

Experimental and Numerical Studies on Integrated Gasification and Combustion of Biomass

Monika Abricka^a, Inesa Barmina^a, Raimonds Valdmanis^a, Maija Zake^{*a}, Harijs Kalis^b

^aInstitute of Physics, University of Latvia, Salaspils, 32 Miera Street, LV-2169, Latvia

^bInstitute of Mathematics and Informatics, University of Latvia, Riga, 29 Raina boulevards, LV-1459, Latvia
 mzfi@sal.lv

Mathematical modelling and numerical simulation of second-order reaction kinetics for fast and slow exothermic reactions has been applied with the aim to estimate the development of composition and temperature profiles downstream of the flame reaction zone. The effects of slow and fast exothermic reactions on the formation of the flame composition and temperature profiles are specified and analysed with account of the combustion of CO and H₂. The effect of the reaction rates on the formation of the flame reaction zone is estimated by comparing the results of numerical simulation with the results of experimental study to assess the main factors controlling the combustion characteristics at gasification and combustion of biomass. An experimental study of the two-stage process of biomass thermo-chemical conversion was conducted using a pilot device with an integrated biomass gasifier and a water-cooled combustor. The primary stage of biomass thermal decomposition provides the formation of an axial flow of product gas entering the combustion section from the gasification section. The secondary swirling air provides mixing of the axial flow of combustible gas with the swirling air flow and initiates the formation of a reaction zone downstream the combustor. The complex local measurements of temperature and composition at different stages of biomass thermo-chemical conversion confirm a faster burnout of hydrogen downstream of the flame reaction zone, determining the dominant combustion of combustibles at the primary stage of the swirling flame formation.

1. Introduction

Understanding the effect of inlet swirl on the development of swirling flow field and combustion dynamics during biomass gasification and combustion is important because swirling flows may affect stabilization of combustion dynamics due to the formation of a toroidal recirculation zone (Gupta et al., 1984), which provides enhanced mixing of the flame components improving combustion conditions and completing fuel combustion (Driscoll et al., 2011). Flame stabilization and control of the combustion characteristics is very important if different biomass types with dissimilar elemental and chemical composition are used as a fuel. The process of biomass thermo-chemical conversion starts with thermal decomposition of biomass particles producing a fuel-rich flow of the main combustible gases (CO, H₂). The axial flow of combustible gases must be perfectly mixed with the air to provide their complete combustion (Houshfar, 2012). Flame stabilization was found to depend on the air co-flow swirl strength (Saediamiri et al., 2014) promoting the combustion with recirculation of heat and chemically active species, which enhances fuel ignition and combustion. The investigations of swirling flows with secondary swirling air supply at the bottom of the combustor provide evidence that the development of combustion dynamics can be affected by air swirl reversing determining the formation of an upstream air swirl (Abricka et al., 2014). The upstream air swirl provides enhanced mixing of the axial flow of combustible gases with the air close to the biomass layer by enhancing their ignition and combustion and by varying the development of the main flame characteristics downstream of the reaction zone. A specific objective of the presented paper is the study of the development of flame composition and temperature profiles with accounting for slow and fast second - order chemical reactions developing at thermal decomposition of biomass and at the combustion of CO and H₂. A mathematical model has been developed for numerical study of the effect of slow and fast exothermic chemical reactions on the formation of flame composition and

temperature profiles. Boundary conditions are specified considering the characteristic parameters of the experimental device, which allow comparison of the results of numerical simulation with the results of experimental study. The main factors controlling the combustion dynamics of swirling flame flow at biomass gasification and the combustion of CO and H₂ are estimated and analyzed.

2. Experimental

The development of combustion dynamics at biomass (wood pellets) gasification and combustion of gases released from thermal decomposition of biomass was studied experimentally using a small-scale pilot device (Barmina et al., 2015). The main parts of the pilot device are: a biomass gasifier (1), which is filled with biomass pellets with a total mass of 250 g and the sections of the combustor (2) of inner diameter $D = 60$ mm and total length up to $L = 900$ mm, downstream of which the dominant burnout of the combustible gases develops (Figure 1). Additional heat energy is supplied by propane flame flow (3) with the average rate 1-1.2 kJ/s into the upper part of the biomass to initiate thermal decomposition of the biomass pellets. The primary air at the average axial mass flow rate 0.4 g/s is supplied below the biomass layer (4) to support the process of biomass gasification which develops under fuel-rich conditions $\alpha = 0.3-0.5$ with the average biomass weight loss rate 0.15-0.2 g/s. The biomass gasification produces the axial flow of combustible gases with the typical composition: 20 % CO, 20 % H₂ and 2 % CH₄. The swirling air supply above the biomass layer (5) at the average mass flow rate 0.8-0.9 g/s initiates the swirl-enhanced mixing of the axial flow of volatiles with the air determining thus the development of the slow and fast reactions at chemical conversion of combustible gases downstream of the combustor at the average air excess ratio $\alpha = 1.3-1.5$.

The experimental study of the thermo-chemical conversion of biomass pellets complexly combines the local measurements (6, 7) of the flame composition and temperature. The flame composition was measured online using a gas analyzer Testo 350 XL. Pt/Pt-Rh thermocouples were used for the local online measurements of the flame temperature using a data recording PicoLog – 1012 plate. The online measurements of the main parameters were made with an average accuracy up to ± 5 %. The average values of all parameters were estimated from 30 measurements.

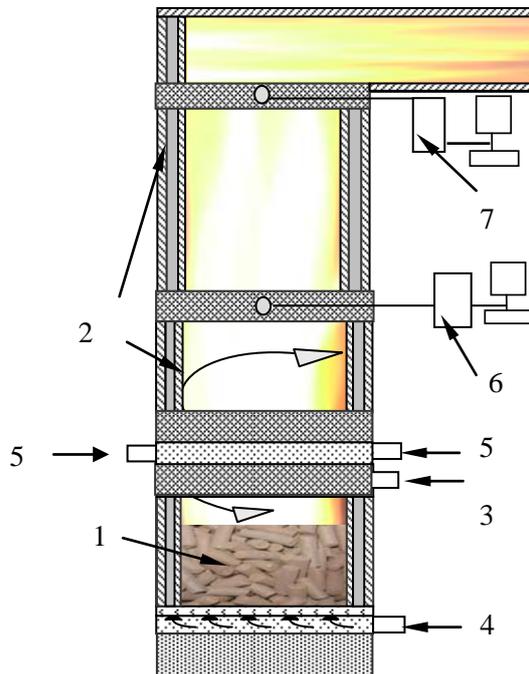


Figure 1: The batch-size experimental device for experimental study of biomass thermo-chemical conversion: 1. - gasifier; 2. - water-cooled sections of the combustor; 3. - primary air supply; 4. - secondary swirling air supply; 5. - propane flame inlet; 6., 7. - diagnostic tools.

3. Mathematical modeling

Mathematical modelling of the combustion processes downstream of the combustor of radius $r' = r_0$ and length $z = z_0$ was performed using a diffusion approximation considering the development of two (fast and slow) exothermic second-order reactions and the Arrhenius equation describing the temperature dependence of reaction rates (Kalis et al., 2015). With this approximation, the mathematical model for swirling flow (Choi et al, 2007) reduces to a system of three dimensionless non-linear partial differential equations:

$$\begin{aligned} \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial x} &= \frac{Le}{\rho Pe} \Delta T + \beta_1 A_1 C_1 \exp\left(-\frac{\delta_1}{T}\right) + \beta_2 A_2 C_2 \exp\left(-\frac{\delta_2}{T}\right), \\ \frac{\partial C_1}{\partial t} + u \frac{\partial C_1}{\partial r} + w \frac{\partial C_1}{\partial x} &= \frac{1}{\rho Pe} \Delta C_1 - A_1 C_1 \exp\left(-\frac{\delta_1}{T}\right), \\ \frac{\partial C_2}{\partial t} + u \frac{\partial C_2}{\partial r} + w \frac{\partial C_2}{\partial x} &= \frac{1}{\rho Pe} \Delta C_2 - A_2 C_2 \exp\left(-\frac{\delta_2}{T}\right). \end{aligned} \quad (1)$$

Where: $Pe = \rho_0 U_0 r_0 / D$, $Le = \lambda / (c_p D)$ ($\rho_0 = 1$ [kg/m³], $U_0 = 0.01$ [m/s], $r_0 = 0.05$ [m], $D = 5 \cdot 10^{-5}$ [m²/s], $c_p = 1000$ [J/(kg·K)], $\lambda = 5 \cdot 10^{-2}$ [J/(m·K·s)]), Pe and Le are, respectively, the Peclet and the Lewis numbers; C_1 and C_2 are the corresponding mass fractions of the two reactants; $T|_{r=0} = T_0 = 300$ [K] ($T = T'/T_0$); $B_1 = 1.5 \cdot 10^6$, $B_2 = 0.15 \cdot 10^6$ [J/kg]; $A_1 = 10^4$, $A_2 = 10^6$ [1/s] ($A = A' r_0 / U_0$); $E_1 = 2.5 \cdot 10^4$, $E_2 = 5 \cdot 10^4$ [J/mol] are the corresponding initial temperature, specific heat releases, the reaction-rate pre-exponential factors, and the activation energies for two reactions; $\beta_1 = 5$, $\beta_2 = 0.5$ ($\beta = B / (c_p T_0)$) are the dimensionless heat release parameters, $\delta_1 = 10$, $\delta_2 = 20$ are the scaled activation energies ($\delta = E / (R T_0)$; $R = 8.314$ [J/(mol·K)]); $\rho = 1/T$; and $x = z/r_0 \in [0, 2]$ ($x_0 = 2$), $r = r'/r_0 \in [0, 1]$.

The approach seeks a steady solution as the time asymptotic limit of the solutions of the unsteady equations. Discrete problems were solved with the finite difference and Douglas and Rachford (Douglas et al. 1956) ADI methods using uniform grid 80x160 in the space.

For the 1D reaction-diffusion equation 2 ($w = 0$, $T = T(x)$, $C_1 = C_1(x)$, $C_2 = C_2(x)$, $x \in [0, 2]$) with BCs $T(0) = 1$,

$$C_1(0) = 0.8, C_2(0) = 0.2, \frac{\partial T(2)}{\partial x} = \frac{\partial C_2(2)}{\partial x} = 0 \quad (r_1 = r_0 = \infty),$$

and summarizing the equations yield: $Le T''(x) + \beta_1 C_1''(x) + \beta_2 C_2''(x) = 0$, $Le T'''(x) = -\beta_1 C_1'(x) - \beta_2 C_2'(x)$ and, in the limit case, we obtain that the maximum temperature is $T(x_0) = 1 + \frac{\beta_1 C_1(0) + \beta_2 C_2(0)}{Le}$. Using the Matlab solver "bvp4c" it was also found that an increase in axial velocity results in an increase in maximum value of the temperature for $Le > 1$ and in a decrease for $Le < 1$.

4. Results and discussion

4.1 Results of numerical simulation

For numerical simulation the boundary conditions (BCs) are the following:

- 1) along the axis of the combustor $r = 0$: $\frac{\partial T}{\partial r} = \frac{\partial C_k}{\partial r} = 0$ (symmetry conditions);
- 2) at the wall of the combustor $r = 1$: $\frac{\partial T}{\partial r} + Bi(T - 1) = \frac{\partial C_k}{\partial r} = 0$;
- 3) at the combustor outlet $x = x_0$: $\frac{\partial T}{\partial x} = \frac{\partial C_i}{\partial x} = 0$;
- 4) at the combustor inlet $x = 0$: $u = 0$, $w = T = 1$, $C_1 = 0.8$; $C_2 = 0.2$; $r \in [0, r_1]$; $u = w = 0$, $T = 0.5$, $C_1 = C_2 = 0$, $r \in [r_1, 1]$ - uniform jet flow by $r < r_1$, $x \in [0, x_0]$ and both reactants by $r < r_1$, $x = 0$; here $i = 1, 2$, $Bi = \frac{hr_0}{\lambda} = 0.1$ ($h = 0.1$ [J/(s²·K)]) is the Biot number, $r_1 = 0.5$.

For 2D numerical simulation the following parameters were used: $Pe = 10$; $Le = 1$; $\tau = 0.0001$; $It = 3000$, where It , τ are the number of iterations and time step. The maximum differences between two iterations are $\nabla T = 1.e - 4$, $\nabla C_1 = \nabla C_2 = 1.e - 8$.

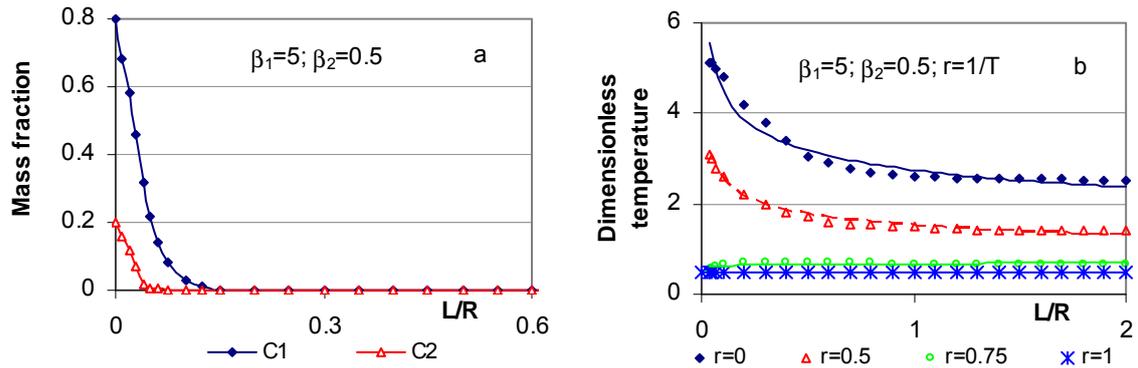


Figure 2: Formation of (a) the flame composition and (b) temperature profiles downstream of the flame with the development of slow and fast reactions at fuel combustion.

Numerical analysis of the distribution of dimensionless temperature for $r = 0; 0.1; 0.5; 0.75$ and 1 showed that the development of the two reactions downstream of the combustor caused the faster decrease of the mass fraction for the reactant 2 with lower activation energy (Figure 2-a).

The formation of the temperature maximum value close to the inlet of the combustor was observed, which refers to the maximum value of the heat energy release at the combustion of reactants (Figures 2-b).

The formation of the reaction zone at combustion of the gases, which are released from biomass thermal decomposition, can be expressed as a global reaction (van Oijen, 2011):



In fact, the process of biomass gasification and combustion proceeds via a large complicated chain of branched endothermic and exothermic, slow and fast reactions developing at thermal decomposition of biomass and combustion of H_2 and CO . The dominant combustion reactions which lead to the formation of the main products (H_2O , CO_2) and their rate constants are as follows:



With the aim to specify the effect of the slow (6) and fast (4) reactions occurring at the biomass gasification and combustion of CO and H_2 on the time-dependent variations of flame composition and temperature, a numerical simulation with account of these two reactions was carried out for the average temperature of product gas entering the combustor $T_{av}=950\text{K}$. The main rate-constant parameters used in the numerical simulation of the reaction rates are: $A = 2.16(08) (\text{cm}^3/\text{mol})/\text{s}$; $E = 14.36 (\text{kJ}/\text{mol})$ for reaction (4) and $A = 2.53(12) (\text{cm}^3/\text{mol})/\text{s}$; $E = 199.71 (\text{kJ}/\text{mol})$ for reaction (6) (Mueller et al., 1999).

The results of the numerical simulation of kinetics confirm the faster burnout of hydrogen with a relatively slow linear decrease of the CO mass fraction (Figure 3-a). In addition, the more intensive heat-energy release is observed from the hydrogen combustion (Q_1), which assisted as a heat source initiating and supporting the combustion of CO . This is confirmed by a decrease of Q_1 with correlating increase of the heat release from the combustion of CO during the primary stage of thermo-chemical conversion of the volatiles ($t < 1$ s). Moreover, during this stage of the combustion of CO and H_2 an increase of the total amount of the heat release up to the peak values is observed (Figure 3-b). The stabilization of the flame characteristics occurs after the burnout of H_2 , when the heat release due to the combustion of CO dominates (Figure 3-b).

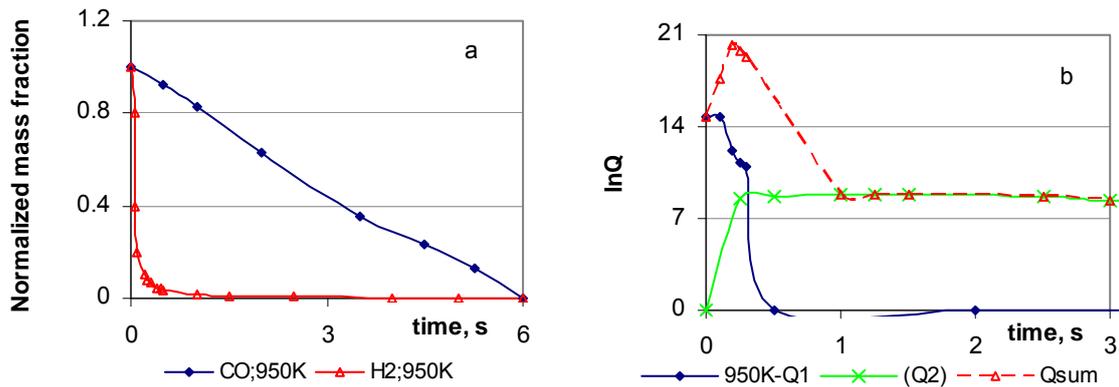


Figure 3: Time-dependent variations of the mass fraction of volatiles (a) and heat energy release (b) at thermo-chemical conversion of volatiles.

4.2 Results of experimental study

The results of the experimental study show that the formation of the swirling flame composition and temperature profiles downstream of the combustor are determined by the evolution of the processes of biomass thermo-chemical conversion. This includes the primary stage of biomass thermal decomposition developing in the gasifier with the formation of the axial flow of volatiles and the next stage of upstream air swirl-enhanced mixing of the axial flow of volatiles with the air. It was found that the upstream air swirl formation (Figure 1) and reflection from the biomass layer (Abricka et al., 2014) enhances the mass transport of the mixture downstream the flow axis ($r/R = 0-0.2$). This leads to the formation of a sharp peak of the mass fraction of the combustible gases (CO, H₂) near the flow axis $r/R < 0.5$ (Figure 4-a). The average temperature of the mixture entering the combustor ($L/D = 2.6$) was about $T = 950-1000$ K with a peak flame temperature near the flame axis (Figure 4-b).

Further development of the flame temperature profiles caused radial expansion of the flame temperature profiles with a gradual decrease of the temperature peak value downstream of the flame axis with a correlating decrease of the mass fraction of the combustible volatiles (Figure 5-a,b). Stabilization of the flame temperature profile was observed at $L/D \approx 6$.

From Figure 5-b it follows that the process of thermo-chemical conversion of the main combustible gases (CO, H₂) proceeds with a faster burnout of hydrogen downstream of the flame reaction zone, as it follows from the results of numerical simulation (Fig. 3.-a). The dominant combustion of H₂ and CO occurs at the primary stage of the formation of the flame reaction zone, close to the combustor inlet: $L/D < 1$, where an intensive heat – energy release (Fig. 3-b) results in the formation of a peak flame temperature (Fig.5-a).

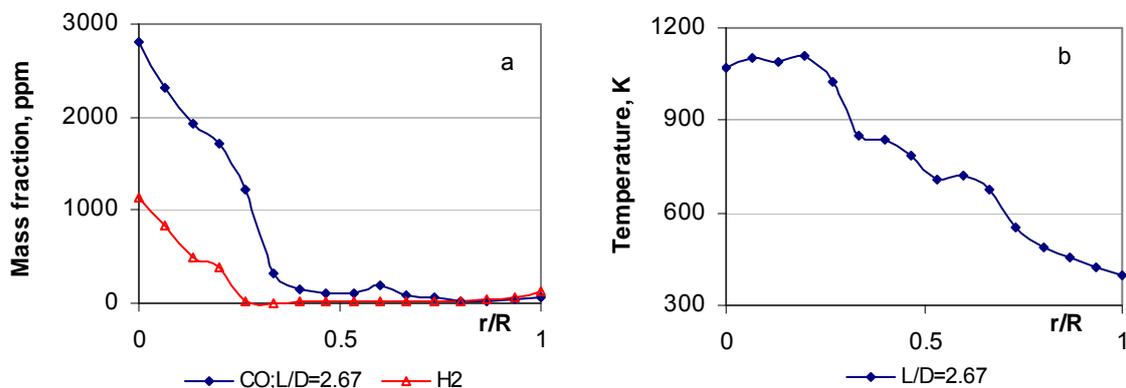


Figure 4: Radial profiles of the mass fraction of volatiles (a) and of flame temperature (b) at the primary stage of thermo-chemical conversion of volatiles.

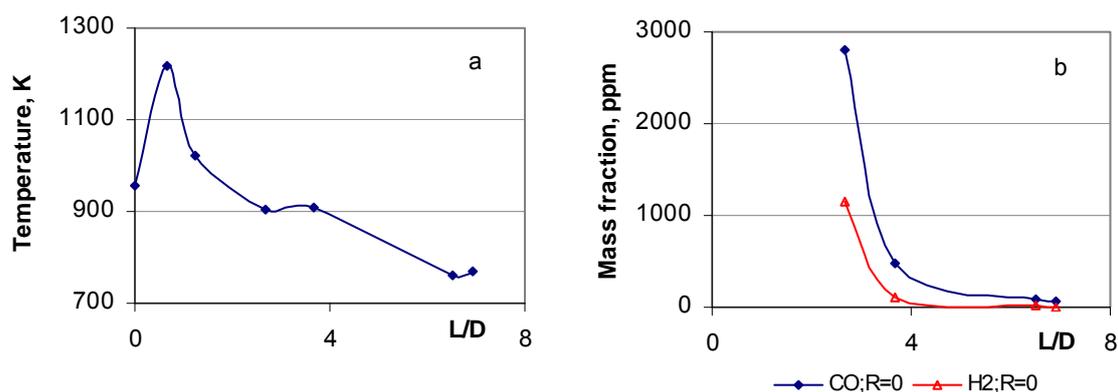


Figure 5: Formation of the axial profiles of temperature (a) and mass fraction of the combustibles (CO, H₂) (b).

5. Conclusions

Based on the results of mathematical modelling, numerical simulation and experimental study a correlation between the development of slow and fast exothermic reactions and the formation of the flame composition and temperature profiles has been observed and considered at biomass gasification and combustion of the product gas.

It is established that the formation of the swirling flame composition and temperature profiles is influenced by the upstream swirling flow formation determining the swirl-enhanced mixing of the axial flow of combustible gases (CO, H₂) with air and the mass transport of the mixture downstream the flow axis.

The results of numerical simulation and experimental study confirm that the fast exothermic reaction of hydrogen combustion helps as a heat source initiating and supporting the combustion of CO. Further development of flame reaction zone is determined by the progress of the slow reaction, which at thermo-chemical conversion of biomass pellets, can be related to the combustion of CO.

Acknowledgments

The authors would like to acknowledge the financial support of the Latvian grant N 623/2014.

Reference

- Abricka M., Barmina I., Valdmanis R., Zake M., 2014, Experimental and numerical study of swirling flows and flame dynamics, *Latvian Journal of Physics and Technical Science*, 51, 25-40.
- Barmina I., Kolmickovs A., Valdmanis R., Zake M., 2015, Combustion dynamics of swirling flame at thermo-chemical conversion of biomass, *Chemical Engineering Transactions*, 43, 649-654, DOI: 10.3333/CET1543109.
- Choi J.J., Rusak Z., Kapila A.K., 2007. Numerical simulation of premixed chemical reactions with swirl. *Combustion theory and modelling*, 6, 11, 863-887.
- Douglas J., Rachford H.H., 1956, On the numerical solution of heat conduction problems in two and three space variables, *Trans. Amer. Math. Soc.*, 82, 2, 421-489.
- Driscoll J.F., Temme J., 2011, Role of Swirl in Flame Stabilization, *AIAA 2011-108*, 1-11.
- Gupta A.K., Lilley D.G., Syred N., 1984, *Swirling Flows*, Abacus Press, London, 1-475.
- Houshfar E., 2012, Experimental and numerical studies on two-stage combustion of biomass, Thesis for the degree of Philosophiae Doctor, Norwegian University of Science and Technology, Trondheim, 1-235.
- Kalis H., Marinaki M., Strautins U., Lietuvietis O., 2015, On the numerical simulation of the combustion process with simple chemical reaction, *Advances in Heat Transfer, Proc. of the 7th Baltic Heat Transfer Conference*, Tallinn, Estonia, 175-180.
- Mueller M.A., Kim T.J., Yetter R.A., Dryer F.L., 1999, *Int. J. Chem. Kinet.*, 31, 411-734.
- Saediamiri M., Birouk M., Kozinski J.A., 2014, On the stability of a turbulent non-premixed biogas flame: Effect of low swirl strength, *Combustion and Flame*, 161, 1326-1336, DOI: 10.1016/j.combustflame.2013.11.002
- van Oijen J., 2011, Energy from Biomass, 4S610, Lecture 3, University of Technology, Eindhoven, 1-35. http://w3.wtb.tue.nl/fileadmin/wtb/ct-pdfs/Energy_from_Biomass/Lecture_3_2011.pdf