapours, etc.

Based on a detailed analysis of individual models energy balance equations were created, the resultant shape of which represents a system of two first order differential equations, namely for the wood biomass and gaseous component

$$\frac{dT_{10}}{dt} = \frac{I_{V1}}{V_1}T_1 - \frac{I_{V10}}{V_1}T_{10} - \frac{k_S.S}{\rho_1.c_{p1}.V_1}(T_{10}-T_{20}) + \frac{m_{H_2O}.T_{20}.c_{P\,H_2O}}{\rho_1.c_{p1}.V_1} + \frac{m_{prch}.T_{20}.c_{P\,prch}}{\rho_1.c_{p1}.V_1} +$$
$$+ \frac{I_{V\,pl}.H}{\rho_1.c_{p1}.V_1} \tag{4}$$

$$\frac{dT_{20}}{dt} = \frac{I_{V2}}{V_2}T_2 - \frac{I_{V20}}{V_2}T_{20} + \frac{k_S.S}{\rho_2.c_{p2}.V_2}(T_{10}-T_{20}) - \frac{m_{H_2O}.T_{20}.c_{P\,H_2O}}{\rho_2.c_{p2}.V_2} - \frac{m_{H_2O}.H_{H_2O\,odp}}{\rho_2.c_{p2}.V_2} -$$
$$- \frac{m_{prch}.T_{20}.c_{P\,prch}}{\rho_2.c_{p2}.V_2} - \frac{m_{prch}.H_{prch}}{\rho_2.c_{p2}.V_2} + \frac{m_{spal}.H_T}{\rho_2.c_{p2}.V_2} \tag{5}$$

where

I_{V1}	– incoming flow volume of gas	$(m^3.s^{-1})$
T_1	– incoming gas temperature	(K)
ρ_1	– gas density	$(kg.m^{-3})$
c_{p1}	– specific heat capacity of gas	$(J.kg^{-1}.K^{-1})$
V_1	– volume of gas	(m^3)
I_{V10}	– outgoing flow volume of gas	$(m^3.s^{-1})$
T_{10}	– outgoing gas temperature	(K)
I_{V2}	– incoming flow volume of wood biomass	$(m^3.s^{-1})$
T_2	– incoming wood biomass temperature	(K)
ρ_2	– wood biomass density	$(kg.m^{-3})$
c_{p2}	– specific heat capacity of wood biomass	$(J.kg^{-1}.K^{-1})$

V_2	– wood biomass volume	(m^3)
I_{V20}	– outgoing flow volume of wood biomass	$(m^3.s^{-1})$
T_{20}	– outgoing wood biomass temperature	(K)
m_{H_2O}	– volume of evaporated water	$(kg.s^{-1})$
c_{pH_2O}	– specific heat capacity of water	$(J.kg^{-1}.K^{-1})$
m_{prch}	– volume of volatile components	$(kg.s^{-1})$
$c_{p\,prch}$	– specific heat capacity of volatile components	$(J.kg^{-1}.K^{-1})$
$H_{H_2O_{odp}}$	– evaporation heat of water	$(J.kg^{-1})$
H_{prch}	– decomposition heat of volatile components	$(J.kg^{-1})$
m_{spal}	– volume of burnt gases formed from the solid component	$(kg.s^{-1})$
$I_{V\,pl}$	– flow volume of volatile combustible component	$(m^3.s^{-1})$
H	– heating value of volatile combustible component	$(J.kg^{-1})$
H_T	– heating value of solid component	$(J.kg^{-1})$
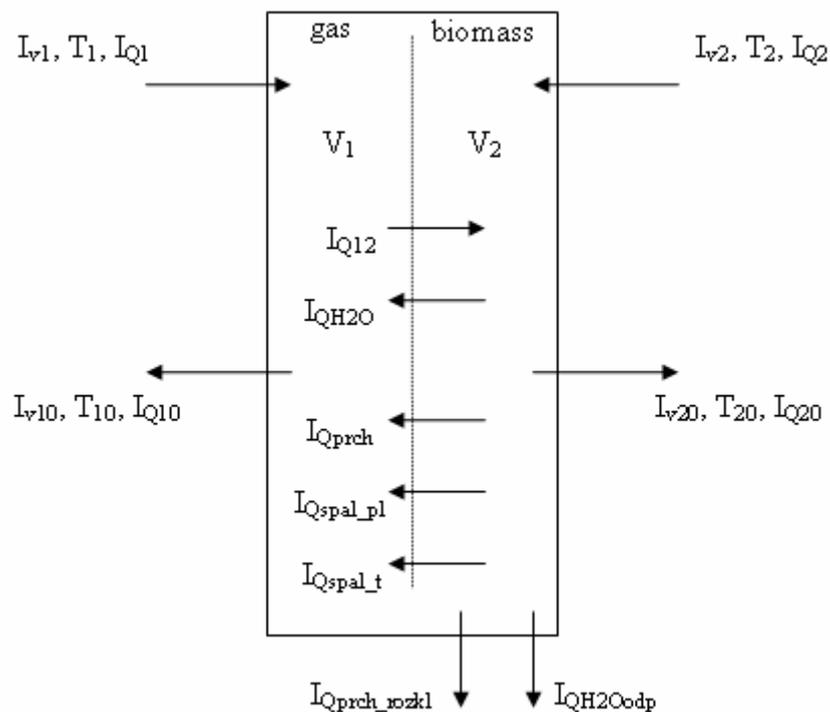
Figure 3: Diagram showing the overall combustion model and gasification of biomass

5 Implementation

Models of elementary processes of the gasification and combustion of biomass have been implemented in the programming environment MATLAB. Implementation was carried out for the static combustion model, heating model, water evaporation model and thermal decomposition model.

The static combustion model of wood biomass consists of individual calculations, which are implemented as functions. For example a function for the calorific value of burned fuel, a function for calculating the amount of oxygen from the chemical fuel composition, a function to calculate the

amount of dry air from the chemical composition of the fuel or calorific value, a calculation of saturated water vapor pressure, a calculation of the moisture of atmospheric air, and so on. Functions are available as Combustion toolbox on Matlab File Exchange [16].

Heating model is represented by the function *heating*. Function declaration with its inputs and outputs

```
function [tau, out]= heating (in, alfa, surface, time)
```

Evaporation model was realized by the function *heating_drying* which is based on the function *heating*, completed with the variables *T10p, T20p, k, kp* needed for evaporation. Function declaration

```
function [tau, out]= heating_drying (in, T10p, T20p, alfa, k,
                            kp, surface, time)
```

Thermal decomposition model was performed by the function *heating_drying_thermal1* which is based on the function *heating_drying*. The header of this function has the following form

```
function [tau, out]= heating_drying_thermal1 (in, T10p, T20p, alfa,
                        k, kp, surface, time)
```

The following inputs are in these functions

`in`	– structure consist of inputs	-
`T10p`	– initial gas temperature	(K)
`T20p`	– initial wood biomass temperature	(K)
`alfa`	– exchange coefficient	$(W.m^{-2}.K^{-1})$
`k`	– evaporation velocity	$(kg.m^{-2}.s^{-1})$
`kp`	– reaction velocity of decomposition	$(kg.m^{-2}.s^{-1})$
`surface`	– wall surface	(m^2)
`time`	– simulation time	(s)

and outputs

`tau`	– temperature	(K)
`out`	– structure of outputs	-

The variable `in` has the following structure in the source file

$\quad$ `in(1).value` – for 1st input value (gas)

$\quad$ `in(2).value` – for 2nd input value (wood biomass)

The variable `out` has the following structure

$\quad$ `out(1).T(i) = T(i,1);` – output 1

$\quad$ `out(2).T(i) = T(i,2);` – output 2

The part of sample calling of function *heating_drying_thermal1*

```
in(2).T      = 20 + 273.15;   % temperature                [K]
in(2).V      =       0.106;   % volume  2                  [m^3]
in(2).W      =        0.20;   % hmot.podiel W - humidity    [kg.kg^-1]


count = 1200;
T1p= 400 + 273.15;
T2p= 20 + 273.15;


for i=1:count

in(1).ro     =       1.200;   % density  1                 [kg.m^-3]
in(1).cp     =      1012.0;   % specific heat capacity   [J.kg^-1.K^-1]
in(1).V      =        1.06;   % volume  1                  [m^3]
in(1).Iv     =       0.375;   % flow                      [m^3.s^-1]
in(1).T     =400 + 273.15;    % temperature                [K]
in(2).ro     =       470.0;   % density  2                 [kg.m^-3]
in(2).cp     =      1800.0;   % specific heat capacity   [J.kg^-1.K^-1]
in(2).Iv     =         0.0;   % flow                      [m^3.s^-1]
alfa         =       300.0;   % exchange coefficient      [W.m^-2.K^-1]
surface      =        1.34;   % wall surface               [m^2]
time         =           1;   %                            [s]
k            =      k_H2O(T2p);
kp           =      k_vap(T2p);


[tau, out]  = heating_drying_thermal1 (in, T1p, T2p, alfa, k, kp, surface,
time);


in(2).T      = out(2).T(end);   % temperature              [K]
in(2).V      = out(2).V;         % volume                   [m^3]
in(2).W      = out(2).W;         % humidity                 [m^3.s^-1]
T1p          = out(1).T(end);
T2p          = out(2).T(end);


nn = length(tau);
for j=1:nn
tauc((i-1)*nn+j)     = (i-1)*time + tau(j);
Temp1((i-1)*nn+j)    = out(1).T(j);
Temp2((i-1)*nn+j)    = out(2).T(j);
end
end


figure(1);


plot(tauc,Temp1-273.15,'r');
hold on
plot(tauc,Temp2-273.15,'b');
xlabel('time / s');
ylabel('temperature / oC');
grid;
```

6 Simulations

Simulations with the different values of inputs were made with the individual partial models.

The first simulation was static combustion and then it was compared with values of literature. Simulations were done for two kinds of wood, spruce and oak. Calculations were done using file *Test.m*. Two types of calculations were chosen for both kinds of wood. The first one was done in terms of elemental composition of wood and the second one in terms of theoretical calorific value of particular kinds of wood from [9]. Subsequently a percentage difference between the theoretical and calculated calorific value of wood was established. Although the results of the simulations were not in close agreement with literature values, they fulfilled the given interval for the heating capacity of wood, whose maximum value is 19 MJ.kg^{-1}. The simulations showed that the proposed static model has been designed correctly.

Simulations of the heating model were realized for spruce weighing 50 kg. Simulations were done for values of input parameters α=300 W.m^{-2}.K^{-1}, V_{vzd}= 1,06 m^3, T_{vzd}=120 °C, for time 60 s, 600 s and 3000 s, and other values α, V_{vzd} and T_{vzd}. The fastest leveling off of temperatures between wood biomass and air occurred at a value α = 450 W.m^{-2}.K^{-1} in a time of 1950 s (Fig. 4). The resulting values of the simulations show that with increasing value of α leads to more rapid stabilization of temperatures.
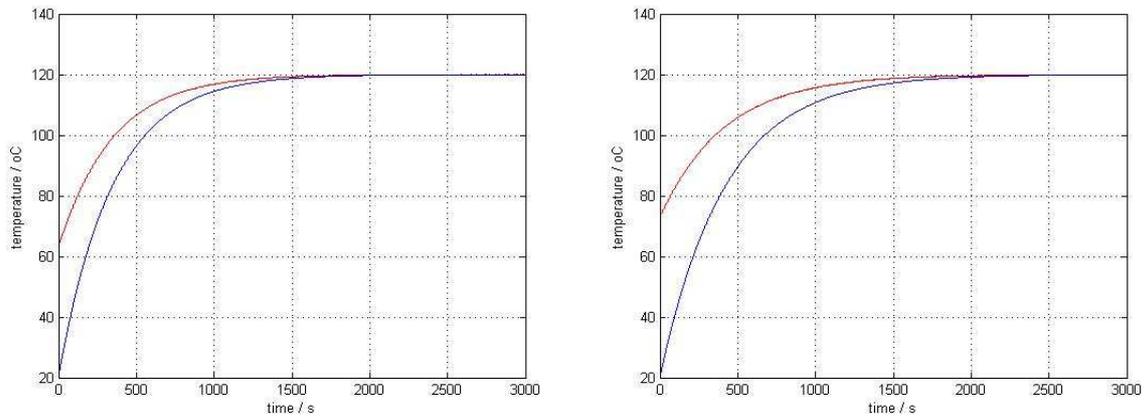
Figure 4: Heating a) *α=450 W.m^{-2}.K^{-1}, V_{vzd}=1,06 m^3*, b) *α=300 W.m^{-2}.K^{-1}, V_{vzd}=0,53 m^3*

Temperature stabilization at 120 °C and α = 300 W.m^{-2}.K^{-1} occurs with an air volume of V = 0,53 m^3 in a time of 2370 s.

An initial simulation with zero velocity of evaporation was made to compare the curves of model simulations of this evaporation. Simulation time was set at 900 s. The course of the simulation is shown in Fig. 5 a). Another simulation was made using trapped evaporation using the theoretical evaporation with a 100 % higher velocity of evaporation Fig. 5 b).
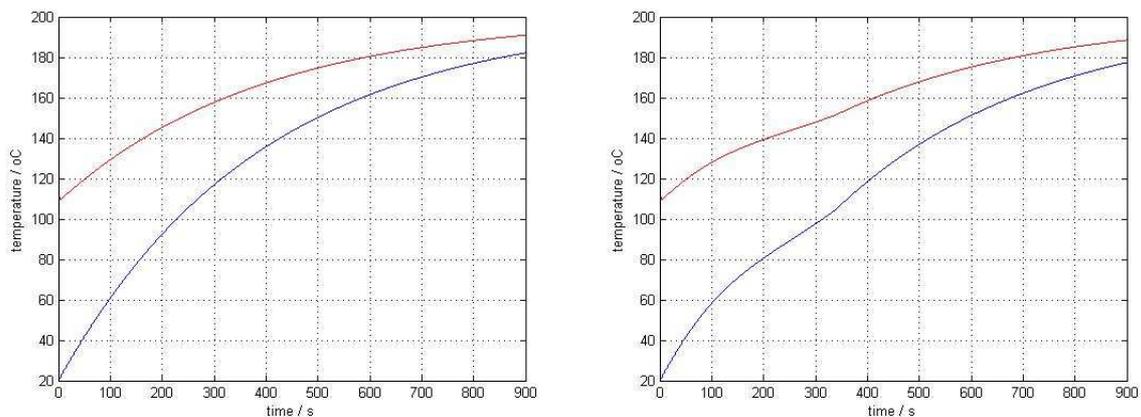
Figure 5: Simulation process a) without evaporation of water, b) with evaporation of water with 100 % higher velocity

From the simulation process in Fig. 5 b) with approximately a 100 % higher velocity the different evaporation rate of water compared with the first process is clear (Fig. 5 a)). In section from 60 °C to 110 °C the increase in the temperature of the biomass was slowed which is caused by evaporation of water from it.

A further four simulations were done. The individual simulation processes were done without thermal decomposition and with it, and also without evaporation of water and thermal decomposition, and with them.

From the curves in Fig. 6 a) and Fig. 6 b) it can be seen that under thermal decomposition the increase in the temperature of the biomass and the gas increases, this is caused by the consumption of heat for thermal decomposition.
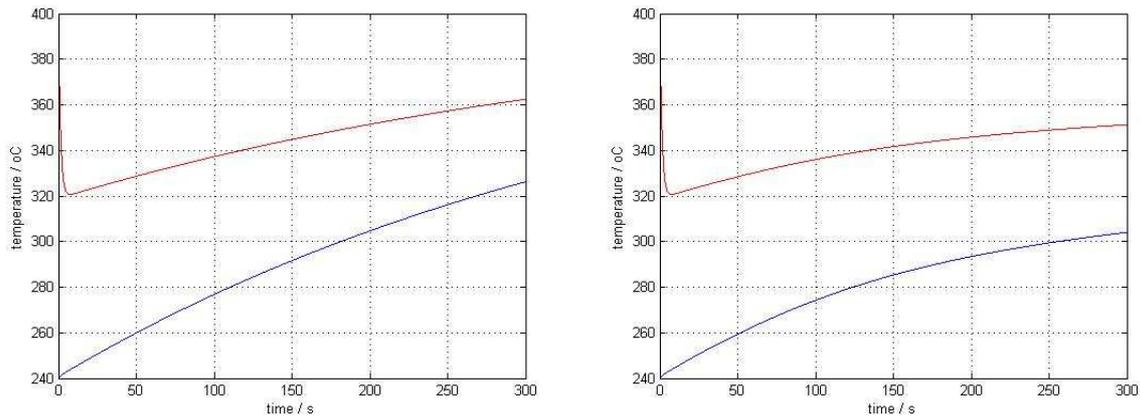
Figure 6: Simulation process a) without thermal decomposition, b) with thermal decomposition
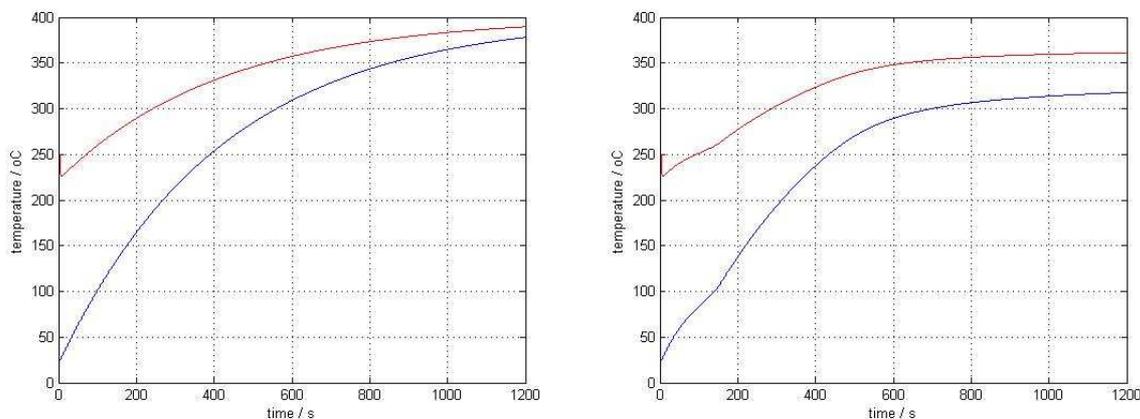
Figure 7: Simulation process a) without evaporation and thermal decomposition, b) with evaporation and thermal decomposition

In Fig. 7 a) and Fig. 7 b) are mentioned complete simulations which were brought about by the association of the three partial models. In the first case (Fig. 7 a)) we disregard the evaporation and thermal decomposition. In the second case (Fig. 7 b)) they are taken into account and the evaporation and thermal decomposition is obvious.

7 Conclusion

Biomass represents a complete alternative to fossil fuel resources.

The purpose of this work has been to create a mathematical model of the combustion and gasification of biomass and to verify its functionality. The results of simulations from three partial models, namely from heating model, evaporation model and thermal decomposition model are listed in this work. Besides these models a model of static combustion has also been created which is an inseparable part in creating a model for the combustion of biomass. A wide range of simulations were

implemented that show the qualitative consistency of the model with real processes. Results of the experiments with the model were compared with literature that was available. It is such a calorific value of biomass for the given type.

Created partial models can be used for process simulations of heating, evaporation and thermal decomposition in terms of analysis of the processes and the study of the impact various parameters have on the partial processes.

Acknowledgement

References

[1] KLENOVČANOVÁ, Alexandra – IMRIŠ, Ivan: Zdroje a premeny energie, Edícia vedeckej a odbornej literatúry – Strojnícka fakulta TU v Košiciach, 2006. 492 s. ISBN 80-89040-29-2

[2] PASTOREK, Zděnek – KÁRA, Jaroslav – JEVIČ, Petr: Biomasa obnoviteľný zdroj energie, FCC PUBLIC, 2004. 288 s. ISBN 80-86534-06-5

[3] TERPÁK, J. – DORČÁK, Ľ. - PALENČÁR, V.: Modelling the gas fuel combustion using Matlab. In: ICCC'2008. – Craiova: University of Craiova, 2008 P. 679-682. - ISBN 9789737468970

[4] Špeciálne jazykové prostriedky počítačov – SJPP: [cit 2008-03-10]. Available from: <http://www.kirp.chtf.stuba.sk/~cirka/vyuka/matlab/kap1.php#sec>.

[5] Humusoft: COMSOL Multiphysics: [cit 2008-03-10]. Available from: <http://www.humusoft.cz/femlab/indexcz.htm>.

[6] Technická univerzita vo Zvolene: [cit 2009-03-15]. Available from: www.tuzvo.sk/files/DF/katedry_df/kchcht/SYMPO/Vladarova.ppt

[7] TRNKA, J. – URBAN, J.: Spaľovacie motory, Bratislava: Alfa, 1992. ISBN 80-05-01081-8

[8] Tepelné vlastnosti dreva: [cit 2009-02-15]. Available from: <http://wood.mendelu.cz/cz/sections/Props/?q=node/49>.

[9] Palivové drevo – Tabuľky: Update 01-10-2008 [cit 2009-04-20]. Available from: <http://drievko.sk/index.php?option=com_content&task=view&id=19&Itemid=60>.

[10] NOSKIEVIČ, Petr: Modelování a identifikace systému, MONTANEX a.s., 1999. 276 s. ISBN 80-7225-030-2

[11] KARBAN, Pavel: Výpočty a simulace v programech Matlab a Simulink, Brno: Computer Press, a.s, 2006. 220 s. ISBN 80-251-1301-9

[12] KUNEŠ, Josef - VAVROCH, Otakar - FRANTA, Václav: Základy modelování. Praha: 1989. SNTL.

[13] MIKLEŠ, Ján - FIKAR, Miroslav: Modelovanie, identifikácia a riadenie procesov I.: Modely a dynamické charakteristiky spojitých procesov. Bratislava: STU, 1999. ISBN 80-227-1289-2

[14] DOŇAR, B. – ZAPLATÍLEK, K.: Matlab - tvorba uživatelských aplikací 2. díl, Ben, 2004, s.216, ISBN 80-7300-133-0

[15] BARTKO, R. – MILLER M.: MATLAB I.: algoritmizácia a riešenie úloh 2. vydanie, Trenčín: DIGITAL GRAPHIC, 2005, s.290, ISBN 80-969310-0-8

[16] Combustion toolbox - File Exchange - MATLAB Central: Update 04-10-2011 [cit 2011-10-05]. Available from: <http://www.mathworks.com/matlabcentral/fileexchange/26492-combustion-toolbox>

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